Combining Qualitative and Quantitative Reasoning to support Hazard Identification by Computer

by

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A Doctoral Thesis

Submitted in partial fulfilment of the requirements for the award of Doctor of Philosophy of Loughborough University

23rd March, 1999

Abstract

This thesis investigates the proposition that use must be made of quantitative information to control the reporting of hazard scenarios in automatically generated HAZOP reports.

HAZOP is a successful and widely accepted technique for identification of process hazards. However, it requires an expensive commitment of time and personnel near the end of a project. Use of a HAZOP emulation tool before conventional HAZOP could speed up the examination of routine hazards, or identify deficiencies in the design of a plant.

Qualitative models of process equipment can efficiently model fault propagation in chemical plants. However, purely qualitative models lack the representational power to model many constraints in real plants, resulting in indiscriminate reporting of failure scenarios.

In the AutoHAZID computer program, qualitative reasoning is used to emulate HAZOP. Signed-directed graph (SDG) models of equipment are used to build a graph model of the plant. This graph is searched to find links between faults and consequences, which are reported as hazardous scenarios associated with process variable deviations. However, factors not represented in the SDG, such as the fluids in the plant, often affect the feasibility of scenarios.

Support for the qualitative model system, in the form of quantitative judgements to assess the feasibility of certain hazards, was investigated and is reported here. This thesis also describes the novel "Fluid Modelling System" (FMS) which now provides this quantitative support mechanism in AutoHAZID. The FMS allows the attachment of conditions to SDG arcs. Fault paths are validated by testing the conditions along their arcs. Infeasible scenarios are removed.

In the FMS, numerical limits on process variable deviations have been used to assess the sufficiency of a given fault to cause any linked consequence. In a number of case studies, use of the FMS in AutoHAZID has improved the focus of the automatically generated HAZOP results.

This thesis describes qualitative model-based methods for identifying process hazards by computer, in particular AutoHAZID. It identifies a range of problems where the purely qualitative approach is inadequate and demonstrates how such problems can be tackled by selective use of quantitative information about the plant or the fluids in it. The conclusion is that quantitative knowledge is required to support the qualitative reasoning in hazard identification by computer.

Keywords: HAZOP Emulation, Qualitative Modelling, Process Safety, Hazard Identification, STOPHAZ, Fault Propagation.

Acknowledgements

I would like, first and foremost, to thank Andy Rushton and Paul Chung for the invaluable guidance they have provided as my supervisors in this work – this thesis would be far poorer than it is without them! I am grateful also to Frank Lees for the valuable advice and inspiration he gave me while I was at Loughborough. I would also like to acknowledge my colleagues at Loughborough, Felim Larkin and Steve Wakeman, as well as the numerous other people around Europe, with whom I had the pleasure of working, on the STOPHAZ project. Lastly, thanks are certainly due to the AI Group in the Dept. of Engineering Mathematics, Bristol University, where I have been working for the past 12 months as a "Post-Doc R.A." – so far without a PhD!

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APPENDICES

Chapter 1 : Introduction

The thesis stated here is that quantitative information is needed to control the reporting of hazard scenarios in qualitative emulation of HAZOP by computer. Without such support, hazards are reported indiscriminately, which reduces the value of the output to human users of the program.

HAZOP is a very useful technique for process hazard identification. However, it requires an expensive commitment of time and resources at the end of the process design phase. Therefore, a strong economic argument exists for automating this technique.

Qualitative methods, among them graph based methods, can be used to efficiently model plant behaviour. By modelling fault propagation in the plant, programs can emulate the hazard identification of the HAZOP study method.

However, qualitative methods are weak representations, which often do not permit unambiguous simulation of the plant. This leads to indiscriminate reporting of process hazards, which reduces the value of the resulting hazard study reports. It is thought likely that this problem cannot be solved without the use of quantitative information of some kind. An example of the type of information often represented weakly in the plant model, is the details of the fluids present in the plant, and their properties. Fluid properties can be used to assess the feasibility of hazards which otherwise would be reported indiscriminately.

The AutoHAZID computer program was developed as part of STOPHAZ, a 3½ year long ESPRIT-funded collaborative project. In AutoHAZID, qualitative reasoning using signed directed graphs (SDGs) is supported by conditions for judging the feasibility of fault-consequence scenarios. These conditions are based on the fluids present in the plant, and are implemented by the Fluid Modelling System (FMS) in AutoHAZID. The FMS also allows verification of scenarios by checking the possible limits of deviations in process variables. The result of applying these conditions is that the results of computer-based HAZOP become more focussed.

The remainder of this chapter introduces some of the ideas expanded on in later chapters. Firstly, some of the terms used in process safety work are defined, in Section 1.1. Hazard identification and risk assessment are introduced as vitally important activities in the design of chemical plants, in Section 1.2. Among the hazard identification methods used in the process industries, the HAZOP study is the most popular method for assessing new plant designs. Section 1.3 describes HAZOP briefly and Section 1.4 makes the case for automation of safety assessment methods, with particular reference to HAZOP studies. HAZOP emulation requires model-based simulation of the plant behaviour. AutoHAZID uses qualitative graph-based models to simulate the fault propagation behaviour that can occur in the plant. Therefore, Section 1.5 gives a description of what is meant by "fault propagation" and Section 1.6 introduces graphs, describing some of the basic concepts of graph search. The chapter concludes with some points of justification for the work done on HAZOP emulation, in Section 1.7.

The chapters following this one deal with the following areas of concern in qualitative modelling as applied to hazard identification:

- Chapter 2 is a review of the literature relevant to hazard identification, qualitative physics and the application of AI techniques to process safety evaluation.
- Chapter 3 describes the HAZID system developed during the STOPHAZ project, including its qualitative modelling system. A significant portion of this chapter discusses the process of developing equipment models for hazard identification.
- Chapter 4 covers some of the problems experienced with the qualitative hazard identification system, and how these problems were addressed.
- Chapter 5 explains an important method for overcoming problems related to fluids in the plant and their interaction with the process itself. The solution is to add conditions to arcs in the SDG models, to execute rule-based checks within the frame of the FMS.

- Chapter 6 discusses topics raised by the work described here, and pinpoints some areas of future work.
- Chapter 7 formulates some overall conclusions about qualitative hazard identification and its extension, using the FMS.

1.1 Nomenclature

Before addressing hazard identification and other aspects of process safety, we must clarify the meaning of some terms used in safety work. A valuable reference for "standard" nomenclature in this field has been prepared by Jones (1992). This guide is the result of a working party set up by the Institution of Chemical Engineers (IChemE), with the aim to help standardise some of the (sometimes rather freely adapted) terminology in use in industry.

The terms of most relevance to this thesis are defined by Jones as follows:

Hazard	A physical situation with a potential for human injury, damage to property, damage to the environment or some combination of these.
Chemical hazard	A hazard involving chemicals or processes which may realize its potential through agencies such as fire, explosion, toxic or corrosive effects.
Risk	The likelihood of a specified undesired event occurring within a specified period or in specified circumstances. It may be either a frequency (the number of specified events occurring in unit time) or a probability (the probability of a specified event following a prior event), depending on the circumstances.
Loss prevention	A systematic approach to preventing accidents or minimizing their effects. The activities may be associated with financial loss or safety issues and will often include many of the techniques defined in this [Jones'] report.
Hazard analysis	The identification of undesired events that lead to the materialization of a hazard, the analysis of the mechanisms by

	which these undesired events could occur and usually the estimation of the extent, magnitude and likelihood of any harmful effects.
Risk assessment	The quantitative evaluation of the likelihood of undesired events and the likelihood of harm or damage being caused together with the value judgements made concerning the significance of the results.

Throughout this thesis, I will attempt to use these terms consistently. It should be noted that there is still a good deal of variability in the usage of these terms in the chemical industry as well as confusion with similar terms in other fields (*e.g.* "risk assessment" as applied to financial risk).

1.2 Hazard Identification and Risk Assessment

Process safety is vitally important to any operating company in the chemical industries, not only because of the human cost of accidents, but also for economic reasons. A serious accident on plant can mean loss of production and consequent loss of customers, compensation payments to injured workers and possibly a serious loss of the considerable investment in plant and machinery.

Such losses can be prevented by two complementary means. Firstly, the philosophy of management of the plant and its personnel should encourage safe working and "good housekeeping" in day-to-day operation. Systems of communication, training and control of access to plant items should be installed, to ensure that people are aware of potential hazards and do their work safely. Increased awareness of safety and operability issues among staff will reduce the frequency of accidents, near-misses and environmentally damaging releases of process materials, thereby increasing productivity and profitability.

Plant safety can also be helped at a much earlier stage by use of safe plant design practices, where the plans for a plant are examined at various stages of the design process. By identifying hazards and possible concerns for plant operation early, and assessing the risks they pose to safety, costly changes in the later design can be minimised, or avoided altogether. Information on potential hazards can be used even before a process or specific product has been decided upon, so that (possibly) a more benign product or an inherently safer process can be chosen for development.

The ICI hazard study review programme, as described by Duxbury and Turney (1989), addresses safety, health and environmental (SHE) issues at all stages of the design of a new plant, from process selection and siting through to commissioning and initial operation. The six stages of the programme, outlined in Table 1.1, include both hazard identification and risk assessment activities in the first three studies. These studies typically produce a large number of actions, ranging from the addition of alarms or indicators to the complete redesign of sections of the plant. The later stages (IV, V and VI) are mostly concerned with checking that all actions have been processed and that the safety measures recommended are appropriate and will function adequately when required on the operating plant.

Hazard Study	When performed ?	What is examined ?
I	Project exploration stage.	Hazardous properties of materials, constraints on siting plant, environmental impact, *etc.*
II	When process flow diagrams (PFDs) are available.	General top events (major hazards) in each plant section. Characterise likely problems and hazards early.
III	HAZOP when detailed Engineering Line Diagrams (ELDs) are available.	Detailed and systematic examination of ELDs and operating instructions using method study approach.
IV	Before start-up.	Checks that all actions from stages I, II and III have been completed.
V	Before start-up.	On-site inspection with regard to access, escape, guarding, emergency equipment, *etc.*
VI	Post-commissioning.	Compare actual plant performance to expected performance, review operating procedures, *etc.* Feedback to design team.

Table 1.1: The six stage ICI hazard study programme

The "hazard identification" part of hazard analysis is concerned with finding out what hazards are possible within a process and characterising the scenarios which allow those hazards to come about. This is a mostly qualitative task, which concentrates on identification and analysis of the mechanisms underlying events, rather than quantifying specific risks. "Risk assessment" is a more pains-taking, quantitative technique, which is applied to a small number of the most important or complicated hazards identified. The objective is to analyse the risk associated with a scenario in terms of the logic for its development, probabilities of various events occurring and consequent losses which could occur.

Figure 1.1, taken from "HAZOP and HAZAN" by T.A. Kletz (1992), neatly illustrates some of the techniques which can be used to identify and to assess hazards. Note that Kletz uses the terms "HAZAN" and "hazard analysis" to denote the quantitative activities classified here as "risk assessment".

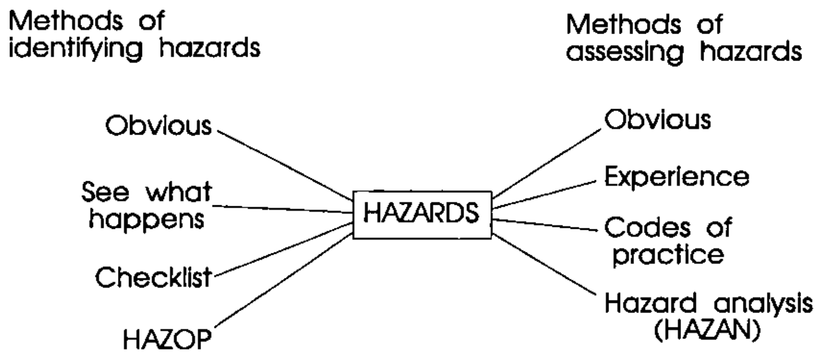


Figure 1.1: Some ways of identifying and assessing or treating hazards

Some of the hazards in a plant may seem to be "obvious" properties of the materials or the process used. However, this assumes that someone looks through the designs with enough awareness of safety issues to notice the problems. Even such "obvious" hazards don't reveal themselves while the plant designs are still just on paper. If checks on the design fail to identify problems, then any hazards may make themselves apparent by the second means, the "see what happens" approach, which identifies hazards by having them cause an accident first. Experience gained from accidents or from recognition of "obvious hazards" can be formally recorded in checklists, so that future plants can be safer than ones in the past. For novel plant designs, other techniques such as HAZOP can be effective in picking out problem areas.

Once hazards have been identified, action must be taken to prevent them or protect against their consequences. Often, preventive measures are readily available and can be easily implemented, or engineers' experience in previous cases can be used to solve the problems. Codes of practice are a more formal approach to design, which ensure safety by avoiding specific known hazards or by managing them using methods known to have been effective in the past. Risk assessment is used to quantify the risks associated with the most significant hazards and decide what action is needed. This approach must be used selectively, however, because of the time and effort required.

To be effective, hazard identification and risk assessment must be integrated with the activity of process design which proceeds *via* a number of stages. Firstly, the design team must obtain a detailed statement of requirements from management or the customer. This allows them to decide what product(s) to make, what reactants to use and the details of intermediates and process chemistry involved. It is also important to decide on the likely siting of the plant, to allow capital cost estimation, environmental impact assessment and safety assessment to proceed from an early stage.

When these basic process details have been decided, the team develops a preliminary process design in the form of a block diagram of the process steps. The block diagram identifies main flows into and out of each plant section, as well as unit operations in each section. This design is refined into a process flow diagram (PFD) by performing heat and mass balance calculations and doing some preliminary equipment selection and design. Several different process options may be worked through to this stage.

After preliminary cost estimation, funds are authorised for one process option. Detailed process design and piping and instrumentation design follows, producing the "Engineering Line Diagrams" (ELDs) for the plant. ELDs are also sometimes known as "Piping and Instrumentation Diagrams" (P&IDs), but the usage of these terms is not standardised in industry - where some companies refer to the P&ID as a more detailed level of specification than the ELD, others use the opposite convention. Further design tasks include layout planning, mechanical engineering and civil engineering. Design is followed by procurement, fabrication, construction and commissioning of the new plant.

As mentioned earlier, awareness of process hazards at each stage can simplify the design and cut down on expensive redesign due to late discovery of problems. A wide range of techniques can be used for hazard identification during process design, as reviewed in Section 2.1. However, HAZOP is described in this chapter because it plays a much larger part in the work described in the rest of the thesis.

1.3 Hazard and Operability Studies (HAZOP)

The most commonly used hazard identification technique in the process industries is the hazard and operability study (HAZOP), which is Hazard Study III in the ICI programme mentioned above. This method has been widely used for many years and is described in detail in many publications, such as Kletz (1992), CIA (1977), Knowlton (1981 and 1992), Lees (1996) and Lawley (1974).

HAZOP is a systematic critical examination of the process and engineering design of a plant, to identify all possible deviations of the plant from its intended operating condition. For each deviation, any possible associated hazards and problems with operability are recorded. The design of the plant is characterised by its Engineering Line Diagrams (ELDs) and operating instructions.[1] The study takes the form of a series of "brainstorming" sessions, attended by a cross-section of project personnel, under the control of a team leader who directs the procedure of the meetings.

The team leader must be familiar with the HAZOP method and be trained for the job of leading a HAZOP team, but he/she need not be involved in the rest of the project. The decisions and points discussed by the team must be recorded – the team leader may do this, but it is generally better to employ a secretary (or "scribe"), to avoid holding up the progress of the study. The remainder of the team should represent all parties with an interest in the project, including each main engineering discipline. The team should not be too large; six members is probably a good maximum.

[1] Operating instructions are an important part of the plant design, which should be available for HAZOP, but frequently are not complete at this stage.

For each ELD in the plant, the team leader chooses the equipment items to be grouped together as "lines", transferring fluid between the equipment items allocated as "vessels" in the drawing. This grouping of equipment should allow the study to proceed at a reasonable pace, without the risk of missing any hazards. The choice of lines is a matter of judgement on the part of the team leader.

The drawing is examined line by line and vessel by vessel, with the group considering deviations from intended operation in each line. This requires that the intentions of all lines and vessels are declared as and when they are encountered. Deviations are formed by combining a guide word (more, less, no, other-than) with a relevant variable in the line or vessel (flow, pressure, temperature, liquid level), or with intended operations or processes (*e.g.* mixing, crystallisation). The following questions are addressed for each deviation:

- Is the deviation meaningful?
- Could it arise, and how?
- What consequences would result, and are those consequences hazardous, or do they prevent efficient operation?
- If so, can the deviation be prevented from occurring, or can the consequences be protected against by changing the design or operation of the plant? Redesign must be avoided in the HAZOP meeting, but may be a recommended action.

Any significant findings of the HAZOP team are recorded, typically in a table including columns for identifying the deviation, possible causes and consequences of the scenario, and any suggested actions to tackle the identified hazard. Common practice in modern HAZOPs also includes listing any existing protections against the identified hazard, such as trip systems, alarms, *etc.*

Figure 1.2, taken from CIA (1977), illustrates the sequence of examination of the HAZOP, emphasizing the methodical and systematic approach of the technique. Clearly, a lot of very creative activity is implied in the central steps (7, 8 and 9), examining possible causes, consequences and detecting hazards, but the method appears highly algorithmic when seen at the level shown here.

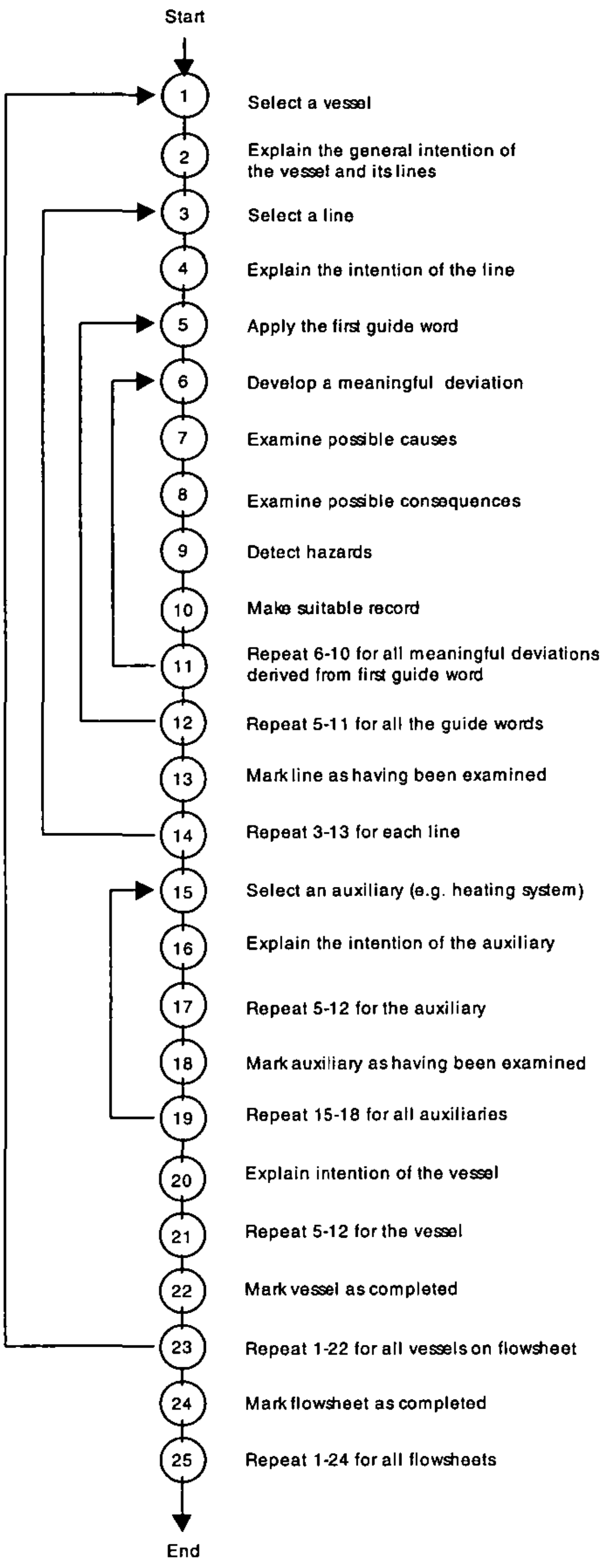

Start
1 Select a vessel
2 Explain the general intention of the vessel and its lines
3 Select a line
4 Explain the intention of the line
5 Apply the first guide word
6 Develop a meaningful deviation
7 Examine possible causes
8 Examine possible consequences
9 Detect hazards
10 Make suitable record
11 Repeat 6-10 for all meaningful deviations derived from first guide word
12 Repeat 5-11 for all the guide words
13 Mark line as having been examined
14 Repeat 3-13 for each line
15 Select an auxiliary (e.g. heating system)
16 Explain the intention of the auxiliary
17 Repeat 5-12 for the auxiliary
18 Mark auxiliary as having been examined
19 Repeat 15-18 for all auxiliaries
20 Explain intention of the vessel
21 Repeat 5-12 for the vessel
22 Mark vessel as completed
23 Repeat 1-22 for all vessels on flowsheet
24 Mark flowsheet as completed
25 Repeat 1-24 for all flowsheets
End

Figure 1.2: Sequence of examination for HAZOP meeting

HAZOP is usually carried out after most of the detailed process design has been completed. Large-scale changes to the design are very expensive at this stage. Therefore, early use of other hazard identification techniques (as discussed in Section 2.1) must have already eliminated the major problems in the process design wherever possible. Simple checks on equipment designs should be dealt with before HAZOP, by checklists relating to equipment items or fluids present in the process. These checks can be performed more cost-effectively by a single engineer than by a team. It is also important to make sure that all information on the safety and control systems proposed for the plant is available before the HAZOP meeting, to avoid delay in getting hold of this information.

Much of the strength of HAZOP arises from systematically examining the interactions between separate parts of the process and from the creative interaction of the team members in looking at the problem. These are factors which are absent from many simpler hazard identification methods. The method involves a lot of redundancy, as the same scenarios are examined from many different viewpoints. This reduces the chance that significant hazards will be overlooked, but the requirement for a group of experts to be present for the full duration of the study means that HAZOP can be rather expensive.

Because HAZOP meetings are so painstaking and methodical, they can be very tiring for the people involved, who must remain motivated and alert throughout. It is not usually productive to run sessions for longer than about three hours, and the frequency of meetings should be kept low, too. The time and personnel required for HAZOP studies at such a late stage in the project often mean that this stage delays final delivery of the project (*i.e.* HAZOP is on the "critical path" of the project plan). Therefore, there is a lot of interest in automating safety verification tasks such as HAZOP.

In the discussion of computer emulation of HAZOP which follows in this and later chapters, a particular approach is taken. This is to consider how deviations of the process variables in a plant could arise, and how they could give rise to hazards.

Although this does comprise a large part of the work of a conventional study, there is more involved. A full HAZOP, conducted by a team of experts, considers *all possible deviations* of the plant from its *intended operation*, which includes many phenomena which are not process variable deviations. Examples include maintenance and operation in abnormal modes, such as start-up, shut-down or process upsets.

1.4 Automation of Safety Assessment

Computers have been used to increase the speed and efficiency of many process engineering tasks. Examples include computer aided design (CAD), flowsheet simulation, layout planning and visualisation, and project planning. The automation of safety-related tasks is an area where appropriate use of computers could greatly reduce costs. Applications of Information Technology (IT) in this area so far fall into four main types:

i. General-purpose office software packages, such as word processors, spreadsheets and databases, are widely used to process and present information in connection with the work of safety assessment.
ii. More structured IT applications have also been developed, to facilitate specific safety tasks, such as documenting HAZOP studies. Here, basic IT has been used in a tightly structured domain, to aid a well-defined task.
iii. Many computer packages exist for performing detailed (often numerical) tasks in risk assessment. These include numerical simulations of vapour cloud dispersal, fires and explosions, or support tools for fault tree development.
iv. The most interesting software developments apply Artificial Intelligence (AI) techniques to diagnosis of process disturbances, real-time monitoring of plant performance using control system data, hazard identification, *etc.* This is the area in which the Plant Engineering Group at Loughborough University has been working. In particular, the group has developed qualitative simulations of plant behaviour for automated hazard identification.

The advantages of using a computer-based approach for hazard identification include:

- Repeatability. Given the same input, a computer program will always produce the same set of results. This is not necessarily true for a human team-based task.
- The computer is impervious to boredom, so that it will examine everything it is asked to, without loss of interest part way through.
- Systematic and thorough approach. Given results from a computer study, we can be reasonably certain that everything has been examined to a consistent level of detail, so that the quality of analysis is consistent throughout.

There are a number of disadvantages to using even a well-designed computer aid for hazard identification. As with the advantages listed above, many of these are shared with programs in other domains of application:

- The results may be lacking in originality, with a "mechanical" feel to them. Partly this is a result of the use of language in the computer results – inevitably the phrases used seem artificial after many repetitions.
- Programs are usually unable to indicate clearly where they do not have the expertise to solve a particular problem, so that weak areas of knowledge may not be appreciated by the human reader of the report.
- The level of detail produced by computer programs can be inappropriate. Often, the report is too detailed in areas which are not very interesting or important.
- Human users often accept, without question, the correctness of results produced by computer. This acceptance is a dangerous tendency in safety-critical work. The assumptions and processing behind safety-related results should be stated, and questioned, wherever appropriate. High quality presentation of results can also mask poor quality content.
- Because of the systematic nature of any computer aid, weaknesses and errors in programs or models will be systematic, too. In this way, single weaknesses can be greatly magnified.

Despite these problems, it is still deemed to be a worthwhile aim to develop computer programs which can automate certain tasks in the safety analysis arena, not least because the attempt at automation may reveal weaknesses in conventional hazard identification approaches and thereby lead to their remedy.

The economic argument for automating HAZOP is that, even if the software can only identify a small class of routine problems, the time and effort saved during the HAZOP study probably makes using the program worthwhile. A consistent quality of hazard identification can also be expected from the software tool. By comparison, a HAZOP team may occasionally have a "bad day".

A software tool for hazard identification should allow initial failures and final consequences to be brought together, to bring potential hazards to light. It should not attempt to model all classes of fault in full detail, but should instead allow the full range of safety concerns to be identified by users when working through the output generated.

HAZOP emulation software could be used by a design engineer, to evaluate a substantially completed design, just before the conventional HAZOP study. Alternatively, the tool could be used at earlier stages of design, before detailed ELDs are available, to screen for problems when the cost of design changes is lower.

1.5 Fault Propagation

To automate the identification of hazards in a process plant design, some formal representation of the plant itself must be constructed. With such a plant model, a computer program can then be designed, to reason about it symbolically or numerically, to determine how the process system could behave in ways that lead to a hazardous situation.

A promising approach is to build a qualitative model of the plant from individual models of the equipment items present and the connections between them. In conjunction with an appropriate computer program (an "inference engine"), the model should predict the behaviour of the plant under normal conditions, as well as predicting its response to individual things that can go wrong. It is not usually necessary to predict in detail what will happen after a hazard has occurred – identification of the hazard is enough.

The approach used in most of our work, to model the development of hazards in process systems, is known as "fault propagation". This is not the only way to model the (sometimes complex) sequences of causes and effects which comprise real-life accident scenarios, but it is a simple approach to tackling many such scenarios. Fault propagation can also be formalised (and therefore automated) quite easily. The wider issues of hazard modelling and how best to model equipment for hazard identification, are discussed in Chapter 3 and, later, in Section 6.4 of Chapter 6.

Fault propagation distinguishes two types of event, or states of affairs, as important: "faults" and "consequences". Both are simply modelled as named events and are usually associated with some equipment item in the plant. Faults model the initial causes of hazards in the plant, such as equipment failures. An example for a pump might be "seal failure". Consequences model the final, reportable, hazards or operability concerns in the hazardous scenario. An example might be "possible explosion".

Faults and consequences are linked together by what is known as a "fault propagation chain". This may be a single link between the initial fault and final consequence, or it may be a sequence of links *via* a number of process variables in the plant. In the latter case, each variable is deviated from its normal value enough to propagate a disturbance from an initial fault to a final, possibly quite remote, consequence.

The single link type of fault propagation chain characterises local failures of equipment which give rise to immediate problems at the same location. For a pump containing a toxic and volatile fluid, we might have:

$$\begin{tikzcd}
\text{'seal failure' (fault)} \arrow[d] \\
\text{'toxic gas release' (consequence)}
\end{tikzcd}$$

The multiple link type of fault propagation chain models more interesting failures, to do with the way the plant is put together. These are the type of hazards which HAZOP studies are particularly good at identifying. A more complicated example, shown in Figure 1.3, will illustrate this type of scenario.

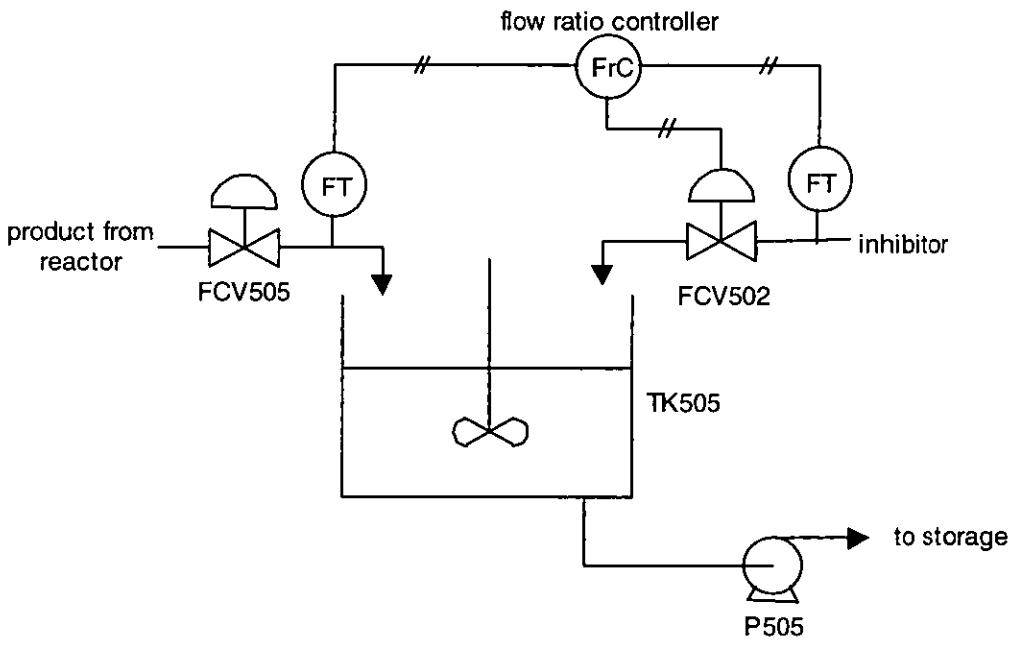
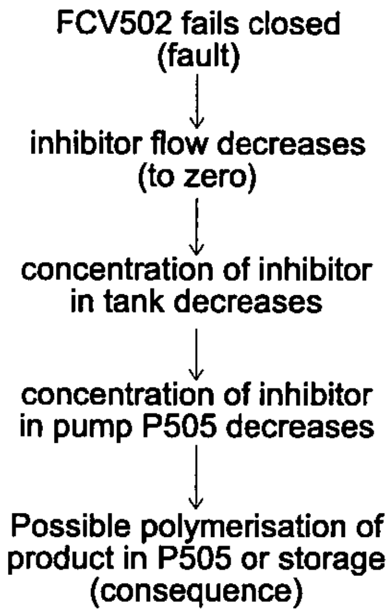


Figure 1.3: Product stabilisation example

A product chemical is stabilised by adding a polymerisation inhibitor before final storage. The flow rate of inhibitor is maintained at a constant fraction of the product flow rate (using ratio control), to ensure that there is a constant small percentage of the inhibitor in the final product. If the inhibitor control valve FCV502 fails closed, the following chain of events may occur:


FCV502 fails closed (fault)
inhibitor flow decreases (to zero)
concentration of inhibitor in tank decreases
concentration of inhibitor in pump P505 decreases
Possible polymerisation of product in P505 or storage (consequence)

Each event between the fault and the consequence is a deviation of some variable in the plant (here we have a flow and two composition variables). Notice that the site of the consequence (the pump P505) is distant from that of the fault (the valve FCV502).

The aspect of fault propagation, as described here, which makes it suitable for use in automated hazard identification, is the use of deviations in intermediate variables to transmit a cause to a possibly quite remote consequence. Because the faults and consequences can be simply modelled as named events, and the variables in the plant can be determined from a model of the process including the connections between its equipment items, the problem of hazard identification can be simplified to finding links between the modelled faults and consequences.

One approach to modelling fault propagation is to model variables in the plant as nodes in a signed directed graph (SDG).[2] Arcs in the SDG then represent causal links between deviations of the variables, corresponding to the physical behaviour of the plant. Faults and consequences correspond to extensions of the SDG, linking named

[2] Graphs are discussed in more detail in Section 1.6.

events to specific deviations of variables. This graph-based representation is the one used in AutoHAZID and is explained in Section 3.3. It allows fault-consequence scenarios to be modelled by paths in the SDG from faults to consequences.

Given a qualitative modelling framework of this nature, there are a number of things one can do with it. One might use a graph search algorithm to search in a model forwards from selected faults to determine their eventual consequences. One might use the ability of the system to qualitatively model process plants and analyse the causation of major hazards to produce fault trees automatically, as Hunt *et al.* did with the FAULTFINDER program (Hunt, 1992, Hunt *et al.*, 1993). Alternatively, one might choose to emulate HAZOP, as we have with the STOPHAZ project.

The approach used in HAZOP emulation is to first compile a list of sensible deviations for each of the process variables in the plant model. Then, for each deviation, backwards search is used to find possible causes, in terms of initiating faults. Any direct consequences of the deviation being considered may therefore be caused by the faults identified. In this way, a list of fault-consequence scenarios can be associated with each deviation. These results are presented in a tabular form, similar to the format used to record conventional HAZOP findings.

The following section discusses graphical representations and the search methods used with them. It can be seen as an introduction to the SDGs used in AutoHAZID models, referred to briefly above and presented in more detail in Chapter 3.

1.6 Graphs, Search and Complexity

Since fault propagation is implemented in AutoHAZID (and in some other systems) using a graphical representation for process variables and their effects on one another, this section gives a brief general introduction to graphs. Graph search algorithms and their complexity are inevitable concerns, and are also dealt with briefly. The descriptions given owe much to “Artificial Intelligence and the Design of Expert Systems”, by Luger and Stubblefield (1989), which gives a particularly clear explanation of these concepts.

A graph can be defined as a set of nodes and the arcs which connect those nodes to each other. It is possible to add information to a graph, in the form of labels attached to either the nodes or the arcs in the graph, or both. This labelling information can be simple or complex, depending on what the graph is to be used for (its "domain problem"). Typically, a directionality is attached to arcs in the graph, in the form of arrowheads, so that arcs can be considered as uni-directional or bi-directional. The nodes in the graph may also be labelled with names. An example of such a "directed graph" is shown in Figure 1.4.

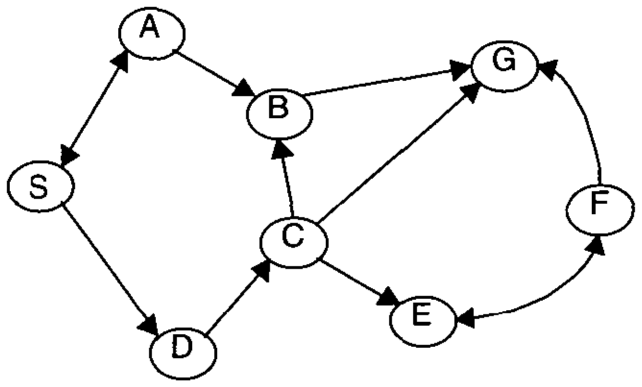


Figure 1.4: An example of a labelled directed graph

The usual purpose of defining graphs is to examine how different parts of a problem are connected, so the concept of a "path" through a graph is usually very important to solving the problems which graphs are used to represent. A path is characterised either by a list of nodes, or a list of arcs in the graph, defining a list of nodes "visited" in sequence, between a starting point and an end point in the graph. An example from Figure 1.4 above is the path from S to G *via* the nodes [S,D,C,B,G]. There can in general be multiple paths between any two nodes in a graph.

An important consideration in solving problems using graphs is the topology of the graph, which includes such questions as whether it contains circuits or not. A path contains a circuit, or cycle, if it passes through some node in the graph more than once. A graph contains a circuit if there is some path in it containing a circuit. A "rooted" graph is one where a single node is identified as the root node, such that there is a path from the root node to every other node in the graph. This sort of graph is usually drawn with the root node at the top of the page.

A "tree" is a graph in which there is a maximum of one path between any two nodes in the graph. This sort of graph is often drawn as a rooted graph, with the branches of the tree drawn out below the root node. A particular example of this kind of "hierarchical" relationship is a family tree, and the terminology of family relationships is usually used in talking about relationships between nodes in a tree, using terms such as "parent", "child" and "sibling" (brother/sister).

Whenever graphs are used to represent a problem in some domain, the interpretation of what the nodes and arcs "mean" is of course dependent on the problem. A frequently used type of interpretation is that of the graph as a "state space representation". In this case, each node represents a possible state of the world, with respect to the problem at hand, and each arc represents a possible change between states, consistent with some rule about the system. Typically, each node stores a description of the state of the world at each point in the graph. Taken as a whole, the graph (which may not contain a finite number of arcs or nodes!)[3] forms a description of the whole scope of the problem. This whole description is often referred to as the "state space" of the problem.

An example of a partial state space representation is shown in Figure 1.5 for the problem of the "8-puzzle". This puzzle consists of a 3×3 grid of tiles, from which one tile has been removed, leaving 8 numbered tiles and an empty space. The tiles can be slid past one another into the empty space, one at a time, allowing the player to rearrange the pattern of numbers in the puzzle. To solve the puzzle, the user must rearrange the tiles from an initial, unsorted configuration into numerical order, as in the "goal state" of Figure 1.5, without removing them from the grid.

[3] Any explicit representation of a graph, in terms of arcs and nodes, must contain a finite number of arcs and nodes. However, where a graph is specified in terms of a node and a set of rules to generate new nodes, then such a graph could be infinite (or extremely large, as in chess, for example).

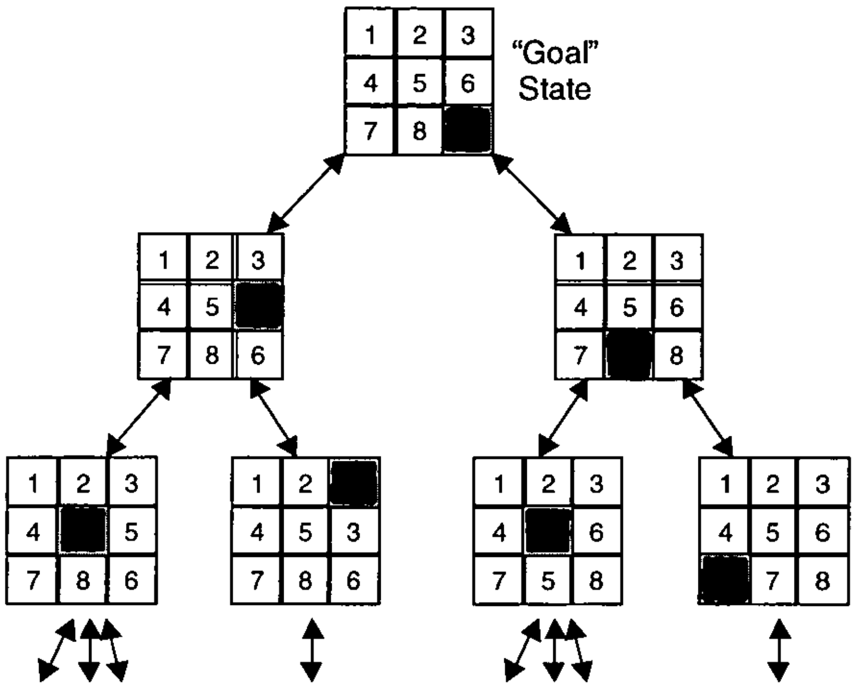


Figure 1.5: Partial state space for the "8-puzzle" problem

In this example, the graph represents the positions of all the tiles at each node. This information gives a complete description of the 8-puzzle "world" in each possible state. Arcs connecting the nodes correspond to "legal moves" in the puzzle (a tile may only be moved into the empty space if the tile is horizontally or vertically adjacent to the space). In this simple puzzle, it is helpful to notice that instead of thinking about moving the tiles, one can consider that this is equivalent to moving the blank space around the grid. There can be a maximum of four moves from any state of the puzzle, corresponding to the directions in which the space can be moved. Notice also that the arcs in the graph are bi-directional, so that any moves are reversible in the puzzle.

A different example of graph interpretation is the signed directed graph (SDG) model representation in the AutoHAZID program, as described in Chapter 3. Here, the nodes are interpreted as variables in the physical system being modelled. Arcs between them represent the causal influences of variables on one another locally. The influences may be "direct" or "reverse", encoded by the signs "+" and "–" attached to arcs.

In the 8-puzzle graph, paths through the graph represent how the state of the puzzle may be changed, which might include solving it. The path corresponding to a solution of the puzzle would therefore terminate at the goal state shown above, and one might imagine that a program could be used to find paths from any other node in the graph to the goal state. Such a program would be able to solve the 8-puzzle problem, or direct its solution, using graph search to find the paths to the goal state.

Paths in the SDG model correspond not to "moves in the game", or changes in a world state, but rather to (possibly remotely propagated) influences between variables. This is quite a different interpretation from the one used for the state space representation above. At no point is there a state description corresponding to the plant being considered, unless the whole graph, with associated variable values at each node, is considered as a description of a state in some larger graph.[4]

Finding paths in a graph therefore serves different purposes dependent on the application domain for that graph. For the 8-puzzle, the goal might be to solve the puzzle from some pseudo-random start position. For the SDG system used in AutoHAZID, the path-finding activity is directed at finding what the wider effects of process equipment failures will be, within the scope of fault propagation, discussed in Section 1.5. Here, finding paths between variables establishes a possible causal influence between potentially quite distant state changes, which may give rise to a hazard by fault propagation.

Graph search algorithms are implemented to find paths through graphs from some set of specified start points, to some set of goal nodes, which may not be fully specified in advance. In the 8-puzzle example, the starting (pseudo-random) position is given, and the goal state is a single known configuration of the tiles. For the SDG-based fault propagation model the starting positions are the faults known about in the models of the equipment in the plant model. The goal nodes correspond to deviations which can give rise to consequences in the plant model.

[4] Even in such a larger "super-graph" it would be difficult to describe or define the arcs which connect the states of the system, defining "legal changes" in the state of the world.

The specification of a search problem must include the following information:

- The nodes and arcs which comprise the graph itself, also known as the "search space" of the problem.
- A set of starting information defining the starting node(s) of the problem.
- Some definition of the goal of the search, either in terms of a list of nodes, some property of the nodes, or some property of the paths to be found in the graph.
- Some definition of the termination conditions for the search as a whole. This may involve finding the first path, the shortest path, or the "best" path with respect to some scoring criterion, or it may involve finding all solution paths in the graph, by exhaustive search.

Given this specification, the next choice is what direction to search the graph:

- **Either :** Work from the starting nodes using the data given to develop the problem forwards, hopefully finding the goal state(s) at some stage (this is known as data-driven, forward chaining search).
- **Or :** Work backwards from the goal, producing successive subgoals, in order to find the starting nodes (this is goal-driven, backward chaining search).
- **Or :** Some graph search procedures develop paths simultaneously from goal nodes backwards and from start nodes forwards, until a path is found which meets up in the middle (this is known as "bi-directional" search).

The choice of which direction to use is dependent on the nature of the problem. Some problems can only be formulated in one direction, and some may be very difficult to express in anything other than the "obvious" form. The "branching factor" of the search space in forwards and reverse directions will also influence the choice of whether to search forwards or backwards, for computational reasons.

The branching factor of a graph is a number expressing the (typical or maximum) number of arcs attached to each node in the graph. If the arcs have an associated direction, there will be a forwards and a backwards branching factor for the graph, which may have quite different values, depending on the problem being considered.

The reason branching is important is because, unless an algorithm has perfect judgement at each step in the search, each node offers many possible paths to explore, most of which will not lead to a solution path. Therefore, the wasted search effort involved in exploring these paths is the main computational cost in searching a graph. This effort can be reduced by reducing the number of alternative branches to be considered at each node. Some problems have a characteristically larger branching factor in one direction than the other, meaning that a clear-cut decision can be made between forward and backward chaining search.

As an example, if we want to check the truth of the proposition "I am a descendant of William Shakespeare", we need to find a path of lineage between the "I" and the "S" (there is a maximum of one such path). Considering that Shakespeare was born in 1564 and I was born in 1968, there are about 400 years between us. Assuming a gap of about 25 years between generations, this means that the line of descent (if there is one) will be about 16 steps long.

The choice is therefore between searching backwards from "I", to find out if "S" appears as an ancestor, or of searching forwards from "S" to find if "I" appears as a descendant of "S". We can analyse the branching factors in each direction to decide which is the best way to search. Everyone has exactly two biological parents, so the branching factor for backwards search is 2. However, in the past, people tended to have more than 2 children, so that the branching factor for forwards search is greater than 2. If we assume that the forwards branch factor is 3, the potential number of steps in exhaustive forwards search could be $3^{16} = 43{,}046{,}721$, compared to $2^{16} = 65{,}536$ for backwards search. Clearly, the backwards search will be more efficient in this case, but still of exponential complexity.

Note, however, that the notion of a typical branching factor can be misleading in some problems because of the nature of the search space. A particular example is the travelling salesman problem described in Section 1.6.3 below, and illustrated in Figure 1.6.

One factor which affects the choice of how to conduct search is the possibility of finding either multiple or cyclical paths between nodes in the graph. Multiple paths which do not include cycles are mostly a nuisance, giving rise to repeated search, or overhead in checking for previously seen nodes in the search. But cycles can cause infinite cycling in the search if the algorithm does not include a check for previously seen nodes within the same path. If it is possible to say with certainty that the graph is a tree, then the overhead of looking for previously seen nodes can be eliminated from the algorithm. Therefore, it is important to consider the topology of the graph before implementing any search algorithms for it.

Having decided whether to search forwards or backwards, the next decision is what search algorithm to use. Two of the most common are discussed briefly below.

1.6.1 Depth-first (backtracking) search

This search procedure works by expanding paths as far as they will go, until either a dead-end is reached or a solution path is found. In the case that a dead-end is found, the search "backtracks" to the nearest node which still has unexamined branch nodes. If a goal node is found, the search finishes, returning the path developed to that node.

This is best explained as a search which recursively examines each of the nodes attached to the current node in turn, to see if there is a solution path along that route. Whenever possible, the search goes deeper in the graph. The general algorithms which implement this search must include a record of nodes which have already been examined, or found to lead to dead-ends, so that cyclical and redundant paths can be avoided in the search.

Depth-first search is not guaranteed to find the shortest path in the search space, unless the search space is finite and search continues until the whole space is searched. The strength of depth-first search lies in the fact that it does not require much storage, because it only stores one partially completed path at any time.

In the example of Figure 1.4, forward-chaining depth-first search from S to F might examine the following nodes in turn: S, A, B, G, no way forwards - backtrack to B, to A, to S, then D, C, (B and G already visited), E, F (goal found - stop).

1.6.2 Breadth-first search

In breadth-first search, the paths examined in the graph are all extended by one step before any of them is further examined. This results in an expanding "search front" of nodes to be examined next, and guarantees that search progresses through the graph so that the shortest paths between start and goal nodes are found first.

This method typically uses a lot more storage space than the depth-first method, because all the paths still under consideration have to be stored at the same time. It can therefore be intractable for highly branched search spaces, but is guaranteed to find the shortest path between start and goal nodes before any longer paths.

In the example of Figure 1.4, searching breadth-first from S to F would examine the following nodes in order: S, A, D, B, C, G, E, F (goal found).

1.6.3 Complexity Analysis

Much of the theoretical work of computer science is concerned with the development of algorithms for performing well-defined tasks on large amounts of data. Computer scientists are therefore concerned with the following questions about an algorithm:

- Is it guaranteed to terminate in a finite amount of time?
- What is the maximum length of time the algorithm will take?
- How much space will it need?

The first question is the most difficult one to answer in general for algorithms and I will therefore not consider it further, beyond making the point that any search on a finite graph must terminate in a finite amount of time if it does not examine cyclical paths in the graph. The time and space required for exhaustive search in this case may make such an algorithm intractable for any realistically sized computer, but the problem is not in any fundamental sense insoluble.

The computational complexity of an algorithm is a measure of the amount of time or space it requires for it to do its job. This is usually expressed in terms of the size of the problem to be solved. For example, the complexity of a procedure for sorting elements in a list may be expressed in terms of the number of elements in the list, N, such that the time taken is " of the order of N^2 ", or $O(N^2)$, meaning that the most significant part of the time taken is proportional to N^2.

The estimation of search complexity depends heavily on knowledge about the topology of the search space, as well as the termination conditions and the goals of the problem at hand. It is not always possible to use a typical branching factor constant in assessing the number of paths to be examined.

As an example, consider the travelling salesman problem, as illustrated in Figure 1.6 below. A travelling salesman has to start at his home city (A) and visit all the other cities in the graph once only before returning home. The distances between the cities are used to label the arcs between them. The objective of the problem is to find the route which minimises the total distance the salesman must travel.

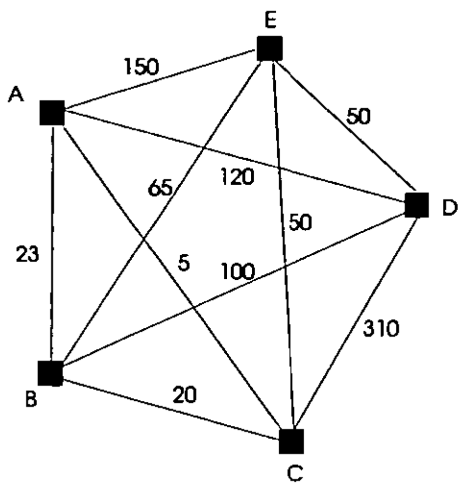


Figure 1.6: Example travelling salesman problem for 5 cities

In the travelling salesman problem, the number of arcs in the solution path to be found is fixed at N, where N is the number of cities in the problem. To assess how much time it takes to find the minimum distance path, it is necessary to observe that the total length of the path is not known until the end of the path is found. Therefore, finding the minimum length path could require expanding all possible routes covering the N cities, computing the total length of each one and choosing the shortest one.

There are (N – 1)! different paths through the graph covering each of the cities, so the time required to check these (the time complexity) is of the order of (N – 1)!, which becomes impossibly long for quite small values of N. The storage required (the space complexity) is of the order of N because all that is required is the list of cities to visit in order, for the shortest path found so far and for the path currently being considered.

However, various strategies for the travelling salesman problem have been developed to make this problem more tractable. An example is the "branch and bound strategy", which at every stage of path generation checks the length of the partially generated paths against the minimum total path length found so far. Any path (partial or complete) which is longer than the minimum length completed path can be rejected immediately. This has been found to reduce the time complexity to exponential, rather than factorial values, $O(1.26^N)$.

Exponential complexity is typical for exhaustive graph searches in search spaces where a branching factor is found which remains more or less constant throughout the search space. In cases like these, the time complexity for finding a path of length N in a graph, with a branching factor of B branches for each node, will be $O(B^N)$. This is equivalent to the number of nodes which will typically have to be examined in the graph to find the first solution path. This time complexity applies equally well to depth-first as to breadth-first search, but the space complexity of breadth-first is $O(B^N)$, while that of depth-first is only O(N).

Despite the space requirements, breadth-first search is often a good choice for problems where the aim is to generate (and store for later reference) all the shortest paths between a number of starting nodes and a number of goals. This is the case with the fault propagation model used for AutoHAZID.

1.7 Justification

HAZOP is an effective means of identifying hazards, but it is also very expensive, in terms of personnel, time and money. The technique is also highly structured and, in overall structure, appears almost algorithmic in nature. These considerations support the view that HAZOP automation is a useful and feasible task to attempt.

The techniques for qualitative modelling of process plants developed at Loughborough are novel and therefore exploratory in nature. However, they promise efficient hazard identification for test cases much larger than those commonly reported in the literature. The model formalism used is a graph-based one, which uses the well-proven AI technique of graph search to reason about fault propagation in the plant.

The Plant Engineering Group at Loughborough University has been active in fault propagation modelling and the automation of safety assessment tasks for many years now. Some of the early work, reported by Parmar and Lees (1987a, 1987b), used rule-based systems to identify equipment hazards. In parallel, Hunt *et al.* (1993) developed the FAULTFINDER system for synthesising fault trees from models of the behaviour of plant components. The latest hazard identification system, AutoHAZID, was based on the QUEEN codes developed by Chung (1993) and in turn builds on the work of Zerkani and Rushton (1992, 1993).

So, Loughborough has extensive experience in this area, the techniques we are using build on mature AI techniques of knowledge representation and inference by search, and there is a strong economic argument for automation. These are the main reasons for the effort, in the STOPHAZ project, to build a prototype HAZOP emulator capable of analysing reasonably large problems. Our partners in the STOPHAZ project were Aspentech (Belgium), Bureau Veritas (France), Hyprotech (Spain), ICI Engineering (UK), Intrasoft (Greece), SfK (UK), Snamprogetti (Italy), TXT (Italy) and VTT (Finland).

Chapter 2 : Literature Review

This chapter reviews three main areas of work which form a background to this thesis:

- Conventional hazard identification, as practised in the process industries (Section 2.1).
- Qualitative Physics and the problem of emulating commonsense reasoning within a computer program (Section 2.2).
- Applications of ideas from qualitative physics and knowledge based systems to hazard identification, process engineering and particularly to emulation of the HAZOP study (Section 2.3).

This review does not attempt to comment at any length on related areas, such as failure diagnosis or process monitoring by computer. There is also no attempt to review the various "new technologies" of fuzzy matching, neural networks, *etc.* The number of papers in these areas is huge, and they are of only limited relevance to the work presented here.

2.1 Conventional Process Safety Methods

This section covers some of the methods used to identify potential hazards in a process design and to ensure the safe operation of chemical plant. A particularly good overview of the commonly used techniques is given in Chapter 8 of "Loss Prevention in the Process Industries" by F.P. Lees (1996), which has been used as a guide for the material given here.

As discussed in Section 1.2, the safety of a process plant can be promoted by two complementary means: management systems which encourage safe practices in the workplace, and safe plant design methods.

A broad range of hazard identification and risk assessment techniques are available, covering all stages of design, from process selection through to fully detailed process design. Some of these techniques can be seen as complete methods, while others are supporting methods to deal with detailed identification/analysis tasks or specific classes of problem. Event trees and fault trees, in particular, are more often used in risk assessment than hazard identification. The table below lists some of these methods, with references to the sections where they are described.

Complete Methods
What If? Analysis (Section 2.1.6)
Preliminary Hazard Analysis (Section 2.1.7)
Coarse Hazard Studies (Section 2.1.8)
Hazard and Operability Studies, HAZOP (Section 1.3)
Failure Modes, Effects and Criticality Analysis (Section 2.1.9)

Complementary Techniques
Event Tree Analysis (Section 2.1.10)
Fault Tree Analysis (Section 2.1.10)
Computer HAZOP (Section 2.1.11)
Sneak Analysis (Section 2.1.12)
Human Error Analysis (Section 2.1.13)

Table 2.1: Commonly used hazard identification techniques

There is a good deal of overlap between techniques, in terms of applicability to each stage of design. Any particular organisation should select appropriate techniques for each stage of the design process, and for plant operation.

In addition to the choice of which methods to use, engineers and managers must organise a system of safety management so that hazard studies are performed by the right people at the right time. The necessary information to carry out hazard studies and the results of those studies should be made available whenever needed, and actions produced by the hazard studies should be executed. The safety management system of an organisation and the technical means it uses to find hazards are both important in ensuring the safety of employees and the wider public.

A further level of checks and balances is usually employed, in the form of management and safety audits (discussed in Section 2.1.1), which are used to check through the procedures in the organisation to see that they are being used appropriately.

Following on from the discussion of audit methods is a discussion of materials properties and how they can be used to screen process options for early process route selection, in Section 2.1.2. Knowledge of material properties is required in any case, for adequate assessment of the hazards in a process. Hazard indices (Section 2.1.3) are another instrument used to assess the hazards presented by a process or its equipment, and pilot plants (Section 2.1.4) can also provide valuable information about the hazards of novel process options.

Checklists, as mentioned above and discussed in Section 2.1.5, are a good way of preserving the "lessons learnt" information gained from accidents, but only if they are used and maintained regularly. The subsections following Section 2.1.5 cover each of the techniques mentioned in Table 2.1 in turn, and in Section 2.1.14 the techniques discussed are put in the context of the activities which go on during the design of a new process plant.

2.1.1 Management and Safety Audits

As a part of the management structure of an organisation, procedures and codes of practice for management and operation of plant, as well as the more technical aspects of process engineering, are important in maintaining a safe place of work for employees. In the UK, management has a responsibility for the safety of employees covered by the Health and Safety at Work Act, HSE (1990).

Audits of the safety systems in use in an organisation are directed at discovering areas of strength, weakness and vulnerability in the activities of that organisation. Typically this sort of investigation will cover the control of maintenance through a permits to work scheme, reporting procedures for accidents and "near misses", *etc.* The safety audit can be quite detailed in its scope, including some identification of main hazards as well as the assessment of site systems of work and reporting. An example of this type of check is given in "Safety Audits", by BCISC (1973).

Management system audits are usually focused on a wider range of commercial activities, but also form the main type of inspection carried out in the UK by the HSE.

All techniques are directed at ensuring the optimum levels of performance throughout the company, including profitable and safe operation of its plant.

2.1.2 Materials Properties and Process Screening

Many hazards associated with a process are related to the properties of materials or intermediates used. Therefore, considerations of safety, operability and environmental problems can take place even before process chemistry or plant siting have been decided.

By considering safety problems for each process option, designers can choose an inherently safer plant. This could be achieved by using a more benign process, which avoids extreme temperatures and pressures, or by eliminating hazardous chemicals altogether. Alternatively, process intensification can be used to reduce inventories of hazardous materials, or plans for siting the plant can be changed to minimise the impact of accidents on local people or the environment.

Screening process routes requires that certain information is available about the process materials, such as physical and chemical properties, as well as safety related information, relating to flammability and toxicity. Standard safety data sheets usually provide some of this information, and some of the rest can be found in reference books. It should be noted, however, that information on likely impurities and their effects on the process chemistry and safety can be difficult to obtain.

According to the EC Safety Data Sheet Directive, CONCAWE (1992), the contents of a material data sheet should include the following items:

- Identification of substance/preparation and company
- Composition/information on ingredients
- Hazards identification
- First-aid measures
- Fire-fighting measures
- Accidental release measures
- Handling and storage
- Exposure controls/personal protection

- Physical and chemical properties
- Stability and reactivity
- Toxicological information
- Ecological information
- Disposal considerations
- Transport information
- Regulatory information
- Other information

Information about the thermal stability of materials in the process can be vital to ensuring the operability of a process as well as its safety. Two factors come into play here. One is the inherent stability of single components, with regard to physical changes in plant and storage conditions. The second factor is the stability of reaction mixtures in the reactor environment and the question of exothermic runaway. For some compounds explosion caused by mechanical shock, rather than straightforward thermal stability may be the dominant issue. Care must be taken to identify what sort of hazards will be present due to the compounds and reactions in the system.

A certain amount of "desk screening", using book data, guidance on chemical bond groupings, computer programs, *etc.* can be used to filter out compounds which are likely to be highly unstable. Then, preliminary tests can be performed to detect the presence of an exotherm or gas evolution when a material is heated. Further tests can also be used (using various forms of calorimetry) to get more detailed information about the stability of compounds or reactions of interest.

2.1.3 Hazard Indices

A number of index methods are available to assess the losses that could be caused by fires, explosions and releases of process materials. These are applicable where a preliminary flowsheet and site plan are available, so that process fluids, inventories, pressures and temperatures are known. Examples of these techniques include:

- Dow Fire and Explosion Index (Dow Chemical Company, 1994).
- Mond Index – Similar to the Dow Index, for fires, explosions and the acute toxicity effects of releases.
- Dow Chemical Exposure Index.

- Instantaneous Fractional Annual Loss (IFAL).
- Mortality Index, which relates to materials with a major hazard potential.

These indices can be used to inform process selection decisions or to identify the main hazards in the process design, with a view to controlling them.

2.1.4 Pilot Plants

A large quantity of potentially useful data can be gained from pilot plant studies, which help in clarifying the safety and operability issues in a process, as well as informing the scale-up of the process from lab experiments to full scale operation. It is very important that the experience gained on the pilot scale is used to good effect when full scale production is considered. Due consideration must also be given to the hazards presented by the pilot plant itself, before it is built.

2.1.5 Checklists

If used appropriately, checklists are an effective way of passing on information about the characteristic hazards of a process or piece of equipment. They are based on past experience of hazards or accidents and may therefore be less useful when developing novel processes, than when reusing or modifying an existing design.

Checklists are often used at the design check stage, when developing a process flow diagram into an ELD, to quickly examine the proposed design for any problems. They should therefore be used only as a final check that nothing has been missed, and not as a protocol to guide the design process itself.

Some guidance on the use of checklists is given by Miller and Howard (1971). There are a huge number of references on the subject, a selection of which is offered in Table 8.4 of Lees (1996).

A useful checklist should provoke enough thought to prevent the user from simply answering "yes" or "no" to each question. This requires a careful choice of questions, which must be worded appropriately. The user of the checklist must of course raise appropriate actions if he/she finds any problems with the design.

Lastly, checklists must be used regularly and updated as necessary, in the light of experience with their use. Ownership and responsibility for the lists need to be maintained and passed on within an organisation.

2.1.6 What If? Analysis

This method is described by Burk (1992) and by CCPS (1985). It is best used at the stage in design when a process flow diagram (PFD) has been produced. All available design information is examined, including the PFD, any operating instructions and equipment design parameters.

The objective is to produce a list of potential safety problems or actions to be considered in revising the design, by considering the effect on the plant of abnormal situations. A group of design team personnel meet to examine the design and ask questions about possible things that could go wrong. The method uses the team's collective imagination to identify more obscure problems than might be possible using a checklist alone.

Burk (1992) combines the "What If?" method with a checklist approach, to give more comprehensive coverage of process hazards. This method can be used to evaluate new plant designs, review an operating plant periodically, or to check for hazards when making modifications. The study is performed by a multidisciplinary group, aided by a team leader to conduct the meetings and a scribe to record the questions raised. The analysis proceeds through a number of stages:

- Organisational Meeting – The team leader explains the method to be used, and the scope of the review, to the whole group. Information packages, containing all necessary drawings, technical details and a timetable of meetings, are distributed to each team member.

- In-Depth Review of Process – For team members unfamiliar with the process, the main features of the plant are explained and a tour of the plant takes place, if appropriate.
- Question Formulation Meeting – When the team members have familiarised themselves with the information available, the plant is studied in detail, from feed to product storage. The team formulates questions focusing on potential hazards or incidents, and their causes:
    - There is no attempt to answer any questions at this stage, as this impedes the generation of further questions.
    - Questions are recorded in full sentences on a flip-chart visible to the whole group.
    - All points raised are recorded, even if they appear to be "dumb questions".
    - Questions do not have to begin with the phrase "What If?".
    - Closely related questions are grouped together, as some questions will give rise to other related ones.
- When the whole process has been reviewed in this "brain-storming" way, the team leader hands out a checklist of possible areas of concern. The group works through the list, to see if any further questions are raised by this. Burk provides an example of a list which could be used here.
- After the question formulation meeting, questions are allocated to team members, who take them away and prepare draft answers to them. When the answers have been prepared, they are distributed to all team members before the next meeting.
- Question Response Meeting – The group reviews the questions raised and answers produced, to agree on what to do about each problem area. It is very important that all agree with the actions produced by this meeting.
- The report should (at minimum) document the identified hazards, their causes and the agreed actions to eliminate or control these hazards. Burk suggests that the report should not be presented in a tabular format, but instead should use complete sentences to record the questions and answers. This is felt to be more effective in communicating the full meaning of what has been discussed.

2.1.7 Preliminary Hazard Analysis

Methods for identifying hazards during early design, when only a block diagram of the process may be available, vary widely. Therefore, use of the term "preliminary hazard analysis" (PHA) is quite loose. The usual objective of PHA (as described by, for example, CCPS, 1985) is to raise awareness of the major hazards in equipment proposed for the design, as early as possible. Analysis should produce a set of causes and consequences of specific scenarios, with associated corrective measures.

The following aspects of the design should be considered, with regard to the hazards that may be present:

- Properties of the raw materials, intermediates and products in the process, as well as utility fluids such as steam, nitrogen, fuels, *etc.*
- Types of equipment used in the process, their temperatures and pressures.
- Interfaces between components of the designed system, such as fluid interactions and compatibility with materials of construction, fire initiation and propagation, *etc.*
- Operating environment. Consider external factors such as temperature limits, humidity, earthquakes, *etc.*
- Operation of the plant (maintenance, testing, start-up and shut-down, *etc.*).
- Facilities support, such as storage, staff training, utilities required.
- Safety Equipment (*e.g.* emergency shutdown instruments, personal protective equipment, fire protection).

2.1.8 Coarse Hazard Studies

Coarse hazard studies, such as the method outlined in Section 4.1 of the CIA Guide to Hazard and Operability Studies (1977), aim to identify problems caused by missing data or hazard information, or features of the basic design, layout and plant siting.

This assessment is carried out early, when a block layout of plant items and (possibly) a basic flowsheet is available. It should clarify to all those taking part what the main sources of hazards and problems with operation will be, as well as indicating deficiencies in data about the process and the materials in it.

A method study approach similar to that used in HAZOP (Section 1.3) is common, where a team of experts reviews the design under the supervision of a chairman. Guide words provoke generation of ideas in combination with the general design parameters decided so far and a number of potential hazards. The guide word lists given by Knowlton (1981), as the "creative checklist" approach are:

General Design Parameters:

- Materials
    - Raw materials
    - Intermediates
    - Products
    - Effluents
- Unit Operations
    - Mixing
    - Distillation
    - Drying
    - *etc.*
- Layout
    - Arrangement between unit operations within the plant
    - Spatial relationships with other facilities

Potential Hazards:

• Fire	• Noise	• Explosion
• Vibration	• Detonation	• Noxious material
• Toxicity	• Electrocution	• Corrosion
• Asphyxia	• Radiation	• Mechanical failure

The actions produced by the study may be queries for information on equipment or materials, or actions to plan for, or design out, certain hazards highlighted in the study.

2.1.9 Failure Modes, Effects and Criticality Analysis (FMECA)

Failure modes and effects analysis (FMEA) reviews specific failures of system components and the consequent effects of each failure mode on the whole system. Criticality analysis can be added to this cause-effect analysis, so that the severity of the effects of failure, and the frequencies of the root cause failure modes, are estimated. When this additional method is used, FMEA becomes FMECA, "failure modes, effects and criticality analysis".

The two methods are described in the CCPS hazard evaluation guidelines (CCPS, 1985) and are also covered by a British Standard, BS5760: Part 5 (BSI, 1991). An example of the results of application of FMEA to a liquefied natural gas terminal is given by Aldwinckle and Slater (1983). An example for a differential pressure transmitter is given in Appendix 3 of Green (1983).

FMEA is a systematic and laborious procedure which requires detailed design information. It therefore can only be used selectively, late in a project, on the more critical parts of the process, control or safety system.

Before starting the study, it is important to decide what equipment is to be examined and in how much detail, as well as collecting all available information on the functions of the equipment items.

Each element of the system is examined in turn (by a team or a single analyst), and all conceivable failure modes are noted. Failure modes are malfunctions that change the normal operation or function of equipment items. For each failure, the effects on the system are determined and the results recorded in a standard format. This requires a detailed understanding of the events involved in the fault-consequence scenario. For

FMECA, the criticality of each failure mode is added, in terms of a severity and probability class (*e.g.* a rank number in the range 1-4), for each identified scenario

The results of the study should record the failure modes of equipment, causes of these failure modes and the further effects on other components, and the system as a whole. It is also important, if possible, to classify the failure mode in terms of how it can be detected, the possibility of testing or replacing components to eliminate the problem, and any provisions made to compensate for the failure if it occurs.

FMEA and FMECA are best for considering components whose failure could have a serious effect on a large part of the (process) system. They are good for serial failure logic, where causes and effects chain together one after another but for more complicated logic, fault tree and event tree analysis are more suitable techniques.

2.1.10 Event Tree and Fault Tree Analysis

Event trees are logic diagrams illustrating the development or escalation of a hazardous consequence, or scenario. Fault trees are logic diagrams which show the mechanisms by which a hazardous event can be caused (sequences of events in the fault tree are known as "fault paths").

Both types of tree are used mainly for risk assessment, to quantify the risk or the losses resulting from an incident. Nevertheless, constructing them can be a useful exercise in focusing thinking during hazard identification. The use of event trees and fault trees for hazard analysis is described in Chapter 9 of Lees (1996).

2.1.11 Computer HAZOP

The failure modes of computer systems can be quite different to those of process or mechanical equipment, and the use of computers in modern process plants is increasingly pervasive. For this reason there has been a lot of recent interest in techniques for analysing the reliability of programmable systems, and in methods to identify the hazards which could arise due to failure of components in computerised systems.

A number of factors combine to make safety assessment of computer-controlled plant more complicated than for plant which does not involve any programmed component. Relevant considerations include:

- Failure of process equipment.
- Failure of computer hardware.
- Common mode failures across the whole plant, related to problems with the computer control system, other services or plant-wide utilities.
- Latent errors in computer programs. These coding errors are systematic and are only revealed under certain conditions of operation.
- Errors in specification of the computer software due to poor communication between engineers and programmers.
- Communication errors between machines, due to unforeseen conditions in the plant, or within the equipment items themselves.

Computer HAZOP is carried out at the same time as, or after, the process-related HAZOP of a plant. Details of the instrumentation and control systems, including loop diagrams for instruments and control program documentation, must be available. The project instrument and control engineer and someone responsible for the technical programming and configuration of the computer system must be present, as well as the usual HAZOP team members.

The method deals with computers by adding extra guide words to the traditionally used set, describing possible failures in relation (normally) to instrument signals and the output signals from controllers. Normally the computer has no power to affect the operation of the process, except through actuators connected to the process. In this sense, the guide word approach proposed by Andow (1991) makes sense for inputs and outputs.

Chung and Broomfield, in Chapter 2 of "Computer Control and Human Error" (Kletz *et al.*, 1995), present a methodology for HAZOP of computer-controlled systems. Their approach concentrates on examining each of the functional requirements of the system in turn, decomposing the requirement into tasks which must be accomplished in sequence, and then asking questions derived from analysis of incident reports. An interesting idea used in this work is that of decomposing a system into components, each of which maps onto a component class and a corresponding "functional layer" in the system as a whole. The layers of the system define the classification of tasks and incidents in the approach, with communications to/from the computer defined as arrows on an "event time diagram", as illustrated in Figure 2.1.

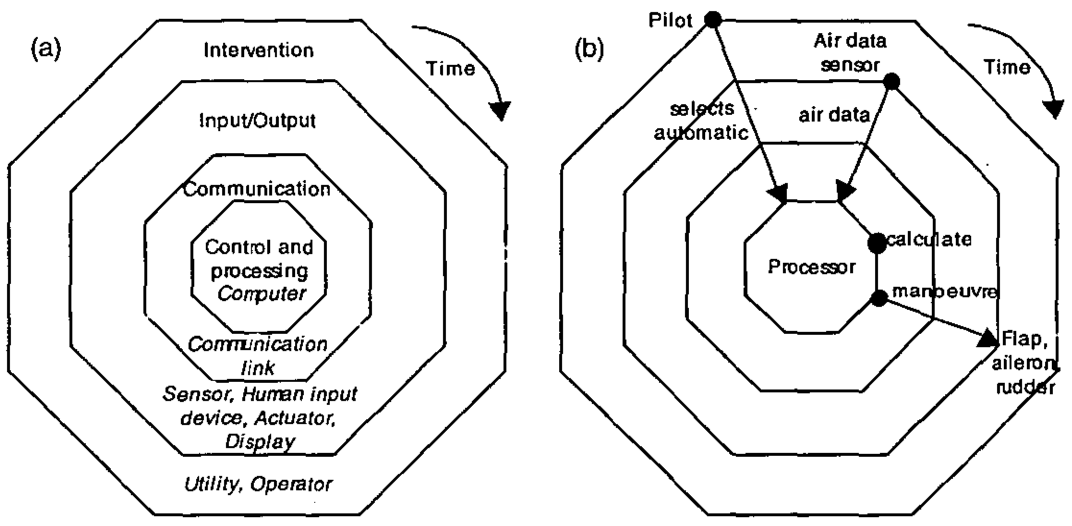


Figure 2.1: (a) Functional Levels and Basic Components of the Event Time Diagram, (b) An Example ETD for a Flight Management System

2.1.12 Sneak Analysis

An account of sneak analysis in process plant is given by Whetton (1993). The technique is adapted from "sneak circuit analysis", a method for finding design errors in electronic circuits, developed in the aerospace industries in the 1960's.

Sneak analysis is a niche method which can be seen as a supplement to other methods of process hazard identification, such as HAZOP, "What If...?", *etc.* A sneak is defined as "an undesired condition which occurs as a consequence of a design error, sometimes but not necessarily in conjunction with a failure".

For process systems, Whetton (1993) identifies six categories of sneak. The categories may occasionally overlap, for some incidents:

1. **Sneak Flow** – An unintended flow from a source to a target location, possibly due to a valve being opened erroneously. A simple example of this is shown in Figure 2.2. If the two drain valves are opened simultaneously, fluid from the high pressure vessel can get into the low pressure vessel, with potentially hazardous results.
2. **Sneak Indication** – Incorrect or ambiguous indication by instruments or safety systems. An example of this type of problem is one from the Three Mile Island incident, where an indicator intended to show the state of a remotely operated valve actually showed the state of the switch operating the valve (Figure 2.3). Clearly if the valve is faulty and cannot operate, the lamp does not indicate this.
3. **Sneak Label** – An incorrect or ambiguous label on instrumentation or process equipment.
4. **Sneak Energy** – Unintended presence or absence of energy. Examples of this include reactor vessels where a mixer, which has been switched off for a while, is reactivated causing a reaction to run out of control, or cases where pressure remains in a system after shutdown, injuring personnel when the process is opened for maintenance.
5. **Sneak Reaction** – Unintended reactions, such as side-reactions in a reactor, or reaction of materials outside the reactor environment.
6. **Sneak Procedure** or **Sequence** – Where events occur in the wrong order or in conflict with one another.

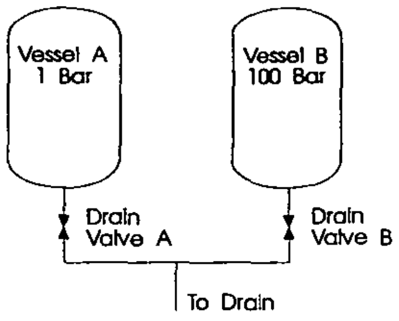


Figure 2.2: An example of sneak flow

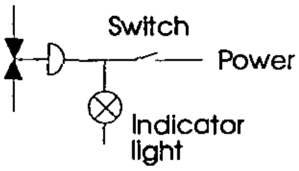


Figure 2.3: An example of sneak indication

By analysing incident reports, a list of clues to identifying sneaks can be prepared, and stored in a database, indexed according to the type of sneak (flow, indication, label, *etc.*), the type of equipment, process parameter (temperature, level, pressure, *etc.*) and deviation (high, low, none as in HAZOP). This clue list database can be used to access the clues relevant to each deviation when conducting a HAZOP study and to provoke identification of sneak faults in addition to the usual "brainstorming" method. Whetton calls this method "sneak-augmented HAZOP".

In addition to the clue list method mentioned above, "sneak flow analysis" can be used to systematically identify sneak flows. This method partitions the process as built into sections and identifies all possible sources and destinations for fluid in each section. Then, each pairing of source and target within a section is examined to see if fluid could flow from one to the other (assuming that all valves are open). Any resulting problems with regard to overpressure, fluid reactions with other fluids and with materials of construction, are noted as sneak flow problems.

2.1.13 Human Error Analysis

Human error is often implicated in the root causes of accidents and in their development. However, techniques to deal with this type of problem are difficult to apply, perhaps because of the vast range of errors which can occur. Two methods are mentioned here which can be used to identify operator error problems. It should be noted that this class of error by no means covers the whole field.

Task analysis can be used to look at the actions performed by an operator and to identify potential problems. It is a technique which breaks down high level tasks into successively more detailed subtasks, forming a plan on a number of levels of detail. This technique is not used a great deal for hazard identification, but was developed as a training tool.

Action error analysis, developed by Taylor (1979), is a method of looking at the operating procedures of the plant and considering the possible errors which could take place in the sequence, using a guide word approach. The procedure is modelled as a sequence of actions and their associated effects on the plant. An error is then developed with regard to a particular action, and the consequences of this error are evaluated. Particularly important in considering the effects of errors is whether they can be detected or corrected afterwards.

For any assessment of human error in a particular plant, reasonably detailed operating instructions must be available, as well as a full specification of the instrumentation systems and (ideally) a layout diagram of the control room instrumentation and alarms, *etc.* This means action error analysis is only possible at a late stage of the project. Recommendations from the study may include modification of the operating instructions, changes to the operating sequence and operator training schemes, extra field instruments, or changes to the organisation of control room instrument panels.

Chapter 6 of Taylor (1994) offers an analysis of the subject of human error in process plant, reviewing some of the techniques which can help, such as action error analysis and sneak path analysis.

2.1.14 Hazard Identification in the Context of Process Design

The methods discussed so far form a menu of options from which safety managers can choose in formulating their own system for safe plant design. These will now be put in the context of the time-line from process conception through to checking on the final, detailed process design.

First of all, the design team must decide what product to make, where, and with what process chemistry. A basic process outline must be produced for a number of candidate options. At this stage, collecting data on process materials, screening them for potential hazards and testing for thermal stability are important concerns.

Experience gained in pilot plant studies, or from previous operation of similar processes, should also be used, at this process definition stage and later. The use of checklists should also be encouraged at all stages of the project where a process design exists at such a level that specific aspects of it can be usefully questioned.

Once a block diagram of the process has been developed, index methods such as the Dow Fire and Explosion index can be used. These inform decisions on inventories of hazardous materials, layout of plant sections, *etc.* Later, when a PFD has been drawn, a more specific view of the hazards to be expected in the plant can be gained by using either "What If?" Analysis, PHA, or a Coarse Hazard Study method.

For hazard identification on the detailed process design, HAZOP can be combined with a number of the supporting methods, as appropriate for the plant being designed:

- Sneak analysis can help to look at potential hazards from a different angle.
- FMECA can be used to investigate the more important components of the system, to evaluate the implications of their failure.
- Fault trees and event trees may be chosen for risk assessment, or to clarify the causation of complex events.

- Computer HAZOP may be used to review the potential problems associated with programmed components in the plant, including the control system.
- Human error analysis is most useful for plants involving a lot of operator intervention (*e.g.* batch or semi-batch operations).

There must be a sensible choice of a range of the above techniques, to cover the specific characteristics of the plant being designed. The technical studies must be integrated into a system of management and communication, so that all involved are aware of how the information generated is to be used.

2.2 Qualitative Physics

Qualitative Physics (QP) is an active field of research in Artificial Intelligence (AI). In QP, models of physical systems are based on qualitative variables with discrete values, rather than the real numbers typically used in the differential equation models of classical physics (De Kleer, 1992). Study in this area is justified by a number of points:

- QP can provide more causally satisfying explanations for physical behaviour than the mathematical equations most often used in classical physics.
- Solutions to problems in QP may be simpler to obtain, compared with those of quantitative physics problems.
- Computationally, QP simulations are cheaper than numerical simulations.
- More intuitive explanations of behaviour may be offered by QP. It seems likely that the mental physical understanding we use (our own "naïve physics") is fundamentally qualitative in nature.
- QP may be able to solve problems where only an incomplete specification is available.
- The precision required in specifying parameters in a quantitative simulation ensures that only one behaviour is produced from any given starting point. By contrast, a qualitative simulation can deal with uncertain or imprecise values and can therefore represent a wider range of physical scenarios. This means that QP

can be made to produce all physically possible behaviours of the physical system corresponding to the qualitative model studied.

- QP models can be used to focus attention on areas of concern and simplify later quantitative analysis.

2.2.1 General Issues to be Tackled by Qualitative Formalisms

Whatever approach is chosen for studying Qualitative Physics, a number of important issues must be addressed (De Kleer, 1992). Firstly, there is the question of what to represent in the QP system — for instance, whether the fundamental "units" in the system are physical processes which may or may not be in operation (Forbus, 1984), components of a mechanism (Kuipers, 1986), or constraints operating between variables (De Kleer and Brown, 1984). These three most common standpoints in the field are discussed later, in Sections 2.2.4, 2.2.5 and 2.2.6 respectively.

A second issue is the treatment of variables and values. We have established that the values of variables in QP are discrete, but what values those variables may take, under what conditions, *etc.*, is a separate argument. Most of the time, the qualitative variable under consideration is produced by segmentation of the real number line (corresponding to the related quantitative variable) into a number of non-overlapping intervals.

The most commonly used value set is {−,0,+}, corresponding to quantitative values which are negative, zero or positive. For a particular material in pure form and at ambient pressure, there may be five qualitative temperature values, corresponding to the temperature ranges where the material is solid, melting, liquid, boiling or gaseous. The points on the number line where the qualitative value of the variable changes are known as "landmark values" and they usually correspond to significant qualitative changes of applicable laws or behaviour.

In addition to the definition of qualitative variables, algebraic axioms and rules must be provided to allow mathematical operations to be defined on the variables. Often, these axioms and rules are derived from the mathematical analysis of real numbers.

Some generic and some problem specific constraints must also be brought into play in order to establish relationships between the variables in the model system. How constraints are expressed depends on how the concepts of "structure" and "mechanism" are treated. Some workers (*e.g.* De Kleer and Brown, 1984) represent constraints directly, avoiding the construction of a constraint set from some other form. In the component based approach to modelling, constraints are specified between variables within the same component, and inferred from linkages between components, so that a network of constraints is formed in the composite system.

The principle of "no function in structure" is a guiding principle for developing models. The laws of individual parts of a system (its "units") must never presuppose the function of the whole. The purpose of this principle is to prevent the development of context-specific models where the answers to questions put to them are built into the laws governing individual units and their linkage. In such a situation, difficulties will be encountered when the unit is presented with a different context.

A major problem with QP systems is that of representing time, and therefore change, in physical systems. As variables change, they may reach landmark values, changing the behaviour of the system. Which variables reach landmark values first is the question addressed by transition analysis, or limit analysis (Forbus, 1984). Time is usually represented qualitatively as a sequence of "intervals", optionally separated by "instants". Having decided on a representation for time, predictions can be made using a qualitative calculus which allows simulation of behaviour forwards in time from a given initial state. This is particularly illustrated by De Kleer and Brown (1984), who describe the concept of "envisioning" the behaviour of a mechanism.

Causality (the issue of what events can cause other events in the system) may or may not be addressed explicitly in a QP model, as with any physical explanation. There is a problem here, in that the scientific community has not yet come up with a satisfying formal definition of causality. As a minimum for causal linkage, dependency must be demonstrated between two events. If A and B are assignments of values to qualitative variables ("events"), then for A to cause B, the occurrence of B must depend on A occurring. Usually, the constraints of spatial and temporal order are also imposed to determine if the causal link exists: only physically connected components may interact, and for A to cause B, A must precede B.

2.2.2 Ambiguity

Ambiguity in qualitative simulation arises when the simulator cannot decide which of a number of possible outcomes actually takes place. This leads to a branched "tree" of possible states of the system being simulated, where every one of the possible outcomes must be considered. Computational complexity becomes a problem when this sort of ambiguity is widespread.

Ambiguity of various kinds is inherent in the nature of most models in Qualitative Physics. One important type of ambiguity is that of certain arithmetical operations, such as addition. If two qualitative variables A and B each take values from the set {–,0,+} then their sum, (A+B), is highly ambiguous (the sum of a "+" and a "–" may be "+" or "–", or even "0"). This is a problem when considering mass balances around dividers or headers in simulations of chemical plant, for example.

Another significant source of ambiguity is where a model uses a very loose functional constraint between two variables. Such constraints are needed to allow a wide range of mathematical functions to be generalised within the qualitative framework. The downside is that a whole family of functions are implied, every time the qualitative constraint is used, so that the simulated behaviours of the system include all those consistent with the different interpretations of the constraint.

Temporal ordering of state changes in qualitative simulations also increases ambiguity. Where the system is unable to decide which of a number of possible changes in the system will occur first, it must consider each of them as equally possible. This occurs when a number of variables are changing, moving towards different landmark values, so that there is a problem in determining the order in which these landmarks are reached.

In QP, we want to be able to distinguish real behaviours of the system as specified from physically impossible predictions. There may actually be multiple real behaviours consistent with the model used, in which case we want to know about them all. Impossible behaviours may arise due to the inability of the model to capture real constraints which exist between objects in the world.

Usually, such constraints are high level ones, such as conservation of mass or energy, which cannot be captured very easily in localised qualitative models. However, some attempt to capture these types of constraints may be made by inspecting the configurations of units in the model of the system as a whole.

2.2.3 Naïve Physics and Commonsense Reasoning

In his "Naïve Physics Manifesto", Hayes (1979) criticises AI research for being too limited to so-called "toy worlds" and simple, well-defined puzzles and games. While the programs developed may possess an ability to play chess, or to reason about blocks on a table top, there is no sign of the general intelligence we are accustomed to making use of in the real world. As a first step towards intelligent systems, Hayes proposes formalising large parts of the commonsense knowledge we have about the world (our "naïve physics").

Among the many interesting topics discussed by Hayes (1979), the idea of histories is particularly useful for its potential in tackling a long-standing AI problem known as the "frame problem". A frequently used representation in AI models the state of the world using a set of propositions about individuals in that world. Rules are used to define possible transitions between states of the world, in terms of changes in the set of propositions. This model of change is known as the "situational calculus" and is described by (among others) McCarthy and Hayes, (1969).

Although this model is mathematically and computationally attractive, it suffers from a serious problem: one must specify, for each individual in the world, whether it changes or does not change in response to each possible action defined in that world. This is known as the frame problem, and it causes an explosion in the number of rules, as each variable must have a “frame axiom” to state if it does or does not change when some particular operation is carried out. The situational calculus allows the state of an object to depend on all the other elements of the world model.

The real world (when viewed in a deterministic way) is somewhat different. We intuitively know that two objects must physically interact with one another, typically through the action of some force or exchange of material, in order to affect their behaviour. Hayes calls for a state representation of objects that includes a limited spatial extent, but potentially unlimited temporal extent. This is the idea of a “history”: a projection of the spatial extent relevant for an object through time.

Histories are associated with an object and the places which can physically interact with that object over the temporal history of the object. These places are not necessarily fixed in size and they can overlap or be nested inside one another - and therefore so too can histories. The history of a composite object is defined as the union of the histories of each of its component objects.

Objects may only interact if their histories intersect in space-time. This substantially tames the frame problem because it restricts candidates for variables changes to those changes caused by the intersection of histories of adjacent objects in the world. Such a restriction embodies the two important causal considerations of spatial and temporal order, mentioned in the previous section.

2.2.4 The Process-Based Approach

“Qualitative Process Theory” (QPT) was developed by Forbus (1984). In this theory, changes in the world are caused by the operation of physical “processes”, corresponding to such phenomena as motion, heating, bending, boiling, *etc.* According to Forbus, this model of change is more descriptive than solving constraint equations to yield evolving patterns of variation in state variables (as in QSIM, for example – see Section 2.2.5 below). Hayes’ idea of spatially limited histories, described in Section 2.2.3, is used to tackle the frame problem, so that only objects whose histories overlap in time and space are permitted to interact.

Variables in QPT are defined in terms of a "quantity space" representation. An arbitrary number of landmark values are placed on the real number line of the quantitative variable being modelled. These define a number of non-overlapping intervals, which correspond to the values of the qualitative variable in question. Landmark values may mark places where significant changes in the physical model of the system occur. They may also be discovered during simulation, so that the quantity space may be extended dynamically.

Time is modelled using ideas from Allen's work on time and action (Allen, 1981 and 1984) and makes use of the concepts of events, instants, intervals and episodes. Significant landmarks on the time axis are not predetermined, but instead are uncovered by simulation, as points in time when significant changes take place. This is similar to the way in which the qualitative value sets of other variables are modified by the addition of new landmark values during simulation.

The objects in the world of process theory are termed "individuals". These represent physically real objects such as containers, substances, fluids, as well as more abstract objects, such as events, heat paths or processes themselves. Individuals are associated with a type, stating what sort of object they are.

"Individual views" (also known as "views") model situations and changes in individuals that may be dependent on the value of some quantity in the system. Each view is specified in four lists, as shown in Figure 2.4, taken from Forbus (1984), which shows a simple view for describing the fluid contained in a cup.

```
;; We take amount-of-in to map from
;; substances and containers to quantities

Individual View Contained-Liquid(p)
  Individuals:
    con a container
    sub a liquid
  Preconditions:
    Can-Contain-Substance(con,sub)
  QuantityConditions:
    A[amount-of-in(sub,con)]>ZERO
  Relations:
    There is p ∈ piece-of-stuff
    amount-of(p) = amount-of-in(sub,con)
    made-of(p) = sub
    container(p) = con
```

Figure 2.4: Qualitative process theory view for fluid in a cup

Views form templates for the realisation of "view instances". For every collection of objects that satisfies the descriptions of the individuals specified by the view, a view instance (VI) is created, which relates the individuals. Unless the preconditions and quantity conditions of the view are satisfied, the VI remains inactive. When the VI is activated however, the specified relations apply between the individuals.

Note that preconditions are used to specify how the view depends on events or situations that may occur outside the scope of the dynamic model of the system. Quantity conditions, on the other hand, may be satisfied or broken by changes predicted within the simulation itself.

Processes are used to describe how changes occur. Examples of physical processes include fluid and heat flows, boiling, motion and stretching. They are specified in a similar way to individual views, but have an extra part in their specification, for "influences". Two examples of process specifications are given in Figure 2.5, taken from Forbus (1984), for heat flow between two objects and a contained fluid boiling.

```
process heat-flow

Individuals:
  src an object,Has-Quantity(src,heat)
  dst an object,Has-Quantity(dst,heat)
  path a Heat-Path,Heat-Connection(path,src,dst)
Preconditions:
  Heat-Aligned(path)
QuantityConditions:
  A[temperature(src)]>A[temperature(dst)]
Relations:
  Let flow-rate be a quantity
  A[flow-rate]>ZERO
  flow-rate ∝Q+ (temperature(src)-temperature(dst))
Influences:
  I-(heat(src),A[flow-rate])
  I+(heat(dst),A[flow-rate])


process boiling

Individuals:
  w a contained-liquid
  hf a process-instance,process(hf)=heat-flow
                          ∧dst(hf) = w
QuantityConditions:
  Status(hf,Active)
  ¬A[temperature(w)] < A[t-boil(w)]
Relations:
  There is g ∈ piece-of-stuff
  gas(g)
  substance(g) = substance(w)
  temperature(g) = temperature(w)
  Let generation-rate be a quantity
  A[generation-rate] > ZERO
  generation-rate ∝Q+ flow-rate(hf)
Influences:
  I-(heat(w),A[flow-rate(hf)])
  ;; The above counteracts the heat flow's influence
  I-(amount-of(w),A[generation-rate])
  I+(amount-of(g),A[generation-rate])
  I-(heat(w),A[generation-rate])
  I+(heat(g),A[generation-rate])
```

Figure 2.5: Process specifications for heat flow and boiling fluid

As with individual views, processes form templates for the definition of "process instances", so that a process instance is created for each collection of individuals in the world which satisfy the description in the "individuals" section of the process definition. Process instances remain inactive until their preconditions and quantity conditions are satisfied, when the relations and influences specified come into effect.

Quantity conditions for processes may include inequalities between parameters of individuals (typically stated in terms of the "amount of" certain parameters, as in "A[var1]>A[var2]"), or conditions on the status of processes and individual views. "Relations" may include constraints imposed on parameters of the individuals and any new entities created by the process. The indirect effects imposed by functional relationships are represented in the "Relations" part of the process description. The "Influences" section is for specifying the direct causal effects of the process. In the heat flow example of Figure 2.5, influence statements describe how the heat flow negatively affects the heat content of the source object and positively affects the heat content of the destination object.

Implementation of QPT requires a simulator which is capable of monitoring a set of individuals and their parameters, automatically creating and activating appropriate view and process instances as appropriate. The views and processes should be taken from a library of models, the "process vocabulary", which defines the sorts of phenomena that can be modelled by the theory.

Simulation of system behaviour typically involves a process called "limit analysis". Changes in variables are observed, to determine which landmark values could be crossed, and in what order, and thereby determine the behaviour in the new qualitative state. This may give rise to more than one possible outcome from any particular state, so that simulation may produce a branching, tree-like pattern of possible behaviours. Limit analysis may uncover new landmark values during simulation, requiring that the quantity spaces of the variables are added to. It is not clear whether all these new landmarks necessarily correspond to physically significant events with respect to the variable concerned.

2.2.5 Qualitative Simulation - QSIM

Kuipers (1986) describes the approach taken to qualitative simulation in the QSIM algorithm. QSIM models the constraints represented by ordinary differential equations (ODEs), using analogous qualitative relationships. An ODE model can be directly translated into a system of qualitative constraints, suitable for processing by QSIM, as illustrated by the following example:

The differential equation

$$\frac{d^2u}{dt^2} - \frac{du}{dt} + \arctan(ku) = 0$$

becomes:

Quantitative	Qualitative
$f_1 = du/dt$	DERIV(u, f1)
$f_2 = df_1/dt$	DERIV(f1, f2)
$f_3 = ku$	MULT(k, u, f3)
$f_4 = \arctan(f_3)$	M+(f3, f4)
$f_2 - f_1 + f_4 = 0$	ADD(f2, f4, f1)

In the above, the DERIV, MULT and ADD constraints are self-explanatory. However, QSIM also uses the more general type of functional constraints, M– and M+. M+(f3, f4) above denotes a monotonic increasing functional relationship, where f4 is a monotonic increasing function of f3. M– is used to represent a monotonic decreasing functional relationship in the same way.

What is interesting about M+ and M– is the way that they introduce a whole class of possible functions into the otherwise quite rigidly defined qualitative constraint system. This vastly increases the range of possible problems with qualitative ambiguity, but is unavoidable if a QP system is to be of any general use. Kuipers discusses the different approaches used by researchers to represent this idea of an unspecified functional relationship between quantities, including the qualitative proportionality of Forbus' qualitative process theory (Forbus, 1984) and the confluence representation of De Kleer and Brown (1984).

The variables in QSIM are often known as "functions", because each is a function of time in the system. Kuipers uses the quantity space idea of Forbus (1984) to define qualitative values by comparison with a set of landmark values (a function can have a value at, or between, landmark values, and can be increasing, steady or decreasing). As with Forbus, the quantity space can be extended by discovering new landmark values.

Transitions of variables between states are governed by well-defined rules borrowed from the analysis of real numbers. For example, a variable cannot move from a value of "between l_1 and l_2 and increasing" (`<(`l_1`,`l_2`),inc>`) to a value of "between l_2 and l_3 and increasing" (`<(`l_2`,`l_3`),inc>`) without first passing through "equal to l_2 and increasing" (`<`l_2`,inc>`).

At each step, QSIM uses the basic rules for transitions between function states to generate possible transitions which may be considered for the function. These are then filtered for consistency with the constraint set describing the problem at hand, checked for internal inconsistency and filtered down to a final set of possible successor states. In general, QSIM will produce a branching tree of states, linked by function transitions, as a description of the possible behaviours of a system.

QSIM constrains the relationships between functions in its constraint set models only very loosely (*e.g.* the M+ constraint described above). Therefore, each set of qualitative constraints corresponds to a larger number of equivalent ODE models. Simulation in QSIM produces a branch for every physically real behaviour of each of these ODE models, which means that the tree produced can be highly branched. Unfortunately, physically impossible behaviours are sometimes also predicted. This is due to a combination of localised constraints and qualitative variable values. Localised constraints do not capture global considerations, such as conservation of energy, while arithmetic on qualitative variables is often inherently ambiguous.

As an example, for a frictionless oscillating spring, QSIM produces three branches, for steady, increasing or decreasing oscillation. The three-way branch occurs in the simulation at every cycle, so that the behaviour predicted by QSIM could change arbitrarily, from steady, to increasing, to decreasing oscillation. Steady oscillation is the only physically real solution – the others are produced because the QSIM model does not represent conservation of energy. Kuipers identifies the problem of modelling high level constraints as particularly important for qualitative simulation.

2.2.6 Constraint-Based Qualitative Reasoning - "Confluences"

In the work of De Kleer and Brown (1984), explicitly represented constraint equations (referred to as "confluences") take centre stage, in partnership with a strong component-based approach to modelling complex mechanisms. This is a similar approach to that in QSIM (described above), but De Kleer and Brown's approach to modelling physical components is much stronger.

The objective is dynamic qualitative simulation, using qualitative differential equations (QDEs), which are analogous to the ordinary differential equations (ODEs) of real number physics. As demonstrated for QSIM in Section 2.2.5, direct translation from ODEs to QDEs is possible. However, this is not the only way to derive confluence models - one can develop models specifically for the qualitative domain.

The world view in De Kleer and Brown's ENVISION program is highly mechanistic. Mechanisms are put together from "components" which process "materials" (such as fluids electrons, force, mass, *etc.*) and are connected by "conduits". The task of simulation consists of describing how the attributes of materials in the model change over time. De Kleer and Brown call this activity "envisioning" the behaviour of the mechanism. They also make the observation that attributes often occur in pairs, with one a flow-like variable and the other a pressure-like variable. This shows certain parallels with the fluid modelling approach for AutoHAZID described in Section 3.5.

State dependent behaviour plays a very important role in the ENVISION models. Each component may be in one of a number of different states, depending on the values of its attributes. A different set of confluence equations applies to the component in each of its states, which gives rise to different types of behaviour in simulation. The applicability conditions of the component states are dependent on landmark values of certain variables, so that when a landmark value is crossed, the behaviour may change significantly.

Qualitative variables in ENVISION use a standard set of values, {–,0,+}, rather than any more complicated scheme, such as Forbus' quantity space idea. Using this convention, De Kleer and Brown have developed a large body of arithmetic and calculus theory for confluence equations, based on similar results in the analysis of real numbers.

At the start of simulation, the components in the system are all in known states and the attributes are all known (in terms of their values and directions of change). At each stage of simulation, the constraints applicable to each component are examined, to see what possible changes in attributes are possible. In general, many possible changes are possible, so that the behaviour of the system may branch at each step of the simulation. For each component, the state of the component may or may not change, depending on the constraints in operation. According to De Kleer and Brown, every one of the paths in the envisioned behaviour tree should correspond to a consistent interpretation of some physical system formally identical to the model being simulated.

De Kleer and Brown address at length the problem of how a qualitative system can be made to offer causal analyses of its reasoning. They favour a state transition diagram explanation, rather than any form of symbolic "proof" method using manipulation of constraint equations.

The reason for this preference is that variables in constraint equations must change in such a way that the confluences themselves are always satisfied. Thus, for the value of any variable to change in a confluence, others must also change (simultaneously). This removes the notion of cause and effect from this part of the behaviour, as one cannot establish a temporal or causal ordering between variable changes within a confluence.

The search for a useful way of constructing causal explanations of ENVISION results forms a large part of the De Kleer and Brown (1984) paper. It certainly is an important problem area for "purists" in QP, who want satisfying explanations of which events cause which other events, as well as workable models. The problem of explaining behaviour (changes of attribute values) within a single state is particularly difficult, and the authors invent a system of "mythical causality" to build candidate orderings of attribute changes for this behaviour.

2.3 Applications of Qualitative Physics in Process Safety

The most commonly seen applications of Qualitative Reasoning in Process Engineering are in the area of safety for process plants. Usually, a component-based modelling system, based around models of individual equipment types, is used. The models may use rules of the traditional "IF-THEN" expert system format, or they may rely on a graphical formalism to represent causal links between variables. The application types most commonly seen in the papers reviewed here are diagnosis of faults in operating plants and identification of potential hazards in a plant design. The latter type of application most often uses the framework of a HAZOP study as an organising structure.

In a review for the European Process Safety Centre (EPSC) of work being done in "Knowledge Based HAZOPs", Rushton (1997) identified a number of groups doing work on HAZOP emulation by computer. These were:

- Dow Benelux, Netherlands [Rootsaert and Harrington (1992)].
- Loughborough University, UK [*e.g.* Parmar and Lees (1987a, 1987b), Zerkani and Rushton (1992, 1993), Chung (1993)].
- University of Pennsylvania, USA [*e.g.* Catino *et al.* (1991), Grantham and Ungar (1990)].
- Purdue University, USA [*e.g.* Venkatasubramanian and Vaidhyanathan (1994)].
- Seoul National University, Korea [*e.g.* Chae *et al.* (1994)].

- VTT, Technical Research Centre of Finland [*e.g.* Heino *et al.* (1994), Suokas *et al.* (1990)].

To this list should be added the following groups, active in areas connected with qualitative physics and process safety:

- Taiwan (two groups) [*e.g.* Chang *et al.* (1994), Kuo *et al.* (1997)].
- Argentina [*e.g.* Martinez *et al.* (1992), Vecchietti and Leone (1996)].
- Japan (two groups) [*e.g.* Iri *et al.* (1979), Shimada *et al.* (1993)].

Of the above, Pennsylvania are the only group who have taken a process-based approach to modelling, concentrating on "phenomena" in a plant. This approach may be very powerful in the long run, but suffers from problems of complexity even for very simple systems, because of the frequent need to recompile models.

The other groups have systems which use a component-based "hybrid" approach, typically using some Qualitative Physics and some Expert System ideas. Discrimination between trivial and significant results seems to be an area where problems are often encountered, where a purely qualitative treatment can give ambiguous results.

The following subsections outline some of the work done by the groups mentioned above. Attention has been concentrated on hazard identification and the qualitative modelling techniques of interest in this area. This means that many papers on fault diagnosis, process monitoring, *etc.* have been omitted from this review.

2.3.1 Purdue

The Laboratory for Intelligent Process Systems at Purdue University is led by Venkat Venkatasubramanian. This group has made a good deal of progress in recent years in developing a tool for emulating HAZOP, known as HAZOPExpert. Because of the similarity of this system to the work done at Loughborough on AutoHAZID, this section concentrates almost exclusively on HAZOPExpert, although one other area of application is mentioned at the end.

HAZOPExpert uses Gensym's G2 system as a framework for development. G2 provides an object-oriented shell for development of on-line process-related expert systems, supported by a strong Graphical User Interface (GUI). Using this GUI, users of HAZOPExpert can easily specify process descriptions to the program as P&IDs (an example is shown in Figure 2.6 below, from Srinivasan *et al.*, 1998).

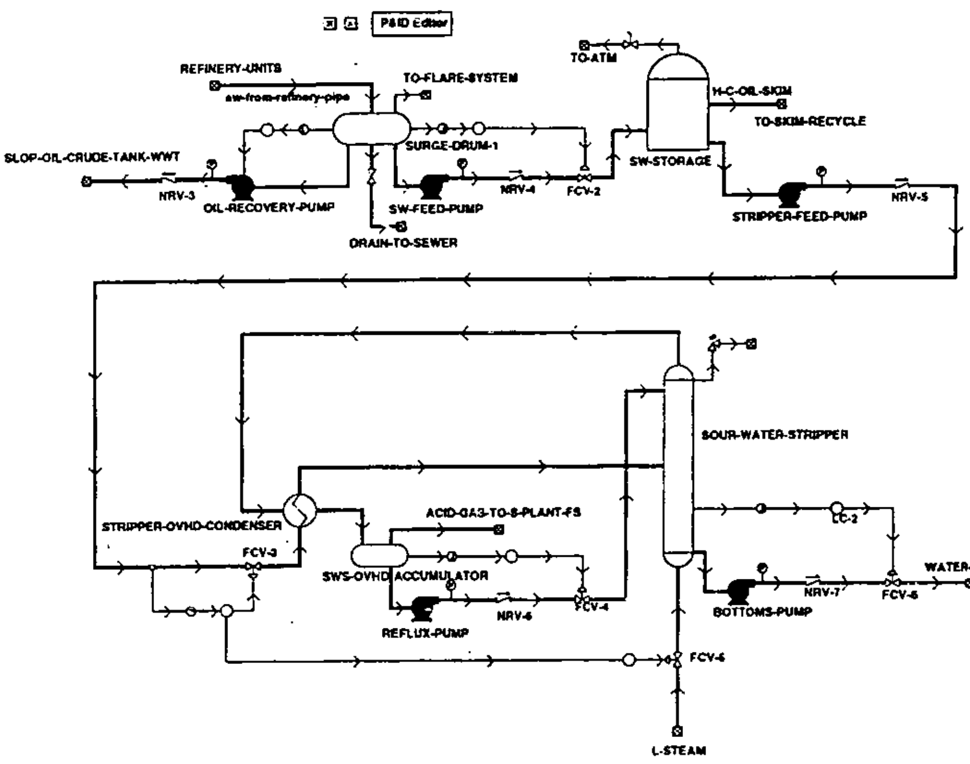


Figure 2.6 : Example P&ID created using HAZOPExpert

Venkatasubramanian and Vaidhyanathan (1994) justify computer emulation of HAZOP by reference to the time-saving potential of a tool capable of automating the routine parts of the HAZOP analysis. Given that all process plant installations in the U.S.A. are now required to formally assess their process hazards at regular intervals, the demand for HAZOP studies is bound to increase.

A principle which underpins HAZOPExpert is the separation of process specific from process generic parts of the knowledge base.[1] This means that models of equipment items and fluids are used which are not dependent on a particular plant and can be used in any plant model. The process specific parts of the knowledge base are the specifications of what equipment items are present, how they are connected together and what fluids are present. Also included are the values of attributes belonging to the equipment in the plant model, to specify information about the operation of those equipment items.

The object-oriented system in G2 allows equipment and fluid models (the generic process information) to be defined as classes of object, which can be related to other classes using inheritance and thereby organised in a hierarchy. Model information also includes methods for diagnosing causes of deviations in process variables, for doing fault propagation through the plant, and for finding possible consequences of a deviation.

The information stored in HAZOPExpert concerning process fluids consists of simple data, such as whether the fluid is flammable, toxic, corrosive, what its physical state is, *etc.* Such information is used in connection with the rest of the plant description to provide better information about the hazards identified by the program. This form of fluid model system adds to the list of hazards found by the system, rather than acting as a filter for ensuring the validity of hazards found (the latter is the approach used in the AutoHAZID program developed at Loughborough).

The first models for HAZOPExpert, described by Venkatasubramanian and Vaidhyanathan (1994), used a propagation equation approach for qualitatively relating variables to one another. This method has also been used at Loughborough by Parmar and Lees (1987a, 1987b) and Hunt *et al.* (1993), for example. Propagation equations can be seen as implementations of the confluences described by De Kleer and Brown (1984). In process systems they typically characterise the relevant balance equations (heat and mass balances) in the equipment. In papers after 1994, by Vaidhyanathan

[1] The importance of this principle was noted in an early paper by Venkatasubramanian and Rich (1988).

and others (1995, 1996a, 1996b and 1996c), the representation used by Purdue changes to the "HAZOP Digraph" (HDG). This is a form of the signed directed graph (SDG) representation to which are added further nodes representing faults and consequences related to process variable deviations.

The HDG allows nodes for process variables to take values from the set {–, +, Normal, Zero}, which correspond to the variable being lower than intended, higher than intended, within the intended range of values, or zero, respectively. This compares with the more usual SDG model, where the value set excludes the "Zero" value, representing only the values "+" and "–" explicitly (all nodes which are not given a value are assumed to be "Normal"). Purdue do not explain how their HDG model handles propagation of "Zero" values in the graph.

The normal mode of use for HAZOPExpert, as described by Vaidhyanathan and Venkatasubramanian (1995), is interactive. A user initiates "HAZOP" of a variable by selecting it on the P&ID and giving it a deviated value (High, Low or Zero), after which the computer performs a search in the HDG and produces results on the P&ID and in a separate window. The program searches in an upstream direction for causes of the deviation and in a downstream direction for adverse consequences. Because causes may not be downstream and consequences may not be upstream in the plant, HAZOPExpert has problems if there are recycles in the plant model, and will fail to identify scenarios where propagation of effects occurs in an upstream direction.

Recycles are examples of feedback in the plant model. Feedback occurs in a physical system wherever a physical variable, such as a flow, has an effect on other variables in the system, such that a part of the original change is propagated back to influence that variable itself. Feedback may arise due to control loops in the plant, which give rise to a link *via* feedback of information, or due to material recycle in the plant, or due to any number of physical phenomena which tend to remain in a stable state if not disturbed.

Feedback mechanisms give rise to cyclical paths in the graph, if the components of the loop are modelled individually. Handling and interpreting cycles as they are found by search is a significant problem in qualitative simulations generally. In HAZOPExpert, control loops are treated as "subsystem" components (described below), but any other paths found in the HDG which contain cycles are ignored. Ignoring causal feedback in this way is rationalised by Vaidhyanathan and Venkatasubramanian (1995) using the rule that "an effect cannot compensate for its own cause", from Oyeleye and Kramer (1988).

The approach used by Oyeleye and Kramer (1988) is to ignore transient effects and other dynamic features of a plant, modelling only the steady state behaviour of the system. This allows them to make the above simplifying assumption about the behaviour of causal feedback, and it probably reduces the complexity of simulations considerably. However, it does not seem to be appropriate for any attempt to model non-steady behaviour of the plant in, for example, hazard scenarios.

The problems presented by control loops when tracing influences through SDG models have been discussed by (among others) Kramer and Palowitch (1987) and Mohindra and Clark (1993). One of these problems is illustrated in Figure 2.7, where a level control loop controls the level in a tank, through which a liquid is passing.

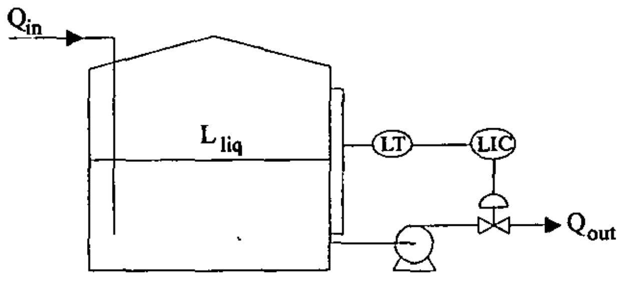


Figure 2.7: A level control problem

The response of the control loop to a change of inlet flow, Q_{in} , is to regulate the outlet flow, in order to maintain the level in the tank at a constant setpoint. Therefore, any deviation in Q_{in} will cause a deviation in Q_{out} due to the action of the controller, but the level, L_{liq} will remain (practically) the same, provided the disturbance in Q_{in} is not too large. The question is how to model this homeostatic effect using the SDG, where influences must propagate *via* deviated variables. Any SDG model which causally links Q_{in} to Q_{out} *via* L_{liq} must deal with the fact that the (steady-state) liquid level does not change and cannot therefore have a deviated value.

Another problem is that of finding the effects of failures within the control loop itself, such as component malfunction or loop saturation. In these cases, the controlled variable belonging to the malfunctioning/saturated loop may not remain normal, while other loops in the plant may remain steady.

In HAZOPExpert, every variable node in the HDG is marked with an attribute stating whether it is controlled or not (see Vaidhyanathan and Venkatasubramanian, 1995). The attribute is set up by HAZOPExpert when it examines the plant for control loops. Additional causes of deviations in controlled variables are added to take account of failure of components in the loop, or control loop saturation.

The action of the control loop (direct/reverse) is encoded in an arc linking the measured variable to the manipulated flow by a single HDG arc and a "valve opening" node, connected to the outlet flow of the relevant control valve. Figure 2.8 shows how this is done for the level control example. In addition, propagation of deviations through the controlled variable is permitted without changing the node from its usual "Normal" value. Vaidhyanathan and Venkatasubramanian do not explain how this is done.

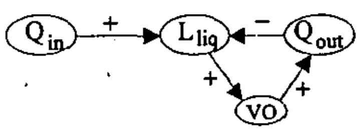


Figure 2.8: SDG feedback loop for level control example

Most recently, Purdue have started to incorporate semi-quantitative information about the process into the rules governing the inference in the system, in order to eliminate unrealistic scenarios and rank the results produced (Vaidhyanathan and Venkatasubramanian, 1996b, 1996c, Srinivasan *et al.* 1997, 1998). The quantities used include design specifications (operating and design temperatures and pressures) and fluid properties (autoignition temperature, boiling point temperature). These properties are integrated into the HDG model of the process and are used to make order of magnitude estimates of whether identified hazards are likely to occur. If loss of containment is identified, for instance, the operating temperature of the unit is compared to the (ambient pressure) boiling point of the fluid (both are stored as single fields in the frame data for the unit). If this temperature is exceeded by a certain (fixed) margin, then the hazard of flashing release is indicated. There is also some order of magnitude reasoning in the treatment of qualitative ambiguity in equipment involving flow splits, based on the relative sizes of the normal flows through the branches of the tee piece.

The work presented by Srinivasan *et al.* (1997 and 1998) uses a quantitative method developed by one of the authors, Dimitriadis, (including "mixed integer linear programme optimisation") to evaluate a small number of chosen scenarios for credibility. The examples given relate to evaluating the time required to overfill a surge drum or the base of a stripping column, based on the mass balance and likely flowrates into or out of these equipment. By considering the time taken for a fault to cause a problem, the importance of the scenario can be evaluated and problems of low importance can be screened out. Additionally, this sort of method may reduce the number of ambiguous predictions made by the system.

It is interesting to note that, in all their work on model-based HAZOP emulation, Purdue view the situation as one where process generic (model based) knowledge <u>interacts</u> with process specific knowledge. The view at Loughborough has usually been that unit models are <u>instantiated</u> by being used in a plant description, so that the plant model used for simulation is an essentially separate entity from the equipment models, which are kept in a library. Another difference is that, while we at Loughborough have organised equipment models into a hierarchy of types, placing similar models close together in the tree, Purdue have not made so much use of this sort of structure with the smaller number of models they have developed.

The whole approach to semi-quantitative reasoning in the Purdue papers is quite simplistic and seems to be based on a small number of ad hoc rules about hazards. It is questionable whether the reasoning methods used are sound enough to reject many of the hazards they do reject. By use of just these simple rules, Purdue claim that they halve the size of the results file for their case study plant.

Other work of interest at Purdue includes that of Srinivasan and Venkatasubramanian (1996). They describe a combination of digraphs and Petri nets, used to model batch processes, and to tackle the mixed continuous and discrete nature of such processes. A batch process consists of a network of tasks comprising the product "recipe", represented as a Petri net. The sequence of tasks need not be entirely linear, as some tasks can be performed in separate equipment concurrently. Each task in the recipe consists of a linear sequence of subtasks.

Within each subtask, the dependencies between variables are represented as a digraph, with additional nodes for quantities such as "amount of mass/heat/time". These nodes are referred to as "integral quantities", because they generally change over time as the subtask progresses. The digraphs for adjacent subtasks may be connected through these nodes, allowing disturbances to be propagated through the different subtasks in the task. The aim of this approach is to capture the different behaviours of equipment items as their uses are changed throughout the batch.

2.3.2 Dow Benelux

The program developed by Dow is known as COMHAZOP (Rootsaert and Harrington, 1992). It is a rule based expert system for HAZOP emulation which produces HAZOP output tables and also makes recommendations for solving the problems it finds.

From the limited information available, it is clear that Dow have recognised the importance of separating the generic knowledge base of information on equipment types, hazards and recommendations, from the description of the plant and its configuration. This separation is analogous to the use, in AutoHAZID, of a library of equipment models and a plant description file.

2.3.3 Loughborough

The Plant Engineering Group at Loughborough University has been working in safety and fault propagation since the early 1970's. Applications of fault propagation investigated during this time include alarm analysis, fault tree synthesis, on-line process diagnosis and hazard identification (typically by emulation of HAZOP).

Andow and Lees (1974 and 1975) describe some early work on the design and organisation of alarm systems. Human factors are often not considered sufficiently in designing alarm annunciator panels or computer displays. In particular, if too many alarms operate simultaneously when a process upset occurs, operators can be unable to identify the true cause of the upset and take appropriate action. Andow and Lees (1975) outline a program used to group process variables together into networks, so that alarms can be assigned to the variables of most use in identifying the root cause of an upset. In this work, cause and effect variables are related to one another using qualitative "functional equations" (or "propagation equations"), similar to the confluence equations described by De Kleer and Brown (1984).

Later, Lees (1984) considers on-line fault diagnosis and analysis of alarms. Two approaches to automatic generation of data structures, suitable for producing fault trees in response to alarm events, are considered. One uses the functional equations and alarm networks of Andow and Lees (1975). The other uses mini-fault trees for each process variable as components for on-line construction of fault trees. Included are many ideas still used in fault propagation modelling, in terms of the pattern of fault initiation followed by propagation of deviations and termination in significant final events. The problems recognised here are also still relevant to current work in fault propagation modelling. Some of these are:

- The problem of ambiguity in qualitative models.
- In fault trees, much useful information about the time ordering of events is lost. Such information can help diagnose the causes of alarm sequences, particularly in batch plant operation.

- Building models is laborious, so a library of reusable models is collected, and methods for systematic conversion of models from one form to another are investigated.
- Models containing just propagation are not much good. Some initiating faults and final consequences must be present, to produce interesting results.
- AND logic is hard to model in mini-fault trees or functional equations.
- Fault propagation must go upstream as well as downstream.
- Instrument failures and control system failures complicate the analysis of disturbances. Instrument reliability is a worry for the operator in interpreting plant disturbances and instrument failure is a possible root cause of deviations on plant.

Fault tree synthesis has been a significant area of work at Loughborough in the past, culminating in the development of the FAULTFINDER program, described by Hunt *et al.* (1993). Kelly and Lees (1986) built on some early work by Martin-Solis *et al.* (1977), producing a fault tree synthesis system based on a component-based equipment modelling system and fault propagation modelling. In a plant model, several units (equipment items) are connected together. Each unit is described by a model taken from a library of commonly used unit types.

Initiation of faults is represented by event statements, propagation of deviations by propagation equations, and undesired consequences are modelled by event models. Each unit model may contain any of these types of entities, as well as decision tables, used for relationships which cannot be covered by the propagation equations, such as AND logic. Fault tree construction proceeds by converting (automatically) all the relevant parts of the unit models into mini-fault trees, which are then combined to construct the fault tree for the chosen top event.

This fault tree synthesis system was further developed by Hunt *et al.* (1993). In FAULTFINDER, decision tables for modelling AND logic were used far more, particularly for problems like reverse flow, *etc.* Hunt also investigated automatic construction of customised vessel models, where a small amount of information about the inputs and outputs of a vessel is used to classify the connections between units into one of a number of types. The connection type determines the flow and pressure relationships appropriate for the associated ports. This work is of interest because a tool was developed for creating new vessel models in the AutoHAZID system.

As an interesting alternative to unit modelling, Shafaghi *et al.* (1984) systematically constructed fault trees based on the control loops in a process, by connecting together sub-trees encapsulating the failure modes of loops. The aim is to produce better structured fault trees which are easier to understand than those produced by a unit modelling approach. However, automatic construction of the plant model may pose significant problems for this method.

Hazard identification is the problem tackled by Parmar and Lees (1987a). They describe an early system which uses fault propagation to emulate HAZOP, by finding causes and consequences for plausible deviations in the plant. The plant model is decomposed quite coarsely into units which correspond to control loops, large items such as storage tanks, *etc.* Propagation equations and event statements are used in models, but are converted to a rule format for fault propagation. Consequence models can be conditional on properties of process materials or materials of construction, and there are models for each type of material in the system to support this. During fault propagation, checks on these properties are used to search for "specific realisations" of hazards in the plant. Parmar and Lees see fault propagation as only one part of the hazard identification solution and suggest that their system could be deployed as part of a larger expert system for hazard identification.

In the case study described by Parmar and Lees (1987b), which is the water separator example also used by Lawley (1974), the authors show how their program can be used to produce HAZOP-like results. The results are compared to those reported by Lawley. They also point out that their program is not able to consider consequences which occur outside the line which the program is examining, meaning that forward fault propagation is limited to components within the line under examination.

Zerkani and Rushton (1992 and 1993) present a hazard identification package for HAZOP emulation developed in Poplog. It uses a unit model library in combination with a plant description file to build a process model which is used in backwards chaining search to find cause-consequence pairs. Backwards, rather than forwards chaining search is used, as this makes it easier to filter consequences for significance.

Each model is a member of an inheritance hierarchy and contains information about process variable deviations, their causes and consequences, and functional equations governing the propagation of deviations. More detailed items of equipment are modelled than in Parmar and Lees (1987a). Zerkani and Rushton recognise that a major problem with acceptability of such systems is that of automating plant data input, through an interface to an existing CAD system.

Chung (1993) developed the "Qualitative Effects Engine" (QUEEN) as a generic toolkit for modelling causal influences in process plants using signed directed graph (SDG) models. QUEEN has been the basis for all further development of hazard identification at Loughborough, including AutoHAZID. Chung presents QUEEN as the core of a number of systems, performing tasks such as fault tree synthesis, alarm analysis, hazard identification, *etc.* It uses a frame-based unit modelling system in which each equipment item is modelled by a mini-SDG. QUEEN constructs the SDG model of the whole plant from the models used and the connections between them.

Jefferson *et al.* (1995) describe a program known as CHEQUER (Computer HAZOP Emulation using Qualitative Effects Reasoning), which was developed from the QUEEN utilities described by Chung. After Jefferson's work on HAZOP emulation, the STOPHAZ project further developed QUEEN and the HAZOP algorithm, converting them to C++ and producing the tool now known as AutoHAZID. This program is described in some detail in the following chapters, and elsewhere by Larkin *et al.* (1997) and Wakeman *et al.* (1997).

2.3.4 Pennsylvania

The modelling approach used at Pennsylvania is of particular interest because it is based around the Qualitative Process Theory (QPT) ideas of Forbus (1984). No other group reviewed here has taken a process-centred approach to plant modelling. The authors claim that this approach avoids some of the difficulties in terms of completeness and correctness encountered in component-based modelling.[2]

As described by, for example, Catino *et al.* (1991), typical input is a structural model of the plant, describing the objects in it. The model system includes the concept of different "zones" in complex equipment, and a classification of equipment items into "homogeneous" (*i.e.* well-mixed), "plug flow" and "stream pair". The structural model is matched to models of processes and views stored in a library, to produce a process-centred description of the plant. The process model can be used to compile a set of constraints between qualitative variables, which are then used to determine the state of the plant and its possible behaviours. The constraints generated can be expressed either as SDG models or as QSIM constraint sets.

One major strength of the approach taken by Pennsylvania is that the process models are produced automatically, so that they can be changed by the program at run-time and therefore used to model the plant in various different states, rather than relying on a single model of the "healthy" plant. This capability may give advantages in diagnostic ability, but comes at the price of increased computational complexity, so that the solution of anything other than trivial problems can be intractable.

The approach usually taken therefore, is to tackle small plant subsystems in detail and to offer detailed explanations of faults, rather than attempting to model large plant sections with many interconnected component units. The authors acknowledge that the component-based modelling techniques investigated elsewhere are more suited to the latter class of problem than their own method.

Grantham and Ungar (1990) consider the problem of fault diagnosis as that of finding sets of assumptions in the plant model which give rise to discrepancies between simulated behaviour and that of the plant itself. A generate and test method is used, where heuristic knowledge is used to select additions or removals of processes from

[2] It seems that this claim rests on the ability of the system to automatically rebuild constraint models and to model state changes in the plant.

the model, to account for the observed differences. After the model is changed, the process model is rebuilt automatically, its behaviour is simulated and compared to the plant behaviour, to evaluate how successful the changes made are in explaining the discrepancies observed. The methods used for comparison are discussed by Grantham and Ungar (1991).

Complexity of qualitative simulations is a particular problem with the Pennsylvania model system. Catino *et al.* (1991) discuss some techniques for focusing the examination of simulation results on more interesting possibilities first. These focusing techniques concentrate on reducing the number of variables in models, limiting attention to only one vessel in the system, or adding further constraints to the system to produce only steady state behaviours, for example.

The "Qualitative Hazard Identifier" (QHI), described by Catino and Ungar (1995), exhaustively tests all possible instances in a plant of a small number of fault types. The applicability of faults in this library is governed by a set of rules, which typically dictate the appropriate equipment where the fault can occur. The consequences of each specific fault are simulated to see if any hazards arise. The procedure is therefore more similar to FMEA than to HAZOP.

The structural plant model used in QHI includes not only the equipment items present and connections between them, but also fluids present and assumptions about the operating conditions of equipment. The process-based model constructed from this structural model is converted into QSIM constraints for simulating plant behaviour, and the results of QSIM simulation are examined to identify resulting hazards.

Faults can either cause a perturbation in some variable, or they can cause some of the assumptions, upon which the current process-based model rests, to be changed. In the former case, simulation of a single model will accurately predict the behaviour of the system. However, if some assumptions have been changed, the process model must be reconstructed, converted to QSIM and simulated, to determine the correct behaviour of the plant.

Because of the frequent rebuilding of process models, computational complexity is a big problem for QHI. However, this approach does have a theoretical advantage over less rigorous systems, in that it simulates fault propagation in a model of the process which accurately describes the faulty condition.

Two simplifying assumptions are used by Catino and Ungar (1995) to reduce problems with interpreting the results of QSIM simulations. The first is the "perfect controller" assumption, where transients associated with controlled variables are ignored, and control is considered to operate instantaneously. The second assumption is the "pseudo-steady state" assumption, which ignores all transients in the plant, so that the results of simulation show only transitions between steady states of the plant.

Despite the complexity and ambiguity problems, the fundamental modelling approach by Catino and Ungar (1995) is sound. To get a workable system, however, it seems likely that some compromises must be made in the modelling and simulation system.

Vinson and Ungar (1992 and 1995) concentrate on on-line process monitoring for fault diagnosis. The "Qualitative Modelling and Interpretation" (QMI) system, takes noisy plant data and interprets it in comparison to qualitative models of expected process performance in different states. By finding the model which matches the observed qualitative state of the plant, faults are diagnosed.

Qualitative models are prepared using off-line QSIM simulation and organised into a tree of system states, each describing the qualitative value of all parameters in the plant. Possible transitions between states correspond to the occurrence of a fault or its development in the plant. Comparing the current state of the plant (extracted from suitably conditioned sensor data) with the states in the tree, the system can tell what fault has occurred in the plant.

The Qmimic system, compared to QMI by Vinson and Ungar (1995), uses semi-quantitative information to rule out some predictions. It uses an updated version of the QSIM simulator to handle the numerical information. An on-line, incremental simulator updates the simulation of the plant one step at a time. This simulation provides candidate model states against which the sensor data are compared. Raw sensor data are preconditioned using a statistical method, Student's t-test.

2.3.5 Seoul

Yoon *et al.* (1992) concentrate on the knowledge structures needed by expert systems for on-line fault diagnosis. Two representations are considered: symptom trees and fault-consequence digraphs (FCDs). Symptom trees are similar to fault trees, representing the conditions which must be satisfied for a deviation in a measured process variable to occur. A symptom tree is produced from a library of mini-trees relating to equipment items in the plant, and used to suggest causes of observed deviations. The fault-consequence digraph (FCD) represents the fault propagation which occurs in the plant. It can be produced either by analysis of results from numerical plant simulation, or from qualitative simulation results (*e.g.* using QSIM).

Nam *et al.* (1996a, 1996b) use the G2 system, in combination with SDG models, for on-line fault diagnosis. Sets of "symptom-fault associations" (SFAs) are produced by off-line search of the plant SDG model. Each SFA associates a variable deviation with the faults which cause that symptom. Diagnosis consists of finding a set of faults which could cause the observed symptoms in the plant. Nam *et al.* (1996a) concentrates on producing SFAs, while Nam *et al.* (1996b) presents two case studies in which these symptom-fault associations are used.

In the first case study described by Nam *et al.* (1996b), complexity is tackled by decomposing the whole plant into a number of semi-independent subsystems. These are typically sections of plant separated by large capacity buffer tanks, or sections which can be shut down without affecting normal operation of the remainder of the process.

The second case study in Nam *et al.* (1996b) uses a model called the "reduced cause effect digraph" (RCED), which is an SDG model in which all nodes corresponding to unmeasured variables are excluded. Additional arcs are added to the digraph to make up for the causal links which are broken by removing these nodes. The RCED is used in conjunction with the "Pattern Graph Through Time" (PGTT) method to do fault diagnosis on an unsteady process. The PGTT is a time series of RCED graphs and diagnosis consists of finding the root nodes of the PGTT which account for the observed phenomena.

Chae *et al.* (1994) describe an interactive knowledge based expert system for hazard identification, which investigates causes and consequences of variable deviations chosen by the user. The user decides the decomposition of the plant into "study nodes" for HAZOP, producing a small number of "vessels" and "transport lines". Generic knowledge about process units and fluids is organised in a hierarchical way, using inheritance, but there does not appear to be any way to connect process units together in the plant. Without this connectivity information, the scope for identifying hazards, by connecting causes and consequences with fault propagation chains through the plant, must be very limited.

The fluid information used includes National Fire Protection Association (NFPA) indices for various classes of hazard, used to evaluate the severity of consequences in the plant. The number of equipment types used in this prototype is small (seven), but the range of causes and consequences modelled appears very similar to the most commonly modelled events in systems developed by other groups (blockages, leaks, fires, toxic releases, *etc.*).

Chae *et al.* (1994) include a system of rules for reasoning about the consequences of certain scenarios, so that initial events can cause intermediate consequences which may go on to produce final consequences. This is a more complex approach than is generally used.

Suh *et al.* (1997a, 1997b, 1997c) also work on an interactive rule based expert system approach to hazard identification. They argue that many workers do not use a particularly strong representation for modelling accident scenarios. Suh *et al.* therefore introduce a system which uses three databases to represent the plant data model: the unit, organisational and materials databases. Three algorithms are used to manipulate this data, covering analysis of deviations, malfunctions and accidents as a whole.

The STARS project is mentioned in a paper by Heino *et al.* (1992) which also presents a short review of expert systems applications in the field of process safety analysis. STARS is a software system operating on multiple levels of process design, to provide a supportive integrated environment for process engineers to do hazard identification and analysis on a plant design, using a number of knowledge bases. It is not a HAZOP emulator, but provides stimulus for hazard identification through guide word prompts, checklists, knowledge of equipment failure modes and access to previously examined analyses.

The KRM project, described by Heino *et al.* (1994), used an object-oriented model of a chemical process to support the provision of safety information to various user groups associated with the plant. The two main areas discussed were safety analysis during the design of a plant, and making knowledge from safety analysis available to operating personnel for troubleshooting and diagnosis during operation. The issue of knowledge-based HAZOP was not addressed in this project, and KRM can be seen more as an integrated framework for organising and communicating the knowledge required for safe operation of a plant in a useful way.

HAZOPTOOL, described by Heino *et al.* (1995), is an integration of some of the previous ideas from VTT, including KRM, STARS and HAZOPEX. It was developed in conjunction with a Taiwanese engineering company, CTCI. The same sort of object-oriented plant modelling is used as in HAZOPEX, but this system also uses multiple knowledge bases corresponding to chemical properties and reactions, as well as those for causes and consequences. The tool is used interactively, displaying the causes of chosen deviations in a tree format and displaying related consequences as lists. Other aspects of safety analysis can also be addressed within HAZOPTOOL, such as conventional HAZOP documentation and checklist management, in addition to the knowledge-based HAZOP system.

2.3.7 Taiwan

There are two groups working on qualitative reasoning for process industry applications in Taiwan.

The group at the National Taiwan Institute of Technology seem to be concentrating on improving resolution in fault diagnosis. Yu and Lee (1991) concentrate on using the fuzzy set membership function in conjunction with qualitative SDG models. Chang *et al.* (1994) present an approach based on equation-based models of the process system, called the "deep model algorithm".

The group at the National Cheng Kung University present a method for fault tree synthesis based on the structure of complex ratio control schemes, in a paper by Chang and Hwang (1994). This does not appear to have been implemented in a computer program, but does use an SDG modelling approach. Digraphs are also used in the system known as IHAS ("Integrated Hazard Analysis System"), described by Kuo *et al.* (1997), which attempts to emulate HAZOP by applying programs for fault tree and event tree analysis to cause and consequence investigation, respectively. IHAS makes use of plant topology and a database of digraph models to construct the internal plant model, and it presents its results in the form of a HAZOP table, including recommended actions generated by a simple rule system.

2.3.8 Argentina

Martinez *et al.* (1992) describe the development of a real-time, on-line expert system (containing about 70 inputs and 90 rules) for monitoring an extraction unit comprised of two columns in a butadiene plant. Of interest here is the way that, during the knowledge elicitation phase, HAZOP and FMEA techniques were used to provoke more detailed thinking from experts in order to "flesh out" the reasoning behind relatively shallow heuristic rules.

In papers by Leone (1996) and Vecchietti and Leone (1996), a system known as SERO is described, which is a HAZOP emulator using a high level, object-oriented representation language to model fault propagation. SDGs represent influences between variables and HAZOP emulation seems to rely on local fault propagation at the interfaces between objects, using message passing. This "distributed" method can be contrasted with the more common approach of compiling a plant SDG from a plant model and then searching it using a global HAZOP algorithm.

2.3.9 Japan

There are a number of research groups working in Japan on problems related to knowledge based safety analysis, fault diagnosis and control. Just two are mentioned here: the group associated with Iri, O'Shima and Matsuyama, and the group associated with Shimada, Suzuki and Sayama.

In a frequently cited paper, Iri *et al.* (1979) describe the SDG-based modelling of chemical processes for fault diagnosis. The state of the plant is seen as a pattern of variable disturbances across the SDG model, and non-deviated variables are of no interest. The problem of finding a cause for the observed deviations in the plant is simplified by the assumption that there is only one root cause for the deviations, and characterised as the search for a "maximal strongly connected" node in the graph.

Iri *et al.* recognise the problem presented by controlled variables which may themselves remain normal while propagating a deviated value to other variables around them. The "trick" of using two extra qualitative values to represent controlled variables which remain normal, but would be deviated in a certain direction if they were not controlled, is introduced in this paper. Some improvements to the basic algorithm presented by Iri *et al.*, in terms of enhanced diagnostic and computational efficiency, are discussed by Shiozaki *et al.* (1985).

In work from another group, Shimada *et al.* (1993) describe a computer system which uses information from fault tree analysis to build IF-THEN rules for use in a rule-based expert system for fault diagnosis. Later work by Shimada *et al.* (1996) moves on to the operability study as an application, and the authors present a knowledge-based system in Prolog for performing a type of HAZOP study. This system contains both process-specific and generic knowledge bases, and uses decision tables for expressing causal relationships in the plant. The user interface is interactive, with the user providing details of the deviation to be examined and the system reporting causes and consequences for that deviation in a tabular format.

2.4 Summary

This chapter has given a review of some of the work being done in the area of process safety and the automation of hazard identification. Firstly, an overview of conventional methods used for process hazard identification was given, in Section 2.1. Section 2.2 introduced the field of qualitative physics research, which seeks out methods for modelling the world qualitatively, instead of using numbers and equations. Ideas from qualitative physics have been used by the research groups whose work is described in Section 2.3. This work covers attempts to automate hazard identification as well as fault diagnosis, using qualitative model-based reasoning to simulate plant behaviour.

Most of the research groups mentioned in Section 2.3 have looked at more than one possible application (from process monitoring, HAZOP, fault diagnosis, simulation, *etc.*), and many have tried a number of different modelling techniques. The most common areas of application have been HAZOP emulation and fault diagnosis, mostly using a graph-based model system.

One notable exception to this choice of modelling system is Pennsylvania, who have concentrated on a process-based system for modelling the phenomena in a plant, combined with QSIM simulation to predict the changes in process variables. The process-based system has certain theoretical advantages, not least that it allows the state-dependent behaviour of the plant to be taken into account. However, Pennsylvania have encountered intractable problems of computational complexity, because of qualitative ambiguity. These problems have limited their programs to tackling "toy" case study plants.

The HAZOPExpert program developed by Purdue aims to emulate HAZOP and uses a SDG-based model system. In terms of development, it is the system closest to Loughborough's AutoHAZID system (described later). It benefits from the graphical user interface of the G2 expert system shell, which allows the same environment to be used for developing SDG models and plant description P&IDs. However, the range of equipment modelled does not appear to be as wide as that attempted in AutoHAZID, and the HAZOP results presented in papers from Purdue suggest that they have not attempted to model a very wide range of failure modes.

In common with Loughborough, Purdue have recognised that quantitative information is needed to improve the focus of HAZOP results and reduce the number of spuriously reported hazards. Their approach to the problem uses a linear programming method based on a quantitative dynamic model of the relevant process units, and relies on optimisation to determine whether scenarios predicted by SDG search are realistic (Srinivasan *et al.*, 1998). The fluid modelling system in AutoHAZID, as described in Chapter 5, adds quantitative conditions to the SDG arcs in order to validate fault paths found by graph search. It seems that the latter approach involves much less numerical computation than the method used in HAZOPExpert, and so may be more efficient.

It is clear that no group has yet succeeded in developing a fully rigorous qualitative treatment of process hazards. Problem areas include modelling the behaviour of plant items in different states, dealing with the sometimes complex logic underlying scenario development, and reasoning with sequences of events in time. There is no reason why these problems should not eventually be solved, once the somewhat simpler problem of modelling continuous plant has been solved.

There remain quite a few methods mentioned in Section 2.1 which can be considered for automation. One example is sneak analysis, which could be integrated into AutoHAZID as a preliminary task – the plant model would be examined, before HAZOP, looking for and reporting sources and destinations of sneak flows. Another possibility is to add further models or rules to an existing hazard identifier system, such as AutoHAZID, to cover computer HAZOP and/or human error analysis. Management of the plant-specific safety data and generic expertise used in safety assessment, is another important area. The work reported in Heino *et al.* (1994), which integrates diverse information resources for common access throughout an organisation, is of particular interest here.

Chapter 3 : Description of AutoHAZID and its Qualitative Modelling System

The HAZID software package was developed for automated hazard identification as part of the STOPHAZ project. Its central module is AutoHAZID, a program developed mostly at Loughborough University, which coordinates the HAZOP emulation that HAZID does.

This chapter first outlines the intended purpose and scope of the HAZID tool. Then the modules of HAZID and the internal modules within AutoHAZID are described. The main part of the chapter describes the qualitative modelling system used by AutoHAZID in modelling plant behaviour. A methodology for model development is described by reference to an example problem – that of modelling flow and pressure propagation. Finally, some conclusions are drawn from the material covered.

3.1 Scope of the HAZID Package

It is intended that AutoHAZID emulate the hazard identification activities of HAZOP, to save some of the time spent by conventional HAZOP teams. Qualitative simulation, using SDG models, is used to find causes and consequences of variable deviations, corresponding to characteristic failure modes of equipment and possible resulting hazards on the plant. An option is also available, to identify items of equipment in the plant (such as trips, alarms, *etc.*) which will protect against the identified hazards.

The range of things detected in conventional HAZOP studies depends on how much previous scrutiny the plant design has been subjected to. Many problems are most cost-effectively detected by simple use of checklists by a single engineer, but are often found at the HAZOP stage. The best use of group time is made by considering previously unexamined combinations of equipment failures and susceptibilities, using the HAZOP guide word method to detect possible hazardous scenarios.

AutoHAZID does not attempt to deal with checklists of concerns relevant to single items of equipment. It also does not seek to check the correctness of equipment designs, except by detecting a small number of errors related to the configuration of equipment. Instead, the approach used in AutoHAZID is to search for links between faults and consequences in a qualitative model of the plant, by constructing fault propagation chains.[1]

Some of the other scope limitations, applying to the type of HAZOP emulation attempted by AutoHAZID program, are listed below:

- The usual emphasis is on predicting the behaviour of a continuous plant during normal operation, where only single faults occur.
- As originally defined, HAZOP examines all deviations from intended operation, which covers a quite wide variety of guide words and considerations. AutoHAZID only addresses the hazards which can be modelled in terms of the effect they have in causing deviations in process variables. To widen the scope, AutoHAZID would have to model the design intent of equipment, as well as the influences between variables.
- Time is not represented in the AutoHAZID models, except in so far as the causes represented in SDG arcs must precede their consequences. It is therefore difficult to reason about sequences of events (temporal ordering), duration and relative speeds of changes, *etc.* An example of the type of problem here is where a leak of fluid out of the process can result in a (later) leak of material into the plant.
- Transitions between states of equipment items, or of the plant as a whole, are not modelled. Because AutoHAZID uses only one SDG model for each equipment item, any serious attempt to model batch or semi-batch processes in detail, is limited. AutoHAZID allows models to be instantiated in particular states, by "sub-typing" them, but does not allow the state to change during analysis. Specifically,

[1] The creation of an environment for integrating and systematically applying software components for hazard identification and risk assessment would be a worthwhile project, but was not an objective of STOPHAZ. The AutoHAZID plant models contain the information needed, but the necessary number of rules and checks is too large to make a system like AutoHAZID practical for this sort of application.

AutoHAZID does not model changes in the behaviour of equipment items when those items have failed.

- Complex fault trees or event trees, involving logic and (potentially) probabilities cannot be directly modelled in the SDG-based system. This is usually not a problem for hazard identification, where enabling conditions for faults can be assumed to be satisfied. Complex logic is more closely associated with risk assessment than with hazard identification.

Some of the above limitations are further discussed in Chapter 6, where possible future improvements to AutoHAZID are considered.

3.2 Description of the HAZID Software Package

HAZID was intended for delivery in a Windows 95 or Windows NT environment. A UNIX version of the AutoHAZID program exists, but this is not able to take advantage of the links to the other modules present in the Windows version.

The various HAZID modules are linked together as illustrated in Figure 3.1. The modules were developed by a number of partners in STOPHAZ. This section explains briefly the connections between the HAZID modules shown, as well as the internal modules within AutoHAZID.

As shown in Figure 3.1, AutoHAZID has a parser, which allows it to read in data from library files and plant description files. It also links to two other modules in the STOPHAZ software package, the Database "Applications Programming Interface" (API) and the Physical Property Calculation packages. These links are described in Sections 3.2.1 and 3.2.2 below, and an overview of the information flows in HAZID is shown in Figure 3.2.

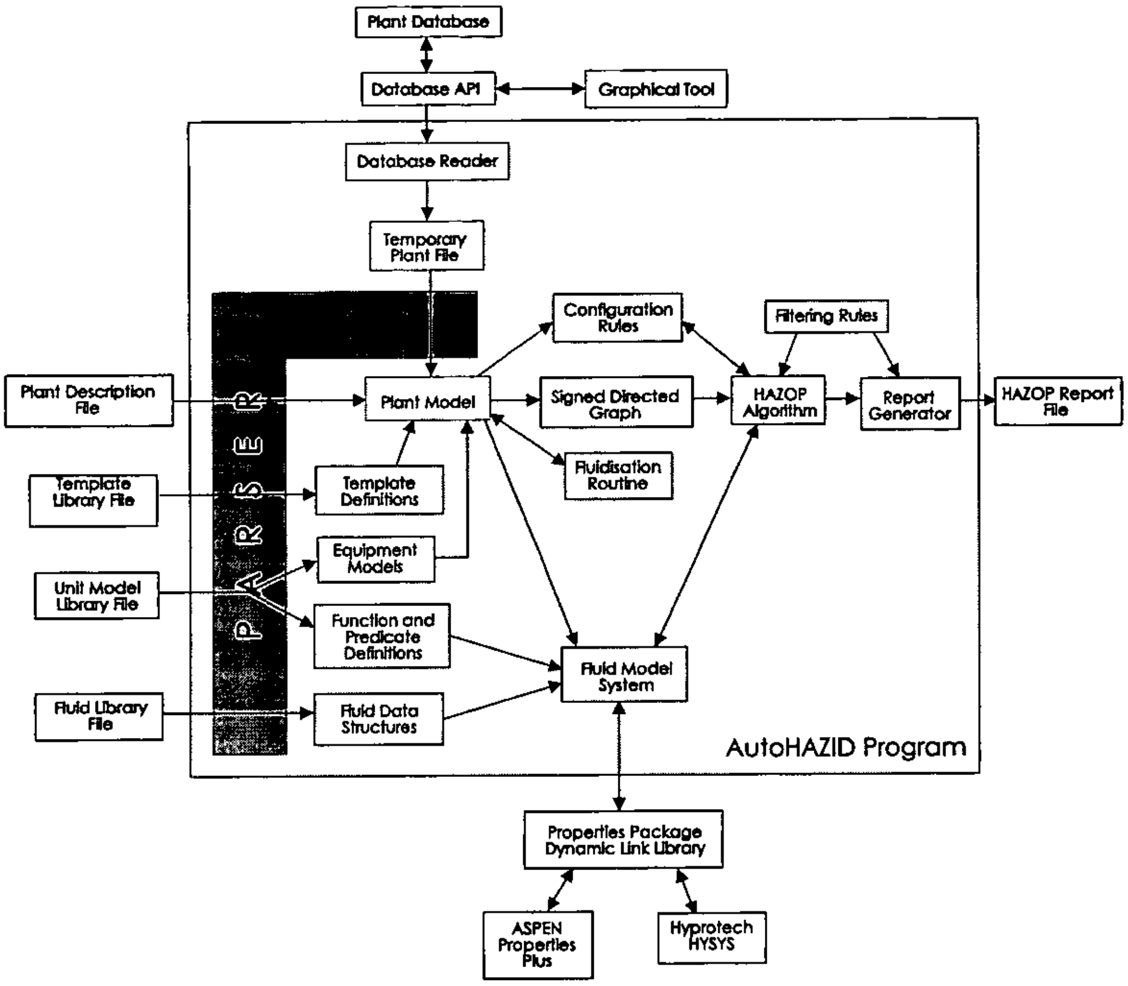


Figure 3.1 : Schematic Diagram of HAZID Architecture

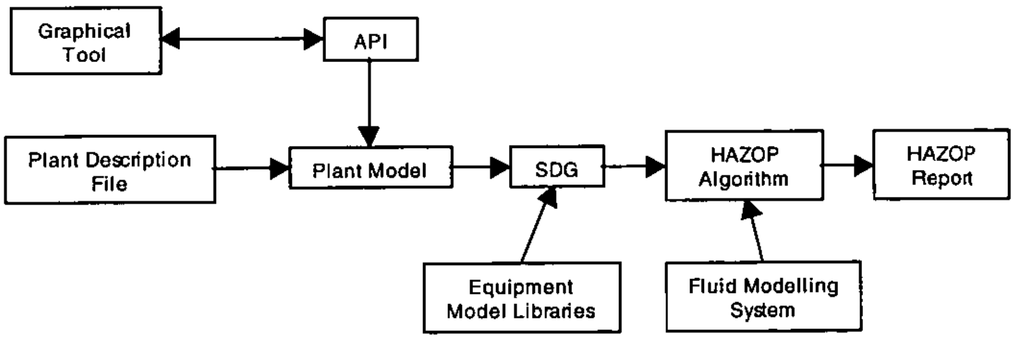


Figure 3.2 : Information Flow in HAZID

The intended mode of use for HAZID is as follows: after starting the program, the user chooses a plant description to examine. This plant description is loaded into AutoHAZID, either from a text file, or from the Database API. Then, the user selects filtering options for HAZOP and initiates the HAZOP emulation stage, which executes without further user intervention. Output is produced in an ASCII text file, in tabular form, with columns for deviation, cause, consequence and (if selected) protections, for each hazardous scenario identified. The start-up procedure and various menu options available in AutoHAZID are described in Appendix A, which also includes (in Section A.8) a sample of the type of output report produced by HAZOP emulation.

The units in AutoHAZID which are treated as potential protections against hazardous scenarios are: alarms, indicators, relief valves (including emergency vent manholes), check (non-return) valves and control valves. When the option to detect protections is enabled during HAZOP, the program looks for any such equipment which respond to the deviations in the fault paths identified by the program. It reports these protective equipment items in the "protections" column of the HAZOP report table.

3.2.1 Plant Descriptions from Database API and Graphical Tool

Plant descriptions can be prepared in the form of graphical ELDs, using the HAZID Graphical Tool (developed by TXT). This is an alternative to laboriously keying in a text file containing the description of the plant.

The plant descriptions produced by the Graphical Tool are stored in a database. Access to the database from the Graphical Tool is mediated by the library of functions known as the Database API. The API was implemented by Intrasoft in the STOPHAZ project. AutoHAZID has access to this API and can retrieve the plant descriptions from the database using the same set of functions.

AutoHAZID first reads all information on a plant of interest, through the API. It then writes a text file containing this information, in the same format as a keyed in plant description. This file is read into AutoHAZID using the parser, to create an internal plant representation. Using this approach allowed AutoHAZID to be developed independently, in a text-based UNIX environment, before the other components of

HAZID were available. It also allowed the links to the API to be tested by examining the text files generated.

3.2.2 Physical Properties Calculations

The Fluid Modelling System (FMS) makes use of physical properties of the fluids in the plant, as described in Chapter 5. These properties can be accessed by look-up in the fluid model library, or estimated by calls to external software packages. The two packages considered in the STOPHAZ project were Properties Plus, developed by Aspentech, and HYSYS, developed by Hyprotech. Both are based on the technology of flowsheet simulators and the property estimation methods used in them.

A library of functions and data structures was defined to implement the property requests interface as a Windows "dynamic link library" (DLL). The library is common to the FMS and the external properties packages, and it allows AutoHAZID to make use of whichever software package is available. The link to a chosen properties package is made when AutoHAZID starts up.

3.2.3 Internal Organisation of AutoHAZID

The constituent parts of AutoHAZID, shown in the shaded areas of Figure 3.1, are:

- **Parser** – AutoHAZID reads most of its input data through a parser. The parser module reads characters from a text file and interprets them to generate the internal models used in the program.
- **Database Reader** and **Temporary Plant File** – The method for reading in plant descriptions from the Database API was described in Section 3.2.1. The database reader is the part of AutoHAZID which does this.
- **Plant Model** – This is the internal model of the plant, composed of a list of instances of equipment models. It is constructed from data read in from external plant descriptions, from the **Equipment Models** and from **Template Definitions** used in the plant. The plant model is the starting point for constructing the **Signed Directed Graph** of the plant, used in HAZOP emulation. The **Configuration**

Rules (for detecting plant design errors) and the **Fluidisation Routine** (for propagating fluid information through the plant) both also make use of the information in the internal plant model.

- **(Internal) Equipment Models** – These are the frame models, defining the types of equipment used in plant descriptions. The models are read in from a library file when the program starts.
- **Template Definitions** – Templates are commonly used groups of SDG arcs which can be used within an equipment model, as described in Section 3.4. When the program starts, all template definitions are read in through the parser.
- **Functions and Predicates, Fluid Data Structures** and the **Fluid Modelling System** – The FMS influences the results of the HAZOP algorithm by applying conditions to check the validity of fault paths produced by graph search. The conditions are defined by functions and predicates, and make use of fluid information from the plant description, the fluid library and properties packages.
- **HAZOP Algorithm** – This module coordinates the graph search which forms the core of HAZOP emulation in AutoHAZID. An exhaustive two-stage breadth-first search algorithm is used, as described in Appendix B. This search produces a record of deviations, faults which cause them and possible consequences of these deviations and faults. The checks in the FMS can be used to improve the focus of results, but AutoHAZID is not dependent on this link. The HAZOP algorithm also initiates a number of extra checks on the configuration of plant items, using the **Configuration Rules**. The results of these checks are integrated with the HAZOP results, and provide a way of detecting elementary design flaws in the plant description, as passed to AutoHAZID. The configuration rules are complementary to the fault propagation approach, permitting the identification of faults which are not easily identified by fault propagation.
- **Report Generator** – This part of the program takes the results of exhaustive search, as produced by the HAZOP algorithm, and formats them in an appropriate order, eliminating duplicated results as necessary. It produces a formatted text file containing the results of the HAZOP study.

- **Filtering Rules** – These influence the HAZOP algorithm and the report generator by controlling the amount of repetition in reports, by dictating the scope of the HAZOP and by defining the order in which deviations are considered.

3.2.4 HAZOP Output Formats

The main output from HAZOP emulation in AutoHAZID is a text file containing two or three sections. The first section is a header, giving details of files used, filtering options selected and settings in use when the results were produced. The next section is the main HAZOP results table, containing identified hazards in a tabular form. The table has columns for deviations, causes, consequences and (if a search for protections has been enabled) protections. The third part of the report is produced by the fluid compatibility checker (see Section 5.2.8), and gives details of adverse fluid interactions detected during HAZOP. This last section can only be produced in the Windows version of AutoHAZID, when given a sufficient plant description.

One alternative, more structured, form of output has been implemented already – an option to produce results in the format required by PrimaTech's "PHAWorks" software package. Information on this package is available on the world-wide web, at `http://www.primatech.com/`. Other types of structured output (as opposed to simple text file formats) could be implemented with little difficulty, when a format has been agreed.

3.3 Models in AutoHAZID

The most basic, qualitative SDG models in AutoHAZID use no information about numerical quantities in a plant, and no numerical calculations. Influences between process variables are modelled by SDG arcs and hazardous scenarios are identified by finding fault propagation chains, by which consequences may result from initial failures.

The real chemical plant can be seen as a collection of equipment items, connected by streams carrying fluids between them. Most of the individual items in the plant are taken from a small set of commonly used equipment types, such as valves, pumps, vessels or pipes. This makes the task of process design much easier and cheaper because standard components are mass-produced and are better understood than customised, one-off items.

Because of this process design method, a component-based modelling approach is used in AutoHAZID for plant representation. Each piece of equipment in the plant is modelled as an instance of an equipment model, taken from a library of process equipment types. The SDG model of the plant is constructed from the SDG models of the units in it and links are added to model the propagation of deviations, *via* streams, to other units. The simplest plant description therefore consists of a list of equipment instances and their interconnections.

Using models for types of equipment in this way is economical in terms of the amount of information required by the program for assessing each plant. Once an equipment model is present in the library, it can be used in a large number of plants, or indeed many times within the same plant. It should be noted, however, that this modelling approach makes the implicit assumption that most interesting causal influences (from the point of view of identifying hazards) propagate *via* variable deviations in streams between units. This assumption is challenged in the case of non-process propagation of faults, which is discussed in Section 6.6.

The decomposition of the plant model is carried one step further for template models, which group together commonly used groups of arcs to model parts of equipment models. Templates are described in Section 3.4.

The failure modes of equipment are modelled in AutoHAZID by including faults and consequences in the SDG models, associating them with deviations of process variables. The elicitation from human experts of the knowledge upon which these failure modes are based, is a very important part of the model development process.

Every variable in the plant model is associated with a port located in some unit in the plant. As an example, the discharge pressure for a pump, `p101`, would be referred to as `[p101,out,pressure]`, where `out` indicates the discharge port. In the library model of the pump, from which `p101` is derived, the same variable would be referred to as `[out,pressure]`, because the unit name is unknown within the model.

Ports are required for locating variables and for connecting equipment items together in the plant, so that deviations in process variables can be propagated to other units. The process ports are of three types: input ports are locations where fluid may flow into the equipment, output ports are locations where fluid may flow out, and internal ports are internal locations not directly connected to other units at all. Only input ports and output ports are used for connecting process equipment items.

When a plant description is loaded, in the form of a number of "instances" of equipment models, the connections specified are translated into SDG arcs connecting the units. The SDG arcs belonging to the units themselves are "instantiated" by adding information about the units to which they belong (unit names and specified attributes). The resulting complete set of arcs is the SDG model of the whole plant, and this is used to simulate the plant's behaviour during HAZOP emulation.

Arcs corresponding to propagation of effects between units allow some deviations to propagate downstream (in the direction of intended flow), some to propagate upstream (against the direction of flow), and some to propagate in both directions. Deviations in some variables, such as level, are not defined in relation to inlet or outlet ports and are not propagated at all between units.

The remaining subsections of Section 3.3 discuss various aspects of the AutoHAZID system as follows:

- The minimum data requirements for generating the plant model are outlined in Section 3.3.1.
- Section 3.3.2 describes the SDG in AutoHAZID in some detail.
- The frame-based system of equipment models, which allows inheritance and a hierarchical arrangement of equipment models, is described in Section 3.3.3. The instantiation of those equipment models, in plant descriptions, is also discussed.

- The hierarchy of models in the equipment model library is introduced in Section 3.3.4.
- The slots which make up the majority of the information given in the models in AutoHAZID, and the mechanism of inheritance operating between models in the model hierarchy, are described together in Section 3.3.5.
- Section 3.3.6 describes the system which allows the basic, generic equipment models to be specialised, based on the values of attributes specified for the equipment item. This is the "attribute conditional model" system.
- Customised models of vessels can be generated in HAZID using the Model Generation Tool (MGT), which is briefly described in Section 3.3.7.
- AutoHAZID allows consequences to be classified in terms of severity, whether the event is a hazard or operability problem, and in terms of a number of standard consequence types. This part of the modelling system is mentioned in Section 3.3.8.

3.3.1 Data Requirements for the Plant Model

The minimum plant specification is just a statement of the equipment items present, their types and the connections between them. This corresponds roughly to the minimum information provided on an ELD and to the basic information required in a HAZOP study. It is surprising how much useful work can be done by AutoHAZID (and by HAZOP teams!) using just this basic information.

Additional information which may be presented in a real-life plant description includes:

- General description of the process and its chemistry.
- Fluid components present, and percentage compositions, throughout the plant.
- Fluid flowrates, temperatures and pressures.
- Physical properties of process materials.
- Materials of construction.
- Operating modes of equipment items.

- Design temperatures and pressures (permitted maximum and minimum values).
- Operating instructions for the plant.

This additional information is not vital to making some progress in hazard identification. However, if the additional information is present, less time will be wasted on unnecessary consideration of scenarios, so that the results of the analysis will be more specific and relevant. Some, but not all, of these classes of information are used by AutoHAZID in HAZOP emulation and are therefore (optionally) present in the plant model.

3.3.2 Signed Directed Graph (SDG)

Nodes in the AutoHAZID SDG represent variables in the plant model which can, in principle, have qualitative values of "+" and "–". The values correspond to deviations in the variable equivalent to applying the HAZOP guide words "more" and "less", respectively. Arcs in the SDG represent direct or reverse influences of one variable on another, according to whether the sign on the arc is "+" or "–", respectively. The arcs are usually found listed in `propLinks` slots within equipment model frames in the unit model library.

Fault propagation is modelled quite naturally using this representation of influences between variable deviations. The local influence of deviations in one variable on its neighbours in the graph models the propagation of disturbances. Paths through the SDG represent potential fault propagation chains. The influence of one variable on a distant one ("direct" or "reverse", represented as a "+" or "–" sign) is the product of the signs of all arcs along the path connecting the two variables, if such a path exists.

In addition to the nodes (corresponding to variables at particular places, or ports, in the plant), three other types of entity are used to construct SDG arcs in AutoHAZID:

- **faults** represent initiating events which give rise to variable deviations in the unit with which they are associated. Faults are declared as textual descriptors, which are the strings reported in the "causes" column of the HAZOP output table.
- **consequences** are the hazardous final events which are to be linked, *via* some fault propagation chain, to deviations of process variables and ultimately to faults at the start of fault propagation chains. Consequences, like faults, are associated with a particular equipment item in the plant and have a textual descriptor, which appears in the HAZOP report when the hazard is reported.
- **deviations** are nodes with an associated HAZOP guide word ("less" or "more") attached to them. They are only used to specify which deviation of a node gives rise to a consequence in the plant.

In addition to the simple text of a descriptor and the name of an associated unit, faults and consequences can (optionally) be linked to conditions for evaluation within the fluid modelling system. The FMS is described in Chapter 5. Therefore, in the discussion below the optional "**`Condition`**" part of the arc definitions is ignored.

Arcs in the SDG can take any of the following forms, as presented in the unit model library of AutoHAZID, depending on their purpose:

- **`arc(Node,Sign,Node,Condition)`** These arcs represent propagation of process variable deviations through the plant model.
- **`arc(Fault,Sign,Node,Condition)`** These arcs represent the deviations caused by initial failures. The given node is deviated in the direction indicated by the sign of the arc.
- **`arc(Deviation,1,Consequence,Condition)`** Arcs representing the termination of the fault propagation chain have this form. The deviation given may cause the consequence given.

- **arc(Fault,1,Consequence,Condition)** Used for failures directly linked to local consequences.

The formats of each of the elements above (Fault, Node, *etc.*), and their subordinate elements, are outlined in Table 3.1 below:

Item	Description
Node	One of two formats: [Port,Property] – The usual form, as seen in the unit model library, where the unit name is not known. [Unit,Port,Property] – Sometimes seen in an instance statement, in a plant description file, or when displaying models of equipment items.
Sign	Usually either 1 (indicating a "+" sign on the arc and a direct influence) or –1 (indicating a "–" sign for the arc and a reverse influence). Other special values exist, and their meanings are discussed in Section 4.2.2.
Condition	A condition which can be tested by the fluid model system, to verify a fault, consequence or arc. If the condition is proven to be false, fault paths containing it are ignored. This is a means of filtering and focusing HAZOP output from the program and is discussed, with the FMS, in Chapter 5.
Fault	One of two formats, depending on whether the fault initiation is conditional on some feature of the plant, or not: [fault,[Descriptor,Condition]] [fault,Descriptor]
Deviation	In the format: [deviation,[DevnCode,Port]]
Consequenc e	One of four formats: [consequence,[Descriptor,Condition]] [consequence,[Descriptor,Condition],Extras] [consequence,Descriptor] [consequence,Descriptor,Extras]
Unit	The name of the equipment item to which the Node refers.
Port	The name of the port where a node or deviation is located.
Property	The name of a process variable (such as flow, pressure, composition, *etc.*)
Descriptor	A string in single quotes to describe either a fault or a consequence. May be accompanied by an integer value between 1 and 5, in brackets, representing the importance rank of that fault or consequence. This rank figure is only used at present to represent the frequency of a fault (1 is infrequent, 5 is frequent) – the importance rank information on consequences is now given in the Extras component described below.
DevnCode	One of the "code words" for variable deviations defined in the program. These include "lessFlow", "moreTemp", "contamination", *etc.*
Extras	A set of information provided for classification of consequences, as an aid to filtering results, *etc.* Comes in the format: [Cat,Rank,StdCons]
Cat	Category of consequence, indicating whether it is a hazard (haz), operability problem (op) or both (haz_op).
Rank	Consequence seriousness rank (from 1 to 5, with 5 the most serious).
StdCons	List of symbols giving standard consequence classes to which the particular consequence belongs, *e.g.* [lc,ed,pi]. The standard consequence classes are explained and listed in Section 3.3.8.

Table 3.1 : Elements of AutoHAZID SDG models

3.3.3 Equipment Models – Frames and Instances

Generic equipment models in AutoHAZID are known as "frames", and their realisations in plant models are referred to as "instances". Both are stored internally in `Frame` objects. The frame models are loaded into AutoHAZID from a single library file when the program starts. Instances are created by reading a plant description into the program, through the parser. Each frame or instance possesses the following data:

- A name.
- A "parent name", which is the name of a frame from which it is derived. Frames are arranged in an inheritance hierarchy, described in Section 3.3.4, which allows closely related models to be placed together.
- A list of slots, which specify all the information comprising the equipment model. These slots are more fully described in Section 3.3.5 below.

So, all frames and instances must be defined in terms of another frame. The one exception to this is the root of the hierarchy ("unit" in Figure 3.3 below), which has no parent frame. Inheritance operates from parent frame to child frame within the hierarchy, and from a frame to instances of that frame in a plant description. This means that the slots (and slot values) of the parent are inherited by the child. The inherited values may then be overwritten or supplemented by information given in slots in the child. Details of how inheritance works are given in Section 3.3.5 below.

The information typically provided in frames is different to that provided in instances, so that the slots used are different. Briefly, frame models specify the information needed to define the SDG of the unit, including the ports in the unit, SDG arcs, default values of attributes, *etc.* The information given for instances of equipment models is related to connecting the unit to others in the plant *via* process port connections, specifying fluids and their properties in the unit, and giving values to the attributes of the unit.

3.3.4 Hierarchy of Equipment Models

Models in the unit model library are arranged into a hierarchy, in which the principles of inheritance operate. Inheritance allows a model to be defined "by exception" from its parent, so that a child frame is the same as its parent, except for specified differences. A hierarchical organising structure helps to group together similar models and to accentuate their similarity by modelling common behaviours of equipment at the highest possible level. Instances of models at any level of the hierarchy can be used in plant models. The current hierarchy of models is shown in Figure 3.3.

A number of guidelines were observed in organising the hierarchy. These include:

- The hierarchy must be intuitively sensible to an engineer, as an end-user. This facilitates rapid and correct selection of an appropriate unit model.
- The lower levels of the hierarchy should correspond to more detailed specification of equipment, the upper ones to more general equipment (*e.g.* a centrifugal pump is defined as a type of a pump, and so appears below pump in the hierarchy).
- The designer should avoid unnecessary proliferation of models, by using attribute conditional model sections, as described in Section 3.3.6.
- Future additions to the library should be anticipated where possible, and appropriate space provided. If necessary, extra layers should be added, to deepen the hierarchy. An example is the `pressureRaiser` model, which was created as a common parent of the `compressor` and `pump` models, even before the compressor model was added to the library.

New models should be placed in the hierarchy nearest to those equipment models to which they are most closely related, functionally. The temptation to maximise the use of the inheritance features of the system, and define models in terms of others which have similar sets of arcs but which are otherwise unrelated, should be resisted.

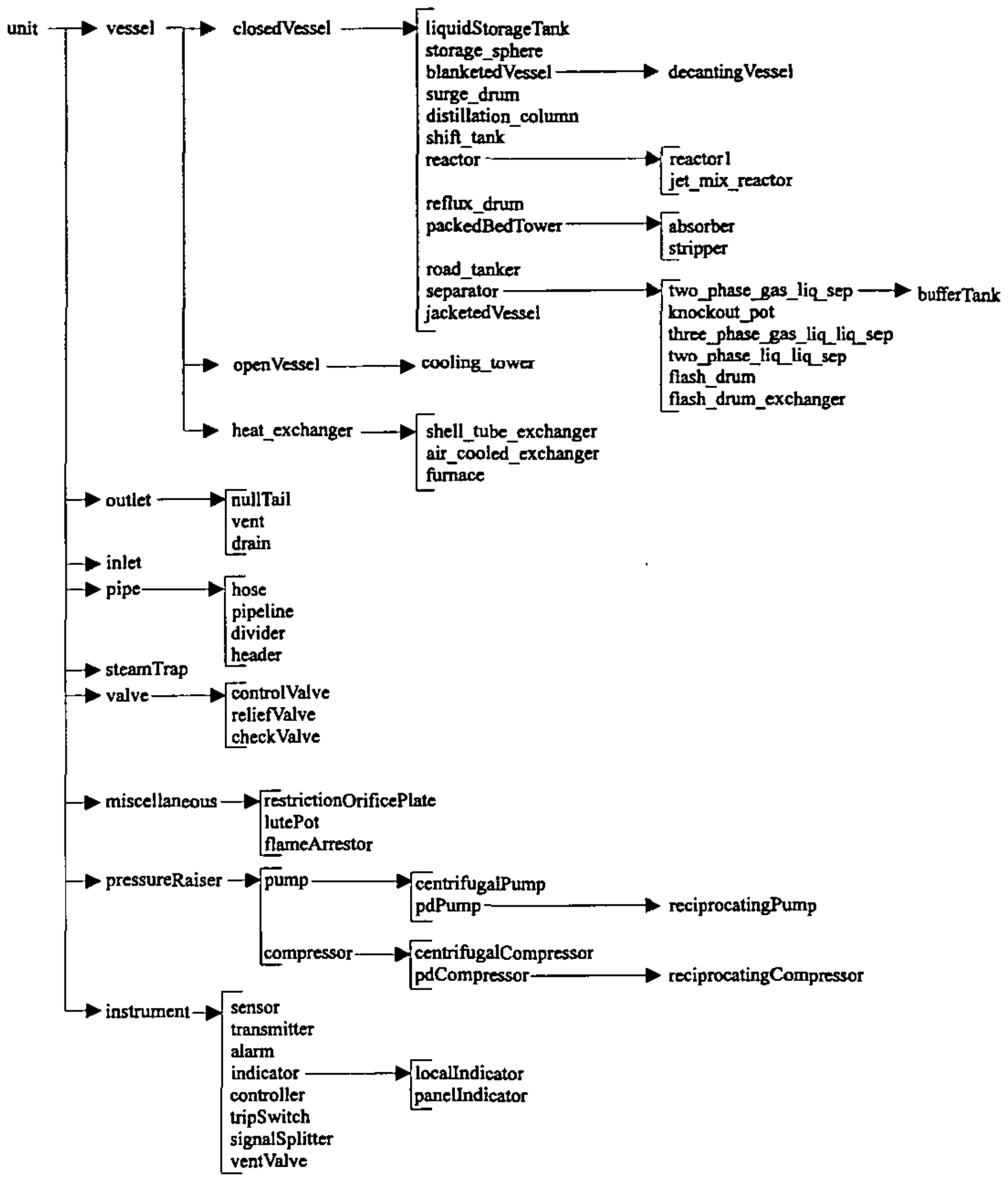


Figure 3.3 : Unit Model Hierarchy in AutoHAZID

The STOPHAZ project documentation contains further information on the hierarchy of models shown above (STOPHAZ Project 1997a, Appendix 4, "HAZID Libraries").

3.3.5 Slots and their Inheritance in AutoHAZID Models

Slots constitute the main body of information stored in unit models. Inheritance operates within the hierarchy of frames and from a frame to instances of that frame in a plant model. The slots of the parent are inherited by all its children, so that the information provided in a child model is in the form of additions or replacements for slots inherited from the parent frame.

Each slot has a name, a type and a list of values. The name of the slot does not have to be unique within a frame or instance, but if there are multiple slots with the same name, they will be reduced to a single slot at run time, giving preference to information supplied later. This principle of slot value resolution applies to inheritance between frames and instances, and to multiple slots within a single model. The values in slots inherited from the parent are considered to be "earlier" than, and therefore subject to overwriting by, the values in slots of the child.

Slots are of three types: "is", "info" and "include". The "is" slots specify simple attributes of the model in terms of constant symbols (*e.g.* for a pump, we may have `status is running`). The "info" type slots each specify a list of values. For "is" and "info" slots, inheritance operates such that every slot which the parent frame has is inherited to the child, but if the child has a slot with the same name, then the value of the child slot overwrites the value inherited from the parent.

The third type of slot is the "include" type. This type of slot has a list of items as its value, in the same way that the "info" slot does, but the "include" slot behaves differently with respect to inheritance. If the child has an "include" slot for some slot name, then provided the parent frame has no slot with that name, the "include" slot is converted to an "info" slot with the same list of values. If the child has an "include" slot for some slot name and there is an "info" slot with the same name in the parent frame, then the value list of the "include" slot is added to the value list of the "info" slot. The resulting list of values is put into the child as a new "info" slot, replacing the "include" slot. This mechanism allows additive changes, possibly specialisations of the SDG model, to be made to the information provided in the parent model.

Although `info` and `include` are implemented as different subtypes of slot, an alternative view of the inheritance system is to consider them to be functional modifiers of the slot. In this view, `info` and `include` determine how the value of the appropriate slot is produced in inheritance.

The "is" type of slot is often referred to as an "attribute" of the model. Attributes can specify additional information about the type of equipment or its operation, and can be used as the basis of attribute-conditional models, as described in Section 3.3.6.

Table 3.2 describes the various "info" type slots which can be used in frames and instances. The columns labelled "F" and "I" indicate if the slot is normally specified for frames in the unit model library (the "F" column), or in plant description files (the "I" column). Some slots are generated automatically by the program and do not exist in any library or plant files external to AutoHAZID. An example is the slot named "location", which is generated by the fluidisation routine described in Section 5.2.2.

Slot Name	F	I	Description
outports	√	√	Specifies the process outlet ports of a model, giving either their names (for frames) or names plus connected port (for instances).
inports	√		Specifies the names of the process inlet ports in an equipment model (frame). Format as for outports.
unitports	√		Names the internal process locations in a unit (frame), such as the vapour and liquid in a tank. Format as for inports and outports.
outSignalPorts	√	√	Defines the signal output ports (and their connectivity) for the instruments on a plant. As with outports above, format is similar, and only the connections for outSignalPorts are specified in the plant model.
inSignalPorts	√		Defines the names of the input signal ports in the model of an instrument (as a frame). Same format as for inports.
script	√		Specifies the templates used to construct the equipment model.
propLinks	√		This slot defines the propagation model of the unit and its failure modes. Used in constructing the SDG of the plant.
conditionLinks	√		This slot is used to selectively include certain parts of the equipment model into the instances when the plant model is put together, based on the values of certain attributes in the model.
sigPropLinks	√	√	Used in both frames and instances to define the propagation of signals in the instrument system.
portTemperatures		√	Allows the temperatures of process fluids to be specified (in °C), for each of the ports belonging to a process unit.
portPressures		√	Allows the pressures of process fluids to be specified (in bar abs), for each of the ports belonging to a process unit.
intendedFluids		√	Allows the flowrates (in kg/hr), component names and compositions of those components (in mole fractions) to be specified, for process fluids at each port in a process unit.
sensedVars		√	This slot is used to flag the variables which are monitored by instruments in the plant model (indicators, alarms, sensors, *etc.*).
material			Intended to specify materials of construction (as a list of names of materials) for the plant items. Not currently in use.
ruleData	√		This slot contains the VTT fluid rules. Each rule is specified as a string in the list. This slot is only present in the models of fluids in the fluid library file.

Slot Name	F	I	Description
location			Records data generated by the plant fluidisation routine, for fluids at various places in the plant model. Not specified in the plant or equipment models.
<generalSlot> (there is no slot with this actual name)			A type of slot defined in the parser so that any named `info` slot can be created without changing the parser. This is a relatively new development compared to the slots named in the previous parts of this table. Note that there is no control over the internal syntax of the items in the value list, so that anything which can be parsed will be accepted – the programmer must take care to check the data appropriately when it has been read into the program.
must_connect	√		Defines the names of the process (inports and outports) ports which must be connected in the plant model. This slot is usually defined in the frame for the equipment model and checked against the actual instance found on plant. If ports are found in the instance which are not connected but should be, this is flagged as an error. This slot is an example of the <generalSlot> type shown above.
comp_connections	√		Specifies the pairs of ports in the model of a unit which are connected together for the purposes of fluid propagation. This slot is an example of the <generalSlot> type shown above.

Table 3.2 : Slots in use in AutoHAZID

3.3.6 Attribute-Conditional Modelling System

When developing increasingly specialised equipment models in a hierarchical system, such as the one outlined above, there is a danger that models proliferate to cover all the possible combinations of optional features in similar equipment. An example is for models of pipe, where the pipe may be lagged or unlagged, welded or flanged, *etc.* If each possibility is addressed by a new model, many models are needed, one for each combination of attribute values. The solution adopted in AutoHAZID is to add a feature to the modelling system which allows sets of arcs and slots to be selected depending on the value of certain attributes in instances of the equipment.

The `conditionLinks` slot provides this feature. It allows generic models of equipment to be specialised in a limited way, by specifying a number of pairings of attribute and value, each associated with a list of slots to be added to the instance if the value of the attribute matches that specified. The values of the attributes are matched when an equipment model is instantiated in a plant.

The attribute-conditional parts of instances are processed after the plant model is loaded and the values of slots are resolved from inheritance and from values supplied by the instance itself. After the matching associated with the attribute-conditional parts of the models, the slots in all instances are resolved again, to integrate any information that has been added. Typically, an `include` slot is used to add new arcs to the model if the attribute condition is met.

3.3.7 Custom Models and the Model Generation Tool

Most equipment items in a plant can be modelled with commonly used models in the unit model library. However, some units may not correspond to models in the library. These are often vessels, made to order as "one-off" items for a particular plant. In these cases, a tool is needed to help the user of HAZID construct a new, customised, model for the equipment item. This is the task addressed by the Model Generation Tool (MGT) program, developed by Dr. F.D. Larkin at Loughborough.

The MGT uses an interactive question and answer session to elucidate a structural model of the new vessel from the user. The structural details include details of internal chambers, their interconnections, fluids present, *etc.* Additional questions are used to add details of equipment failure modes and consequences. The MGT uses the information provided to construct an SDG model of the vessel, which can be added to the unit model library for later use.

Templates (see Section 3.4) are used to model the different parts of the model, and the content of the template library has been heavily influenced by the development of the MGT. Numerous templates were defined to model different types of liquid and gas inlets and outlets for vessels, interfaces between fluids, *etc.*

The MGT is described further in the "Model Generation Tool User Manual", (STOPHAZ 1997b, Appendix 7). The software and its documentation were prepared by Dr. Larkin.

3.3.8 Consequence Types and Ranking

The consequences represented in AutoHAZID equipment models cover a broad range of undesirable events, from minor inconveniences for plant operation to major catastrophic events with the potential for loss of many lives. Therefore, a method for focussing attention on the more important consequences is important in a system which produces a large volume of results, as AutoHAZID frequently does.

For this reason, a consequence classification and ranking system was devised by Prof. F.P. Lees and Dr. F.D. Larkin. Every consequence in the model library is associated with three types of classification information, added to the model definition by the model designer:

- A default[2] severity rank in the range 1 to 5, indicating the scale of the event, where 1 is least severe and 5 is most severe. The user may ask the program to screen out consequences below a certain severity, when reporting HAZOP results. The severity is reported next to the consequence descriptor in the HAZOP report and is used to sort consequences so that the most important ones are reported first.
- A consequence class, which is a symbol defining whether the consequence is an operability problem (`op`), a hazard (`haz`), or both (`haz_op`).
- A list of codes, each one taken from a list of standard consequence types, defining how the given consequence is classified. The standard consequence types are listed in Table 3.3 below. Every consequence should be a member of at least one of these classes.

[2] The rank given is a default because the severity of many consequences depends heavily on process-specific parameters, such as the fluids involved, which cannot be known to the generic unit model. For loss of containment, AutoHAZID can adjust the default severity according to particular process details (if those details are given) using methods from the Dow Chemical Exposure Index Guide.

Standard Consequence Categories	Code
personal injury	pi
loss of containment	lc
equipment damage	ed
operating problem	op
loss of outlet flow	lf
contamination of outlet flow	cf
explosive mixture	em
unintended reaction	ur
vibration	vb
ignition source	ig
device malfunction	dm

Table 3.3 : Standard Consequence Categories in AutoHAZID

3.4 Templates and Scripts for Modelling Parts of Equipment Items

The observation that equipment in a plant tends to be chosen from a small number of types led to the structural decomposition of the plant model into a number of units, each based on one of a limited set of models stored in a library. It is found that models of equipment themselves possess an internal structure, midway between the level of a unit and that of a single SDG arc. Moreover, the structural or functional components of an equipment model are taken from a limited set of possible types (*e.g.* heat transfer between two fluids, flow of a liquid into a vessel, *etc.*).

In AutoHAZID, these repeated structural or functional components are modelled using "template models", whose definitions are read in from a library file when the program starts. Each template is a group of arcs which are often found together, and can be thought of as a model of a phenomenon or of a part of an equipment item.

Templates can be used to build up parts of equipment models anywhere in the unit model library. However, since their context varies, some elements of the arcs (*e.g.* the names of ports in the unit) must be varied also. Therefore, each template is associated with a name, a list of arguments or parameters and a list of associated arcs. The arguments of the template are variables, which also appear in the arcs listed.

When a template is used (in a `script` slot in a unit model), values are given to its arguments. These values are substituted wherever they occur in the associated arc list, before those arcs are added to the SDG model of the unit, as defined by other slots (*e.g.* `propLinks`) elsewhere in the frame.

This approach to "sub-component" model decomposition is limited to the addition of groups of arcs, typically using variable port names, as described above. However, the use of a library of templates does reduce the effort required to make some types of changes to models, significantly simplifying model maintenance.

3.5 Methodology for Model Development

This section builds on the description of the AutoHAZID modelling system offered in Sections 3.3 and 3.4, giving some guidelines on how to apply the tools just described. The objective is to allow for models to be developed in a disciplined and structured way, so that a consistently high quality of model performance may be expected. This method was not used for all models in the unit model library, due to time constraints.

The proposed methodology is described in this section, in relation to an example which was examined in detail during the STOPHAZ project – that of modelling flow and pressure propagation. Firstly, a system boundary for the flow and pressure modelling case study is defined, in Section 3.5.1. Then, Section 3.5.2 discusses the "no function in structure" principle and its application to the flow modelling problem. The formalisation of the flow path model, in terms of the choice of variables in the model, is addressed in Section 3.5.3. The idea of "causal hierarchy", outlined in Section 3.5.4, was found useful in the flow path model, and may be of use elsewhere. The flow path SDG model itself is presented in Section 3.5.5, along with the list of assumptions which define this particular template model.

The conventions used to model no flow and reverse flow in AutoHAZID flow paths, are described in Section 3.5.6. Finally, Section 3.5.7 finishes this section of the chapter by describing the techniques used to discover weaknesses in the models of AutoHAZID, and to direct their improvement. This topic is labelled as "Knowledge

Elicitation" because it consists partly of extracting knowledge from human experts, and partly of formalising that knowledge in SDG models.

3.5.1 Flow Path System Definition

The case study problem for modelling is to "build a model of flow and pressure propagation for chemical plants". A first model for flow cannot be expected to cover all the potential complications of flow geometry, multiple phases, non-Newtonian fluids, *etc.*, so we concentrate on a limited, but commonly occurring, case. The system to be studied first is the simple "flow path" – a path between an inlet and outlet location, through which a fluid can flow. This system is typified by a rigid pipe or an open valve filled with a single fluid.

The restriction assumptions, which define the system, are:

- The model deals with propagation of flow and pressure deviations in a "flow path". Other phenomena, such as heat transfer, *etc.*, must be modelled separately.
- The flow path is an unbranched space, filled with a single phase fluid and enclosed by rigid walls, with one inlet location and one outlet location.
- The fluid may be liquid or vapour.
- Density changes in the fluid are not modelled, so that the fluid is assumed to be incompressible, within the scope of the flow path model.
- The normal direction of fluid movement (flow) is from the inlet location to the outlet location.
- No shaft work is done on the fluid within the flow path.

Known variations on the above assumptions include:

- Where the flow path is branched, so that it has either many inlets or many outlets. These cases are represented by the `header` and `divider` models, respectively, and discussed in Appendix C.
- Where heat transfer, or a phase change, occurs between the inlet and outlet.

- Where the fluid flows in an open channel, as opposed to an enclosed "pipe".
- Where shaft work is done on the fluid, or extracted from it, between inlet and outlet.

3.5.2 The "No Function in Structure" Principle

The "no function in structure" principle, as given in De Kleer and Brown (1984), states that: "The laws of the parts of a device may not presume the functioning of the device as a whole". This means that the model of a device component (such as a unit in a process plant) should be developed free of the context in which it will be placed. In practice, this is an unattainable goal, not only because it is almost impossible to imagine a component functioning completely free of context, but also because the very act of decomposition presupposes the mode of interaction or connection between pieces. Thus, one must at the very least state how components are connected together, in order to construct a feasible model of a composite device.

The principle of locality follows naturally from the no function in structure principle. It states that the components of a physical system can interact only with adjacent components, to which they have a connection. The mode of connection between components therefore determines how causes and effects may propagate.

Clearly, the no function in structure principle is particularly appropriate to unit-based modelling systems, such as the AutoHAZID SDGs. If the principle is violated, the models produced will be of limited use, and may produce erroneous results when used in other plants or other contexts.

In AutoHAZID local causal input-output mappings, expressed as SDG arcs, define the fault propagation functions of the components. Any influences propagated through the model are mediated by deviations in variables present in the ports connecting units together. Physical "adjacency" in this system is therefore defined by stream connections between units. The overall behaviour of the plant model in simulation results from the interaction of the devices in it. The only assumed context information in this model is the mode of connection between units (using SDG arcs in the plant model), and the variables used in those connections.

The no function in structure principle requires that a level of decomposition, a "basic unit", be chosen for the phenomenon to be modelled. In the case of flow and pressure modelling, this is the flow path, and communication with adjacent units is achieved by propagation of pressure deviations.

3.5.3 Choice and Definition of Variables

To build a model of the fault path "basic unit", at least three things must be done:

- Choose a formalism for implementing the models. In this case, the choice has already been made: it is the signed-directed graph (SDG) used in all AutoHAZID equipment models.
- Decide which are the important variables in the problem area and characterise them. Any restrictions imposed on the type of variable, by the choice of implementation, should be considered. Also, the meanings of variables, as well as issues of how and when they should be used, should be agreed by convention. For flow path models, three variables were chosen:
    - **Pressure, P,** is the pressure at a single point in the plant. The qualitative values of this variable are *lessPressure* and *morePressure*, corresponding to the HAZOP guide words. Pressure is an entirely local property of the fluid present at a particular location in the plant.
    - **Flow, Q,** is the variable chosen to represent the bulk flow of fluid from one location to another in the plant. In a HAZOP study, four deviations are commonly used to examine changes in flow (more flow, less flow, no flow and reverse flow). The SDG does not permit variables with more than two qualitative values, so flow has only two associated deviations (*moreFlow* and *lessFlow*). The separate deviations *noFlow* and *revFlow* are modelled using other variables (see Section 3.5.6 below). Note that flow is not modelled as a property of a single location in the plant, but rather of the path between two

points. In that respect it is different from properties, such as pressure and temperature, which can be stated uniquely for any single location.

  - **Flow Resistance, R,** represents the frictional resistance to fluid flow which exists between the inlet and outlet locations. Resistance has two qualitative values corresponding to deviations (*lessResistance* and *moreResistance*), and can be seen as a variable similar to flow in nature, because it is a "path property" rather than a localised property.

- Once the variables have been decided upon, the next task is to link them to each other in an appropriate way. The objective here may be to build a model displaying some known set of behaviours (failure modes, perhaps), or to work from first principles, guided by the assumptions made in the model scoping step.

3.5.4 Causal Hierarchy in Flow Modelling

Previous attempts to model fluid behaviour in process systems have often suffered from difficulty in disengaging the effects of flow and pressure. Frequently, the designer would worry about whether deviations in flow caused deviations in pressure, or *vice versa.* The result could be a poorly explained model (possibly containing circular influences between variables) in which the reasons for different parts, and the action to take when the model failed to produce appropriate results, were unclear.

The practice of stating all known assumptions in a model as it is developed, should help to clarify the influences involved, and prevent the occurrence of confusing circular relationships in the model. In addition, a "causal hierarchy" is introduced here, which is an arbitrary convention governing the allowed causal relations in SDG arcs modelling flow.

The flow modelling causal hierarchy shown in Figure 3.4 states the "can influence" relationships between variables. Deviations in resistance may cause deviations in pressure or flow, pressure deviations may cause deviations in flow or pressure, but flow may not cause deviations in pressure, resistance, or other flows. Outside the scope of the flow path, flow may cause effects on other variables, such as the level of liquid in a tank, temperatures in a heat exchanger, *etc.* Note that the causal hierarchy stated here assumes that the flow in the flow path is steady, and that the fluid is incompressible – otherwise, flow may influence pressure in the system.

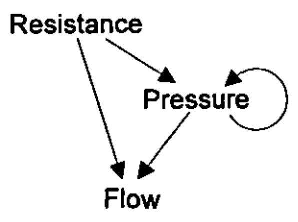


Figure 3.4 : Causal Hierarchy for Steady Flow of an Incompressible Fluid

As a result of this ordering relation, propagation of flow is no longer needed - the information necessary to propagate changes of flow is carried by pressure propagations from other flow paths. This elimination of flow propagations reduces the chance of confusing, "crossed" influences between flow and pressure when a plant model is built from a number of equipment models.[3]

The idea of causal hierarchy may be useful in other problem domains where there appears to be a strong interdependency between variables. The modeller must decide carefully what the dominant causal relationships are in the system, before choosing the ordering of variables in the model.

3.5.5 The Flow Path SDG Model

Having decided the scope of the flow path model, the set of variables to be used in modelling it, and a principle governing how the variables may be connected (the causal hierarchy), the next step is to formalise the model in an SDG. The basic SDG for the simple flow path discussed so far is shown in Figure 3.5 below, where flow occurs from an inlet port, `in`, to an outlet port, `out`. In the figure, `P` represents pressure, `Q` flow and `R` resistance; the subscripts indicate the ports with which the variables are associated.

[3] The use of pressure propagation for flow modelling means that, when adding new failure modes which have an effect on flow, the model builder must think of the effects on pressure which those events have. This ensures that effects on flow and pressure of new failure modes are added at the same time.

$$\begin{tikzcd}
P_{in} \arrow[rr, bend left, "+"] \arrow[ddr, bend right, "+"'] & & P_{out} \arrow[ll, "+"] \arrow[ddl, bend left, "-"] \\
& R \arrow[ul, "+"] \arrow[ur, "-"'] \arrow[d, "-"] & \\
& Q &
\end{tikzcd}$$

Figure 3.5 : Simple Flow Path Model

The arcs shown above are easily used to define a flow path template which can be used in many equipment models. The complete set of assumptions and principles used in the above model is summarised below:

- Flow and pressure are modelled in a "flow path" – an enclosed, filled space with one inlet (*in*) and one outlet (*out*), and a clear path between *in* and *out*.
- The fluid in the flow path is single phase (liquid or vapour) and continuous throughout. Multi-phase flow is therefore excluded from this model.
- The fluid is considered incompressible, so that changes in density are ignored.
- Fluid in the flow path is considered to flow normally from *in* to *out*. Therefore, no flow and reverse flow are exceptions to this condition.
- Pressure deviations are allowed to propagate in either an upstream or a downstream direction in the flow path.
- Flow deviations are not propagated between flow paths – they are generated locally, for each flow path.
- The flow path model complies with the restrictions of the causal hierarchy. These include the restrictions that the flow is steady, and that the fluid is incompressible.
- The relevant variables are pressure, P, flow, Q , and resistance, R.
- The fluid has no external work done on it, and performs no mechanical work on its surroundings.
- There is no significant height difference between *in* and *out*, so that static head is the same at both locations.
- The fluid does not exchange significant quantities of heat with its surroundings.

- Within the SDG model of the flow path, the shortest path between two nodes determines the appropriate influence between those nodes. This "shortest path heuristic" is used in all AutoHAZID models, and is discussed in Section 4.10.
- Friction has an effect on the flow in the flow path, and the amount of friction is represented by the resistance, `R`. Partially blocking the flow path tends to restrict the flow path, increasing `R` and therefore decreasing the flow, `Q`. The increase in resistance also tends to increase the pressure upstream of the flow path and to decrease it downstream.
- The driving force for flow in the path between *in* and *out* is the pressure difference between the two locations, which is not represented explicitly. The upstream pressure P_{in} has a direct effect on the flow and the downstream pressure P_{out} has a reverse effect.

Wherever the above assumptions hold for a path between two locations in a piece of equipment, the flow path model template is used to model the pressure and flow propagation effects. A single equipment model may contain a number of flow paths connected together, with each one declared in the `script` slot for the unit. The flow paths in the plant model are linked together by a pressure propagation "back-bone", which forms a communication path between remote units. This seems to be an efficient method for constructing large models of process flow systems, as all flow related propagation occurs *via* a single network of pressure deviations.

By varying the assumptions in the above list, one can tackle other pieces of equipment. Dividers and headers ("tee" pieces) are exceptions to the single inlet, single outlet assumption – they are addressed in Appendix C.

The deviations no flow (*noFlow*) and reverse flow (*revFlow*) challenge the assumption, in the above flow path model, that fluid flows forward. These deviations are qualitatively different from the cases of *moreFlow* and *lessFlow*, and the landmark value of zero defines the domains of forward flow, no flow and reverse flow. The problem of no flow and reverse flow modelling is dealt with in the following section.

3.5.6 Modelling No Flow and Reverse Flow

The approach used to model the deviations "no flow" and "reverse flow", in the AutoHAZID SDG, is to use additional nodes to represent these deviations, separately from the flow nodes already present in the SDG. The *revFlow* and *noFlow* nodes, whose deviations are also called *revFlow* and *noFlow*, are used for this purpose. By convention, these nodes have only one possible qualitative value, "+". A value of "–" associated with these nodes has no meaning.

Two problems with this new scheme immediately present themselves. The first is that of ensuring that the new nodes are never used during fault propagation in such a way that they are associated with a value of "–". This is solved by adding checks to the HAZOP algorithm which make sure that deviations encountered in all fault paths are permitted ones. The second problem is one of model maintenance. New arcs must be added to all models, so that *noFlow* and *revFlow* propagate through the plant model in the same way that pressures propagate to cause the other deviations of flow. To a certain extent, the use of templates can help with this problem.

The problem of four deviations for flow in HAZOP could have been solved in other ways, possibly using a more powerful graph representation than the SDG. However, the SDG was retained because it is efficient and because it is powerful enough to represent most of the problems tackled in qualitative models for HAZOP emulation.

The deviations of *noFlow* and *revFlow* will now be considered separately.

No Flow

Flow can cease in a flow path because of two physically distinct causes. Firstly, the pressure difference between *in* and *out* becomes zero due to some change in the pressures. Secondly, the flow path may become completely blocked somehow, so that the flow path no longer exists. This is an interesting distinction not explicitly made clear in many descriptions of HAZOP.

The former case is not considered to be an example of the *noFlow* deviation in AutoHAZID, but instead is an extreme case of the *lowFlow* deviation. It is thought likely that this form of zero flow is not distinct from the *lowFlow* condition in any meaningful way, so that the *lowFlow* guide word should capture all the relevant hazards in the HAZOP report.

The second cause of no flow is more important for hazard identification, and defines the only case where *noFlow* takes place in AutoHAZID. Because some event has caused the flow path to be blocked, the plant model has changed in some way, and this may be an important consideration.

Therefore, *noFlow* may not be caused by pressure deviations in flow paths, but must instead be caused directly by initiating faults, or propagated from other flow paths in which such a fault has occurred. The information that a blockage event has occurred is propagated through *noFlow* nodes in the SDG, upstream and downstream.

It is important to bear in mind the special meaning applied to the *noFlow* deviation, when reading the results of HAZOP emulation, and when designing new models.

Reverse Flow

Reverse flow may be caused by a reversal of the pressure gradient in a flow path, for example by leakage out of the path, leading to flow in the opposite sense to that intended. However, the basic flow path modelling system in AutoHAZID, using only pressure propagation, cannot represent the magnitude of a pressure change. This means that it is difficult to judge whether a (qualitative) pressure deviation will cause a decrease in flow, or a flow reversal.

In trials, problems occurred with flow path models which linked pressure directly to *revFlow*. A typical problem was where a partial blockage in a line caused the pressure at a point to change; the pressure deviation then propagated and caused a *revFlow* deviation elsewhere in the line. It is absurd that a partial blockage could cause flow to go backwards in the same line. This is an example where the pressure propagation chain does not carry enough information on the magnitude of changes taking place.

Therefore, *revFlow* is propagated separately from pressure in AutoHAZID, in order to preserve the information that a flow reversal has taken place. For the same reason, pressure and reverse flow are not linked at every point in the flow path chains. The working assumption is made that flow reversals are caused either by faults, such as large-scale leakages from the flow path, by pressure changes in process vessels or in tee pieces (dividers and headers). Ideally, points where *revFlow* is initiated should be tested for the magnitude of change which can be considered to occur (perhaps such tests will reveal that only *lowFlow* is possible in response to a particular change in pressure). These sorts of numerical tests can be carried out by the fluid modelling system, which is described in Chapter 5.

Taking the example of a pressure increase in a vessel causing a flow reversal in an inlet to that vessel: pressure deviations will be propagated upstream, allowing *lowFlow* and *morePressure* to be predicted anywhere in the inlet line. However, *revFlow* will also be propagated upstream, along an independent propagation channel. This arrangement allows all possible deviations to be predicted correctly, if the magnitude of the pressure change is not known.

3.5.7 Knowledge Elicitation Methods

Once an adequate model of the links between variables in a unit has been developed, perhaps from first principles, failure modes need to be added to the unit model. Failure modes are very important parts of the model, and identifying them requires expert knowledge of the equipment.

Knowledge elicitation was traditionally used in developing rule-based expert systems. A "knowledge engineer" would talk to a "domain expert", to extract the most important knowledge, rules, techniques, *etc.* from the expert. The knowledge engineer was an expert in developing expert systems and the domain expert was someone who knew a lot about the subject matter to be encapsulated in the expert system. This type of knowledge elicitation can be very difficult, because often the expert does not use knowledge in any explicitly formal way, but instead relies on rules of thumb, previous experience, *etc.* to guide his/her judgement.

The knowledge elicitation techniques outlined in this section were used to stimulate thought about the nature of equipment, the ways it could fail and the susceptibilities it may have to various conditions. The "domain experts" in STOPHAZ were typically safety and process engineering experts. The "knowledge engineers" were members of the AutoHAZID development team. Many techniques are based around the group "brainstorming" type of meeting, using guide words, as in the method study approach.

Equipment failure is often caused by taking a unit outside its safe operating regime. Therefore, failure modes may be identified by systematically challenging the details of the operating regime, using a "what if?" method. This is partly what the knowledge elicitation techniques are designed to do. By identifying the underlying function of the equipment, it may also be possible to identify "enabling faults" for some items (these are events not leading to immediate hazards, but which reduce the degree to which the equipment is protected against the consequences of some other failure).

The following subsections cover the various techniques used to improve the accuracy and range of phenomena modelled in AutoHAZID. Some require an organised group meeting, and some are better carried out by a single model builder.

Trial and Error in Modelling

The usual means of evaluating library models was to test them out in case study plants and examine the HAZOP results produced by AutoHAZID. By examining the scenarios identified, an experienced model developer can quickly pin-point where an error has been made in a model, where an inappropriate fault propagation path has been produced, *etc.*

This job was usually done by a member of the Loughborough team, after changes to the models, to verify improvement and to see that no unexpected side-effects occurred. Output criticism was also used as a method of provoking comment from safety experts, to get new ideas for improvements.

The test cases used during STOPHAZ are outlined in paper 7 of the series submitted for publication in the IChemE Transactions on "Process Safety and Environmental Protection" (McCoy *et al.*).

Conventional HAZOP Studies

The largest test case plant, analysed so far using AutoHAZID, is a benzene plant taken from Wells (1980). This plant was subjected to a conventional HAZOP study by two separate HAZOP teams early in the project, to provide a set of results for measuring the success of automated HAZOP. These results have been valuable, in setting targets for improvement during the project, though we cannot yet claim to identify 100% of the results produced by the human HAZOP team in these meetings. A P&ID of the plant, as annotated for the HAZOP study, is included as Figure 3.6.

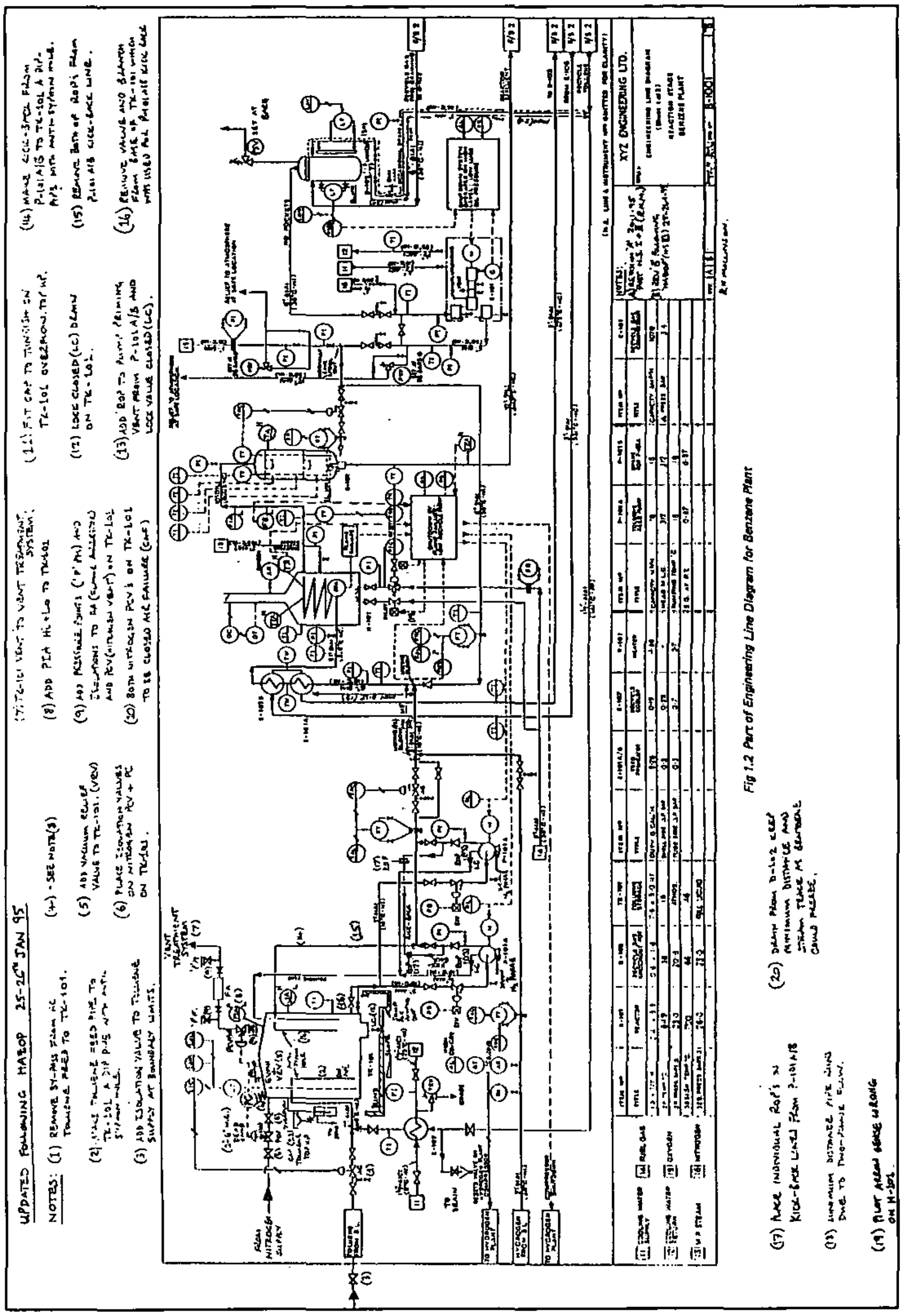


Figure 3.6 : Benzene Plant Test Case (after Wells, 1980) - Annotated P&ID

Equipment Modelling Seminars

Several seminars were hosted by Loughborough, where experts from process-based companies in the STOPHAZ consortium were assembled to look at single equipment models. The objective was to encourage remarks about possible failure modes of equipment and thereby elicit information for improving models.

These seminars were conducted as "mini-HAZOP" studies. A single equipment type would be chosen for study by (typically) two experts and a member of the Loughborough project team. The team would discuss the equipment item in a way similar to that of a HAZOP meeting, but without considering any specific installation of the equipment item (*i.e.* free of any particular plant context).

First, the purpose of the equipment was agreed and the scope of discussions fixed, particularly in order to decide what not to discuss. A number of equipment ports were then identified as study node locations to focus on. Following the HAZOP method, deviations of variables at each study node were considered. The questions of how the deviations could arise, and what consequences they could have locally, were asked.

In all these discussions, it was important to keep the team focussed on the equipment at hand, while also encouraging them to imagine the item in a variety of plant contexts. It was hoped that, if this could be achieved, the model which would be later developed from the notes of the meeting would be as general as possible. The role of the Loughborough team member was to take notes, and to encourage comments which could be easily formulated in terms of rules or arcs in the SDG.

The minutes of these meetings were noted on sheets in a similar format to the HAZOP report sheets typically used during conventional plant HAZOPs. However, this format was very often insufficient to record all the notes which arose during the meeting, because much of the knowledge gleaned from our experts turned out to be in terms of different or more useful ways of looking at situations on the plant. An example is the observation that reciprocating pumps can cause problems with flow measuring devices installed downstream, because pulsations caused by the piston stroke cause such instruments to read too high. This is an important problem which doesn't obviously fit into the fault path model of hazards typical for AutoHAZID scenarios.

The modelling seminars produced material which it was sometimes difficult to implement in AutoHAZID because of the format of the information, or because of the limited stage of development of the program itself. Nevertheless, some of the information obtained could be used to add new failure modes to the existing models, and this has been achieved for a number of cases.

Criticism of Equipment Library Models

Another technique, similar to the modelling seminar approach in some ways, was for a single safety expert to examine models in the equipment model library, and to criticise them, pointing out what was right or wrong, what missing, *etc.* This was attempted in at least two cases, with some success. However, to provide the most useful criticism, the expert needed a quite deep understanding of fault propagation behaviour in plant models, to see how the models were designed to work together. This presented a barrier to effective use of the technique. Nevertheless, some useful pointers were identified.

Although this method was used during STOPHAZ as an "off-line" study of models in the library, it could be adapted so that AutoHAZID would construct a plant model with a single instance of a model to be examined. Then, the user would examine the inputs and outputs of the model in a systematic way, using AutoHAZID results. This approach would also insulate the user from the internal detail of fault propagation.

Expert Criticism of HAZOP Results for Test Cases

At around the middle of the project, when AutoHAZID was substantially complete in its simpler, basic form, a reasonably formal series of test case evaluations was carried out. Critical input from the process expert partners in the consortium was sought, to find out what the shortcomings of the system were.

Automated HAZOPs were performed on a series of plant models, of successively more complex design, using AutoHAZID. The results were sent to the partners for comment. Ideally, comments on one test case would have been used to improve the performance of AutoHAZID before the next test case in the series, so that continual improvement of the system could be demonstrated over a number of weeks. A number of problems were identified and fixed quite quickly, but very often the solutions to the problems involved larger pieces of work, on a longer timescale.

3.6 Conclusions

This chapter has described HAZID and AutoHAZID in some detail, covering the architecture of the integrated HAZID system and the modelling system in AutoHAZID. The models are based on the signed directed graph (SDG), and represent the influences between physical variables, faults and consequences in a piece of plant equipment. The chapter has described all the main features of this qualitative modelling system, as well as stressing the importance of principled development of new models, illustrating this by the example of the flow path model in AutoHAZID.

The component-based modelling approach to the plant model and the SDG includes many useful ideas, such as inheritance, the use of template models and the flow path approach to flow and pressure modelling. The chosen SDG modelling formalism has a natural interpretation in the way it mimics the causal nature of simple fault propagation chains. Luckily, it is also probably the most efficient way of doing the sort of qualitative reasoning required for HAZOP emulation.

In order to manage a potentially quite large and diverse library of models, some form of structured development procedure, in terms of knowledge elicitation, implementation and documentation, should be adopted. This is particularly important when developing novel unit models, as these often contain new assumptions and may require modelling techniques not used elsewhere in the model libraries.

The AutoHAZID program now performs efficiently on large test case plants and, now that the model library has been enriched by the knowledge and experience of a number of process industry experts, the program produces increasingly valuable HAZOP results. There are still many situations, however, where problems arise, which it is difficult to address using the SDG model system described so far. Some of these problems (and possible solutions to them) are discussed in Chapters 4 and 5.

Chapter 4 : Some Problems with Qualitative SDG-based Hazard Identification

This chapter discusses some of the problems encountered with HAZID as described in Chapter 3. Many of these problems are shared with other systems based on a qualitative modelling system, or which use a graph search model for inference. Some of these problems have been tackled successfully – the approaches used to solve these are also discussed here.

However, some of the recognised weaknesses of HAZID have not been tackled. Some improvements were ruled out because they were, strictly speaking, "out of scope" for HAZID (the scope of application for HAZID was discussed in Section 3.1). Other problems were not dealt with because the effort required to do justice to them would have diverted attention away from more important priorities in the project. It was important during STOPHAZ, to keep the development of HAZID focussed on the core objective: hazard identification by HAZOP emulation.

4.1 The SDG represents only two deviations

As discussed in Section 3.5.6, the main case where there is a problem with the limitation of two deviations per SDG node, is that of modelling flow deviations, specifically "no flow" and "reverse flow". However, it is conceivable that other variables, which require more than two deviations, may need to be modelled at some stage.

For the four deviations of flow, the solution adopted is to allow pressure to propagate through the plant, causing *lessFlow* and *moreFlow* deviations, while *noFlow* and *revFlow* are propagated as separate variables in the SDG. Depending on the details of the case, this approach may well be useful with other similar problems.

4.2 Single Mapping Influences

The arcs in the SDG are labelled with either a "+" or "–" sign, implying a direct or reverse mapping between the two possible values of the variable on the left of the arc and those of the variable on the right. Some influences between variables in reality do not conform to this dual mapping. To model these influences properly, some change must be made to the SDG representation.

An example of an influence which does not readily fit into the basic SDG framework is seen in the nitrogen inerting system shown in Figure 4.1. A flammable and volatile liquid (hexane, for example) is stored in a tank. To prevent the formation of a flammable atmosphere in the tank, the vapour space of the tank is maintained at a small positive pressure with nitrogen.

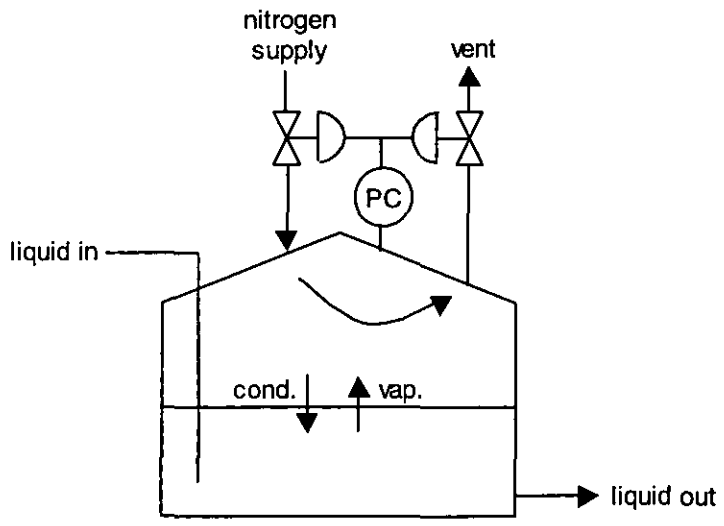


Figure 4.1 : Nitrogen Blanket Example

The nitrogen also accommodates changes in the liquid level in the tank. When the level of the liquid in the tank falls, nitrogen is added to replace the liquid removed. When the level rises, nitrogen containing small quantities of vaporised hexane is flushed out of the tank through the vent. If the level is steady, there is no net flow of nitrogen through the tank.

If the control valve for the nitrogen vent fails open, the other one also opens in response to the low pressure, so that nitrogen flows through the tank at a maximum rate. In this situation, much more hexane vapour than usual is removed and an evaporative cooling effect is observed – the liquid is cooled by the removal of the vapour, and its temperature drops. However, the relationship between flow and temperature does not work both ways. If the flow of nitrogen is low, no change in temperature can be expected.

This phenomenon can be understood by considering that the hexane in the tank exists in vapour and liquid form, and the vapour will tend to equilibrium with the liquid, according to the equation:

$$\text{Liquid} + \text{Heat} \Leftrightarrow \text{Vapour}$$

When nitrogen flows through the tank, vapour is removed, driving the equilibrium to produce more vapour (*i.e.* towards the right hand side of the above equation). In doing this, heat is required to produce the vapour, and this is removed from the body of the liquid, cooling the liquid that remains. When very little nitrogen flows through the tank, the vapour-liquid system is close to equilibrium, so a negligible amount of heat is produced or consumed.

A further example is the overheating problem that occurs if a running pump is not able to discharge its usual quantity of process fluid. In normal operation, any heat generated by the pump is carried away from it by a large volume of process fluid, so that the increase in temperature of that fluid is negligible.

When the fluid in the pump cannot escape, however, all the energy supplied by the pump (including much of that which would otherwise be transferred to the fluid as work) goes into heating up a much smaller volume of fluid. In this case, the temperature of the fluid can rise much higher, possibly causing a leakage or other problem for the plant.

Here a relationship is established where low flow of fluid through the pump causes high temperature in that fluid. High flow through the pump has no meaningful effect on the fluid temperature, as an already negligible temperature rise is made even smaller by the change.

This is another case where a balanced process is perturbed from its normal state, although here the balance point is not strictly speaking an equilibrium, but rather a steady state. It seems likely that wherever the "normal" state of a physical system is at a balance or equilibrium point, as with the nitrogen blanket and pump examples, there will be a problem with representing a single mapping influence within the SDG.

4.2.1 Use of Directed Graph instead of SDG

One approach which solves the problems of modelling single mapping influences described in the examples above, is to use a directed graph representation, rather than the signed directed graph, to model the plant. In this scheme, the nodes in the graph represent deviations of process variables, rather than the process variables themselves.

Therefore, the digraph nodes do not have a range of qualitative values; they represent single qualitative values which would otherwise belong to SDG nodes. A sign is not needed on the arcs between nodes, since arcs in the digraph represent simple cause-effect links between deviations.

In converting SDG models to the digraph system, each SDG arc would translate directly to two DG arcs, in most cases. Exceptions are arcs involving *revFlow* or *noFlow*, which would translate to only one DG arc each. Within the DG, such deviations would look far less out of place than they do in the SDG.

Representing other deviations, where no appropriate process variable relates to both a "+" and a "–" value, would not be a problem for the DG representation. An example of this is *contamination*, where *moreContamination* and *lessContamination* deviations are inappropriate, and the only sensible deviation is *contamination* itself.

The single mapping influences in the examples above would be easily represented in this scheme as $highFlow \rightarrow lowTemp$, for the nitrogen blanket, or $lowFlow \rightarrow highTemp$, for the pump. It seems that all such cases, where only a single mapping between deviations is required, can be dealt with using this digraph method.

In the DG, tracing fault propagation through the plant just consists of finding paths between deviations – there is no need to take account of signs attached to the arcs along the path. The presence of any path between deviations in the graph indicates a causal link between them.

One problem with the digraph representation is that it would almost double the number of arcs in any model of the plant. This may or may not lead to problems with computational complexity in search.

After some experimentation during the development of AutoHAZID, it was decided not to proceed with a change to DG models. Apart from the upheaval of changing every equipment model, and the risk associated with a new system, it was found that moving to a digraph makes it more difficult to detect ambiguous predicted deviations during search. Checking a set of paths for contradictory influences on a process variable (*e.g. lessFlow vs. moreFlow* for the same flow) is more costly, as the deviations no longer correspond to the same node in the graph. To get around this problem would require an association between deviations of the same process variable which would negate the benefits of the DG approach.

4.2.2 Extra Code Numbers for SDG Arcs

The SDG uses two labels for its arcs, usually shown in figures as "+" and "–", but represented in AutoHAZID as two integer values, 1 and –1. These code values represent dual mappings of input values to output values, where the input and output values are both taken from the set {–,+}. To model single mappings between input and output values, a minimum of four possible link types need to be defined.

In AutoHAZID, the single mapping influences problem is solved by allowing SDG arcs to be labelled by four extra code values. The numbers –2, –3, 2 and 3 were chosen arbitrarily to label the single mappings, as an extension to the use of –1 and 1. All six arc codings are shown in Table 4.1 below:

Code Value	Input	Output
+1	+ –	+ –
–1	+ –	– +
+2	+	+
–2	+	–
+3	–	–
–3	–	+

Table 4.1 : Codings for Arc Influences

The arcs which make use of the new code values are often referred to as "coded arcs", and the graph which includes them is strictly speaking not a signed directed graph. This "coded directed graph" approach has successfully solved the single direction influences problems mentioned earlier. In the first example an arc is added, linking the flowrate of nitrogen out of the vent to the temperature of the liquid in the tank:

```
arc([out2,flow],-2,[liquid,temp])
```

The second example contains a single link between the flow through the pump and the temperature of the pump outlet:

```
arc([out,flow],-3,[out,temp])
```

It is worthwhile noting that, using the ±2 and ±3 mappings, it is possible to completely replace the dual mappings represented by the ±1 arcs with equivalent pairs of coded arcs. In a sense, the pure SDG system is included in the more specific single mapping scheme, but the old SDG codes were retained for brevity, for notational convenience and for compatibility with existing equipment models.

Taking this approach, the risk associated with the move to a new system is reduced. Users can continue to use the existing SDG models, whilst deploying the new arcs in a small number of places first, to demonstrate their usefulness before making any large-scale changes. This allows an overall policy of incremental upgrade, minimising disruption to the users, model libraries and the AutoHAZID program code.

The system of coded arcs does not impose any great burden on the search algorithm, as all that is required is a small amount of extra checking when paths are verified. If a coded arc is found in a fault path, the input influence to the arc is determined, from the initiating fault and subsequent arc codes, and checked to see that it has the value ("+" or "–") required by Table 4.1. If not, the path is rejected. This does not impose any significant penalty in efficiency.

Note also that the extra codes for the arcs do not introduce any fundamentally new concept to the SDG models. Arcs still represent influences between variables and those variables are still represented by graph nodes having values from the set {+,–}. Further, the coded digraph is the *most specific enhancement* that can be made, whilst retaining the basic framework of the SDG and the search techniques used on it. Any further change, such as extending or restricting the value set for nodes in the graph, would break the system or be a fundamentally new addition to it.

It would be possible to add new concepts to the system, such as particularly strong influences, transient effects, delays, probability ranks, *etc.* This could also be done by encoding this information in the arc labels, using extra numbers. However, doing this would be a fundamental change to the SDG system and could give problems requiring the SDG models to be replaced entirely by a newer system. This sort of change would involve a higher risk than the single mapping codes discussed here.

4.3 Reasoning through unhealthy units

AutoHAZID relies on the assumption that the single SDG model of the plant it constructs from equipment models is valid, even when the scenario being constructed requires that a fault has occurred in the plant. Even within the equipment item in which the fault originates, the "healthy" SDG model is still used to predict behaviour.

This "single model assumption" is closely related to the "single fault assumption" used to simplify analysis of accident scenarios in hazard identification. The single fault assumption is that there is only one initiating failure in the plant at any time, so that simultaneous independent failures are ignored by AutoHAZID.

Under the single fault assumption, it is reasonable to assume that the only unhealthy equipment items are a subset of those through which the fault propagation path passes. The only equipment item known to be unhealthy is the one in which the initial fault occurred. Most fault paths considered in HAZOP initiate in one place, are propagated elsewhere (to healthy units) and only there, in an otherwise healthy unit, cause a hazardous consequence. This explains why the single model assumption usually produces quite good results when used for HAZOP emulation.

Problems can arise however, when the fault propagation chain passes through a unit in which the initiating fault has caused some part of the model to become invalid. An example of this is the problem with modelling reverse flow caused by major leakage out of a component such as a valve. The relevant fragment of the SDG for this situation is illustrated in Figure 4.2 below.

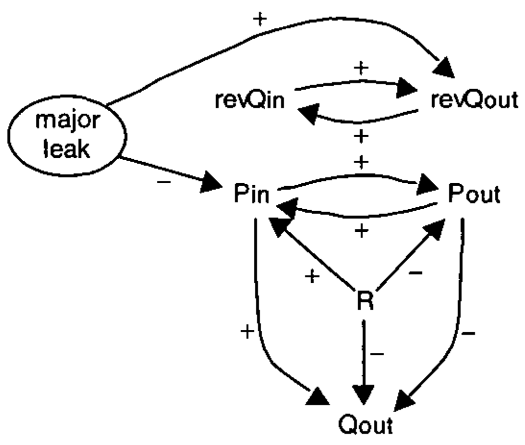


Figure 4.2 : Reverse Flow Problem for a Leaking Valve

The problem in this case is that the fault should give rise to a potential reverse flow at the outlet and downstream of the valve, but not at the inlet or upstream of the valve. Unfortunately, the normal model of the valve allows *revFlow* to propagate in both directions, meaning that reverse flow is predicted upstream as well as downstream of the valve.

The leak event has "invalidated" the normal model of the valve, in the sense that the model should no longer allow reverse flow to propagate through it. AutoHAZID cannot model the sort of state-based model dependency implied by this situation.[1] Instead, it uses a rule in the HAZOP search engine, to detect any fault paths found in the graph which start at a leak fault and subsequently propagate through any two reverse flow nodes in the unit where the leak occurred. Leaks out of pressurised systems or into vacuum systems are covered by the same rule.

This state of affairs is not very aesthetically satisfying, relying as it does on filtering out bad results after they are generated, using a rule which is outside the scope of the models themselves. But, it works well so far. It is not clear if this rule eliminates any valid scenarios which would otherwise be found by AutoHAZID, but it seems sound enough reasoning for any simple single input, single output unit.

Note that, when air leaks into a vacuum system, the leak gives rise to *revFlow* at the inlet to the unit, rather than the outlet from it, so that the SDG model shown in Figure 4.2 is not relevant for the vacuum case. It is still true, however, that reasoning through *revFlow* nodes when a leak into vacuum has occurred, is wrong. The different cases (of pressurised and vacuum systems) are handled in AutoHAZID by using conditional arcs, which are discussed in Chapter 5.

[1] Unlike the systems developed by Pennsylvania and described in Section 2.3.4, which allow the plant to be remodelled automatically whenever such a state change occurs.

4.4 Sparse Results for HAZOP

Early versions of AutoHAZID produced very large HAZOP report files, containing only very few interesting hazards. As a result, users needed a long time to analyse the output, to extract results of only limited value. The large size of the output reports was a result of the systematic nature of the HAZOP algorithm, combined with the inability of the program to filter important results from trivial ones.

The results were perceived as repetitious, due to the narrow range of phenomena tackled by the modelling system at the time. Although all reportings of a particular hazard may have been accurate, they were not necessarily important or interesting new failure modes discovered by the program. Because all results were reported in the same way, the program was unable to distinguish more interesting or important hazards from other, less important ones. Such a filtering mechanism is one of the natural strengths of the human involvement in HAZOP studies and complements the systematic method study approach, ensuring that maximum value is extracted from the study.

When ensuring the correctness of results produced by HAZOP emulation, a lot of time was spent examining scenarios to find the causes of any problems with them. If the report files had been smaller, this task would have been less laborious.

Some of the techniques developed to tackle these problems were discussed by Wakeman *et al.* (1997), who showed significant improvements in the readability of HAZOP results from AutoHAZID. In newer versions of AutoHAZID, the bulk of the report is reduced by a number of filters, each of which can be used or not used, at the user's discretion. These filters are outlined below and further information is given in Section A.5 of Appendix A:

- Scenarios in the HAZOP results are sorted in order of the importance rank of their consequences. This helps focus attention on the most important scenarios first.
- Using the consequence threshold feature allows the user to significantly reduce the bulk of the report, by ignoring consequences below a certain importance rank.

- The Fluid Modelling System (FMS), based on conditional fault propagation, allows fluid properties to be checked so that highly specific failure modes can be included in SDG models and spurious reporting of hazards dependent on fluid properties (such as fires, toxicity hazards, *etc.*) can be reduced. This increases the relevance and importance of the results.
- Identified faults which cause deviations, but are associated with no identified consequences, can be eliminated from the report. Similarly, consequences not associated with any identified faults can also be left out.
- If identification of protections is enabled, the HAZOP report can be reduced by displaying only scenarios against which there are no protective devices reported.
- Repetitions are tackled by removing any fault-consequence pair from the report if that same pair has appeared in the report already.
- During fault propagation, each deviation is associated with a set of faults which cause it. If the deviation itself can cause some further deviation by fault propagation, then the set of faults causing the first deviation will be repeated as causes of the second deviation. This can be a source of significant repetition in the report produced by AutoHAZID. Repetition is reduced by allowing some deviations to be reported as causes of others in the HAZOP report, replacing the set of faults which cause the intermediate deviation. Fault propagation search is effectively stopped at that point in the longer fault propagation chain. Therefore, this method was known (in AutoHAZID) as the "stopping point" method.
- AutoHAZID groups equipment items into "lines" for the purposes of examination, in an attempt to emulate the grouping performed by the HAZOP leader in a conventional study. Equipment items are examined by AutoHAZID in a line-by-line fashion, so that the order in which deviations appear in the report emulates the order of examination in a conventional HAZOP. This makes the report more readable for users with experience of HAZOP studies.
- A frequent source of repetition is where many similar faults are reported as causes of a deviation, for the same type of equipment. An example is where the deviation "*noFlow*" could be caused by the blockage of a number of valves in the same line. AutoHAZID allows such faults to be grouped together and reported for only one of the offending units, adding the string "etc" to the fault descriptor, as in

"`valve8 etc blockage`". All units grouped using "etc" must be in the same line (as identified by AutoHAZID) and they must be the same type.

One of the most important ways of improving the HAZOP results is to add more interesting failure modes to the models. This should not be attempted on an ad hoc basis, but should use the knowledge elicitation and modelling techniques mentioned in Chapter 3. The Fluid Modelling System, as discussed in Chapter 5, can help improve the focus of results, as well as making possible the addition of more detailed, specific failure modes.

4.5 Specific Hazards Flagged Indiscriminately

In the most basic qualitative, fault propagation-based version of AutoHAZID, faults and consequences are paired up and reported solely on the basis of whether a valid fault propagation path can be found between them. This means that the faults and consequences are constrained only by their location in the plant (associated with a particular piece of equipment) and by the SDG which (potentially) provides a causal path between them.

In reality, many hazards are dependent on other factors, such as the nature of the fluids in the plant, as well as the equipment items present and their connectivity. An obvious example is the fire hazard posed by a leak of fluid out of the process. This can only be a true hazard if the process fluid contains a flammable component – a leak of water would not pose a fire hazard.

Clearly, if a tool such as AutoHAZID is not able to refer to information telling it whether the material is flammable or not, it must either report every leak as a fire hazard, or ignore fire hazards altogether. Therefore, information about the properties of the process fluids is used to decide the relevance of specific faults and consequences in the plant model.

This capability has been present in AutoHAZID since an early stage. Initially, the information stored on fluid components included a small number of characteristics which a fluid either possessed or lacked, such as "flammable", "toxic", "corrosive", *etc.* When a fault or consequence was conditional on one of these properties, reference was made to the library of fluid properties for each component of the relevant process fluid.

Now, the fluid modelling system contains more data on the fluids present in the plant model, and has access to a wider variety of information (numerical as well as logical) on the chemical components present in those fluids. The newer system is described in Chapter 5. However, the objective is still to verify specific hazards by reference to fluid properties, in order to make the HAZOP report more interesting and reduce the bulk of irrelevant false positives.

4.6 Hazards do not appear where expected in HAZOP report

Users of the AutoHAZID program who are experts in traditional HAZOP often criticise the form, or order, of the results produced by HAZOP emulation. A typical comment is "Why doesn't the program identify this hazard next to this deviation?". There is probably no acceptable solution to this problem, because experts will disagree over where any specified scenario should be identified, which is largely a matter of personal taste.

AutoHAZID's efforts to make the output table more readable (Section 4.4) partly cause this problem and partly improve it. Sorting process units into lines arranges the HAZOP results into an order which makes more sense to a human reader. However, filtering out repetitions in the report, which vastly reduces the volume of output, sometimes causes deletion of a "preferred" reporting of a hazard.

It would be possible to apply further rules to the report generator in AutoHAZID, so that the program would report certain classes of hazard next to "appropriate" deviations. Such a facility could perhaps be customised to particular user preferences. However, this was never a priority during STOPHAZ, and was never implemented.

4.7 Change the Format of the AutoHAZID Report

A radical approach to reducing the bulk of the results produced by AutoHAZID is to consider abandoning the HAZOP table as a vehicle for these results. Since the results are really only a set of fault paths, linking initiating faults to final deviations or consequences, the faults and consequences could be tabulated against one other, without stating the intermediate deviations.

Alternatively, a graphical user interface could be developed, allowing the user to interactively browse through the fault paths with full access to the fault propagation chain as well as the terminal events. The fault tree is another model of how results could be presented.

Although none of these ideas were developed into software during STOPHAZ, it seems clear that much of the effort made by users to read the results of AutoHAZID could be saved if they were presented in a more concise and usable format.

4.8 Models in AutoHAZID not applicable to early HAZOP on PFD

There is no fundamental reason why a tool like AutoHAZID cannot be used to perform HAZOP-like analyses at an earlier design stage, on PFD-level plant descriptions. Although there was no serious attempt to apply AutoHAZID to PFDs, it is clear that identifying safety problems at this stage can save a lot of time and money.

A PFD is essentially the same kind of input as a P&ID, with less detail on it. The main problem is likely to be that the models developed for HAZOP analysis of P&IDs concentrate on problems of components on a fairly detailed level. Output from the system when examining a PFD may therefore not be very interesting or informative due to lack of detail in the PFD description.

There may also be a problem with PFDs in that the items on the PFD may not correspond to single items in the AutoHAZID library of equipment models. What is required is probably a set of models covering operations at the level of detail likely to apply to PFDs. One issue to be addressed is how to link these models to the existing hierarchy of equipment models. Another is to what extent the PFD models would correspond to functionally distinct "modules" performing well-defined unit operations, specified at quite a high level, in the plant.

4.9 Qualitative Ambiguity

The problem of ambiguity is one that faces all qualitative modelling systems and has been introduced, in general terms, in Section 2.2.2. This section discusses how ambiguity causes problems for AutoHAZID, mainly through increased complexity in graph search.

An example of the ambiguity of qualitative addition, which often occurs in AutoHAZID, is the problem of deciding what flow deviations occur in the branches of a divider or header as a result of a pressure deviation in one of the branches. To resolve this ambiguity requires information (possibly numerical) on components connected upstream and downstream. Sometimes, using higher level qualitative mass balance constraints can reduce ambiguity, as reported by Fanti *et al.* (1993).

It should be noted that this inability to incorporate higher level constraints is due to a great strength of the SDG models in AutoHAZID, namely locality. It is not desirable to build balance constraints into otherwise completely local unit models, but some approach to automatically generating these sorts of constraints, at the level of the plant model, may be useful.

AutoHAZID is not a rigorous qualitative simulation package. It simply attempts to implement hazard identification techniques, searching for evidence that a hazard is possible without simulating the hazard in great detail. Most of the time, ambiguity is a nuisance rather than a threat to the integrity of the results produced. The result of ambiguous models is that the program over-reports hazards which may in fact not exist, rather than missing out hazards.

4.9.1 Multiple Paths in the SDG

The most important type of ambiguity in the SDG is related to the problem of multiple paths between nodes in the graph. Given two process variable nodes, A and B, searching the graph exhaustively may yield a number of paths, of various lengths, from A to B. Each of these paths can be associated with an overall effect of A on B, either a "+" or a "–". There is no guarantee that all the paths found will have the same overall influence, so they may contradict one another.

In assessing the paths produced by exhaustive search, the first task is to eliminate those paths that represent "unreal", or physically impossible, scenarios. The remaining paths may represent "real influences" between A and B, operating *via* a number of alternative causal mechanisms.

Further analysis of how these causal paths relate to one another is not a simple matter. They could be treated as simultaneous and potentially competing influences in the plant, or as alternative (mutually exclusive) situations, only one of which is relevant at a time. This level of analysis is not addressed in AutoHAZID at present.

If possible, the real influence paths should be assessed in terms of their relative strengths of influence, so that the dominant influence between A and B can be identified. At this stage, the most dominant path may be chosen as the only one to proceed with, or a number of the more dominant influences could be considered.

A number of problems arise with this theoretical model for search path evaluation. Most importantly, there is no secure way of deciding within the program if a given path represents a real or unreal influence between variables. Therefore, much of the effort in this area has to be put in during model design and implementation, well before any HAZOP search. In searching the SDG, AutoHAZID must assume that all paths it finds are equally "real". Secondly, the question of comparing paths to find the more dominant influences may be possible in theory, but is not supported by any existing data or models for causal strengths in the SDG.

In the absence of information to allow the strengths of influences to be determined and compared, the path which represents the worst case from a safety point of view can be chosen. Frequently, however, identifying the worst case is not possible until the expansion of all fault paths has been completed, which means that the computational costs of searching the SDG cannot be reduced in this way.

The simplistic approach to the problem of multiple paths used in AutoHAZID is to take the set of paths produced by exhaustive search and eliminate all but the ones of shortest length in terms of number of SDG arcs. The resulting set may still contain more than one path, and these paths may themselves predict contradictory influences between the variables A and B. From the point of view of qualitative hazard identification, however, all that matters is the overall influence between the variables. If this is still ambiguous, AutoHAZID must proceed with the assumption that both influences are possible. This may cause problems with the credibility of the results obtained, of course. This "shortest path heuristic" is discussed further in Section 4.10 and, elsewhere, by Chung (1993).

4.9.2 Cyclical Paths

If the nodes A and B are the same in the above discussion, then the paths produced are cycles in the SDG. Sometimes, these represent the influences that a deviation in one variable has on that variable itself, but this is not always the case. Because the presence of cyclical paths in the SDG is ignored by the search algorithm used in AutoHAZID, models are very often designed to take advantage of this feature. In such cases, no cyclical influence is intended by the model designer.

An example is the frequent use of one variable to propagate deviations in both upstream and downstream directions using the same set of nodes. This situation is illustrated quite well in Figure 4.3 in Section 4.10, where flow nodes are chained together by pairs of arcs forming tight cyclical paths in the SDG at each point along the chain. Making use of such an arrangement is practical, provided that the algorithm used to search the graph ignores the presence of cycles.

Real plants certainly do include real cyclical influences. They are in operation in every feedback loop in the plant, including many of the physical processes as well as the control loops which maintain the plant at steady state.

Cyclical paths are ignored in the search procedure in AutoHAZID because they potentially lead to fault paths of infinite length. It is also rather difficult to deduce anything from the presence of a cyclical path unless some of the numerical properties of the feedback system are understood, so that questions of dynamic behaviour and stability can be answered.

In other work, feedback loops (particularly control loops) have formed an integral part of the decomposition of plant models, in Shafaghi *et al.* (1984), for example. There may be some value in identifying feedback in the plant in order to simplify the analysis of behaviour, but this idea has not so far been developed within AutoHAZID.

4.9.3 Ambiguous Predicted Flow Deviations

Within the flow path modelling system in use within AutoHAZID models, pressure deviations can give rise to changes in flow. However, it is often impossible to check whether reverse flow (*revFlow*) or simply reduced flow (*lessFlow*) are possible in a given scenario, because of lack of specific (numerical) information about the cause. At other times, both deviations are genuinely possible given the situation as specified. In either case, ambiguous predictions are produced.

One must bear in mind also that deviations of process variables are defined in terms of their sufficiency to cause some final consequence. The sufficiency of each deviation can only be judged in the context of a complete fault path, and may depend on the magnitude of the deviation or on other factors, including the nature of fluids in the plant. Therefore, the sort of uncertainty shown when we cannot decide which of *revFlow* or *lessFlow* occur, is an example of the more general problem of deciding the magnitude of deviations in a fault path. The issues of reasoning with fluid properties and the quantitative magnitudes of deviations, in order to assess the sufficiency of fault paths generated by SDG search, are discussed further in Section 5.3.

4.10 Shortest Path Heuristic Not Sound

The shortest path heuristic is a rule that considerably simplifies the job of simulating fault propagation in the SDG. It states that the shortest path between any two nodes in the SDG is the dominant one and should therefore be taken as the effective path of influence in the model.

This means that when AutoHAZID expands paths by backwards chaining search, to find the causes of a variable deviation, it takes notice only of the shortest path leading from a particular node or fault to the deviation of interest. The program may find more than one path with the same length, so all of these are accepted as equally valid, but all longer paths are rejected.

The shortest path heuristic does away with most of the ambiguity in influences between variables in the plant model, but sometimes two or more shortest paths can be found, including paths with differing overall influences. In this case, AutoHAZID reports that both deviations of the final node can be caused by the initial cause.

In addition to its effect on ambiguity, the shortest path heuristic helps to control the complexity which would otherwise affect the efficiency of search. The problem is that we have no reliable theoretical foundation or guidelines to support the use of the heuristic, just the observation that it works most of the time. Interestingly, there are very few problems where the shortest path heuristic produces an answer which is actually wrong. An example is shown in Figure 4.3.

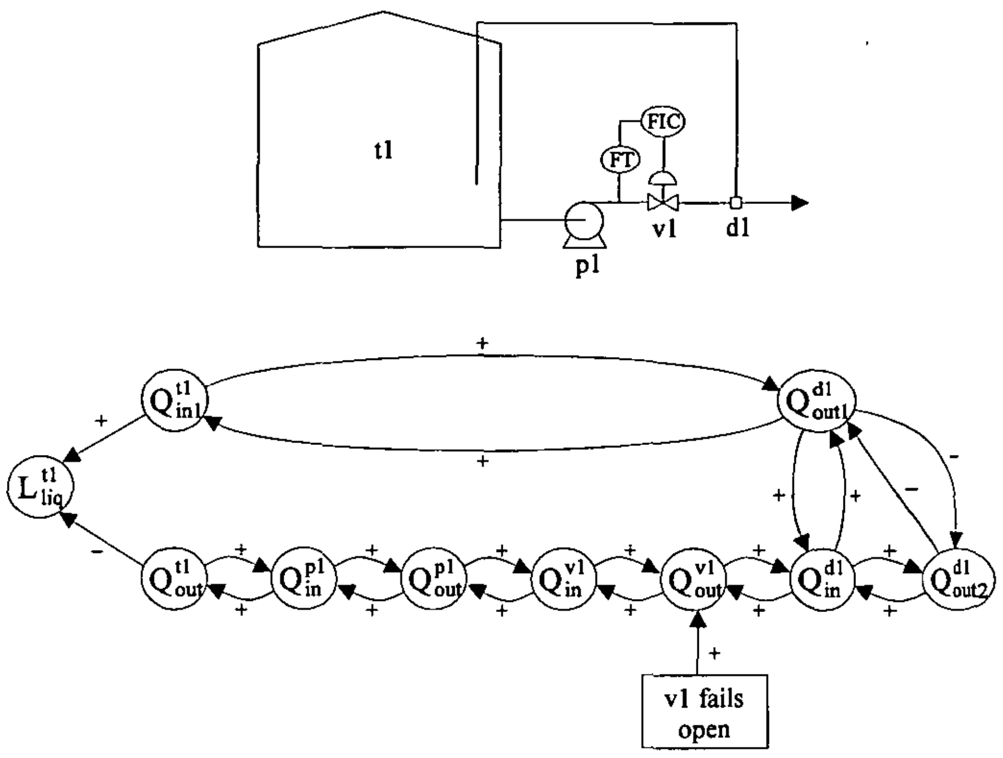


Figure 4.3 : Problem Plant for the Shortest Path Heuristic

In this constructed example problem, liquid is being pumped out of the tank t1 using pump p1, through the valve v1. A spill-back line is shown from the divider d1, taking a proportion of the liquid back to the tank. Other inlets and outlets from the tank are not shown in this example. Considering how the level in the tank is affected by the valve v1 failing open, it is most likely that the flow downstream of d1 increases, causing the level in the tank to drop. However, depending on what units are connected downstream of the divider d1, the flow could also remain constant.

The plant SDG in Figure 4.3 is simplified to show only flow (Q) and its effect on level (L) in the tank t1. For clarity, this example does not use the flow modelling technique described in Section 3.5, but similar examples have been used to demonstrate the occurrence of the same problem with AutoHAZID models which do use the flow path templates.

In searching backwards from the level node, two paths are discovered which lead back to the fault, "v1 fails open". One depends on upstream propagation of flow deviations through v1 and p1, to t1 at the main outlet of the tank. The other path propagates flow downstream *via* v1 and the divider d1, through the spill-back line and into the tank t1.

The former path is the correct one, leading to a low level in the tank – what we would expect if the valve were to open fully. However, the propagation path *via* the spill-back line is the shorter one (5 arcs, compared to 6 for the other path), so it is the one which is reported. That is, in this example, the valve failing open is reported as a cause of an increase in the tank level.

In AutoHAZID, this problem is solved using rules which are activated by the HAZOP algorithm itself. The rules look out for situations where a path has been found which propagates deviations through the "feedback" section of a loop, from an event in the "forward" section of the loop. If such a path exists, in conjunction with another path having a contradictory influence and not using the feedback section of the loop, then the longer path is adopted in preference to the potentially erroneous shorter one.

The use of ad hoc rules for fixing problems like this is not very palatable, especially when they are resident in the inference engine part of the system, rather than embedded in the model system. It may be that there is little option in this case, because of the non-local nature of the problem – the real behaviour of the tank level depends on a mass balance over the elements of the loop which cannot be expressed in the unit models at a local level.

One reason for the success of the shortest path heuristic is that models are usually designed in the knowledge that the heuristic will be applied. That is, the modeller makes the assumption that the shortest path is the most valid, as well as the most efficient, link between nodes in the SDG. Therefore, good practice in modelling means using the minimum number of arcs necessary to represent the influences present in the unit, without allowing false influences to be created in the model by unintended paths.

Even assuming that models are constructed using the best practice in modelling, the question still remains: "Why does the shortest path between two nodes in the plant SDG usually represent the correct causal influence between them?"

To look at the problem in more detail, the first thing to note is that the plant SDG consists of a number of mini-SDGs, representing equipment items connected by links which correspond to stream connections between the equipment items. All the stream connection links are parallel sets of SDG arcs connecting variables in one unit to the same variable in another unit. The "cross-over" between variables, representing interesting physical influences, takes place within the units themselves.

Next, we observe that the shortest paths between node pairs within the same unit are likely to be correct because the models were designed in this way, with all variables visible to the model builder at the same time. It should be part of the methodology used whenever constructing or updating models of equipment, that every distinct pair of nodes in the model is checked to see that there is at most one shortest path between them. The influence represented by this shortest path must also be correct (or at least feasible), and appropriate for the model.

Given these observations, we can go on to examine how alternate paths between two nodes, a_i and b_j, arise in the plant SDG. If a_i and b_j are present in the same unit, then the shortest path must be the correct one, as the model builder made it so.

If a_i and b_j are in adjacent units, then these units are connected by a stream, represented by a parallel set of arcs, each arc linking a propagation variable in one unit to the same variable in the other unit. The simplest case is shown in Case I of Figure 4.4, where node a_1 in unit A is connected to a_2 by a shortest path of 0 or more arcs. a_2 in unit A connects to b_1 in unit B *via* a single arc, and b_1 is connected to b_2 *via* a shortest path of 0 or more arcs.

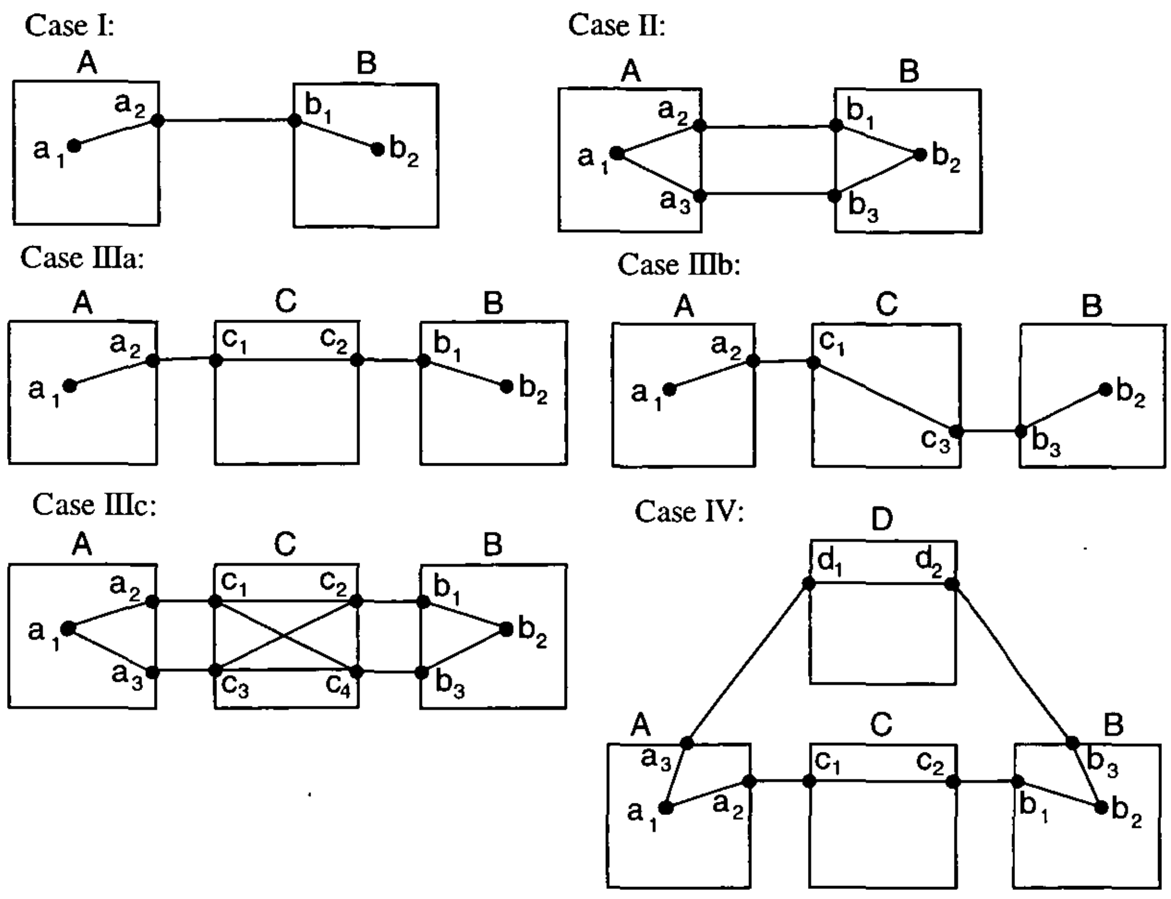


Figure 4.4 : Propagation Paths between Units

Since the shortest path between nodes in the same unit is designed to be the only valid influence between those variables, the path between a_1 and b_2 in Case I must be a valid one. For a particular variable (*e.g.* pressure, temperature) propagating between units A and B (as represented by [a_2-b_1] in Case I above), there is only one arc linking the two units. Thus, there can be a maximum of one path per propagation variable linking the nodes present in adjacent units, and this path is valid.

This does not prevent there being another path between a_1 and b_2, *via* some other propagation variable, as shown in Case II. Each path is a feasible causal influence, by virtue of the argument for Case I above, but there is no guarantee that [a_1-a_2-b_1-b_2] and [a_1-a_3-b_3-b_2] will be the same length.

If the two nodes are separated by any number of intervening units in series, as in Case III, there are at least two subclasses to consider. Firstly (Case IIIa), if there is no cross-over within the intermediate unit C, then propagation goes straight through C and the system is equivalent to Case I. Secondly, if the propagation crosses over from one variable to another within unit C, as in Case IIIb, the path [c_1-c_3] is still a valid shortest path and a valid path in C between those nodes, by virtue of the same argument as before. Therefore, the path [a_1-a_2-c_1-c_3-b_3-b_2] is valid.

Systems where there is more than one unit interposed between units A and B can be dealt with in the same way as Cases IIIa and IIIb. Case IIIc shows that, as units are increasingly separated, there is more scope for ambiguity. In this case there are four possible paths between a_1 and b_2, all of which can be shown to be valid. Not all of these will necessarily have the same length or path influence, so some will normally be neglected using the shortest path heuristic.

A similar argument to that used with Cases IIIa, IIIb and IIIc, can be used for the example of Case IV, which is similar to the example problem of the tank in Figure 4.3 above. The propagation paths *via* unit C and *via* unit D are both equally valid as far as the information in the SDG models is concerned.

Thus, to make an informed judgement of which paths are appropriate, all possible paths should be examined, and information outside the scope of the pure SDG model is required. The information required should support the evaluation of which paths are most “relevant”. This question could involve some evaluation of the relative strengths of causal influence in candidate paths, or assessment of time-based aspects of the system, such as transient behaviour and ordering of the events which may occur, rate information, *etc.* As mentioned in Section 4.9.1, causal analysis of this depth was never attempted in AutoHAZID.

It should be noted that preliminary results with AutoHAZID indicate that the shortest path heuristic can be made into an “option” without too many computational penalties. Comparing the results of running the program on the test case plant reported by Lawley (1974) reveals that without using the shortest path heuristic, the HAZOP report produced is not much more bulky, and the HAZOP run time is only doubled.

Analysing the Lawley results file reveals that the only problems caused by the loss of the shortest path heuristic concern the flow path templates used in the plant. The flow path allows two conflicting paths linking pressure and flow, one of which is eliminated by the shortest path heuristic. Therefore, the predicted flow effect due to a pressure deviation sometimes operates in the wrong direction. The use of the shortest path heuristic has been effectively designed into the flow path template (see Figure 3.5). Unless an alternative flow path model can be produced without multiple internal paths, it is impractical to discard the shortest path heuristic.[2]

4.11 Computational Complexity

The problem of complexity has been described in general terms in Chapter 1. It is not clear whether the complexity of the search space examined by AutoHAZID is exponential, or less complex than that (*e.g.* polynomial). This judgement is dependent on the nature of the SDG, which in turn is ruled by the connections in the plant model and the models of equipment items in it.

It is easy to see that an upper bound on the branching factor for any given plant can be identified, as the maximum branching factor in units within the plant. For a range of plants of various sizes, using the same library of unit models, the maximum may be identified as the maximum branch factor of nodes in equipment items modelled in the library. Therefore, the branching factor has an upper bound which is not dependent on size of the plant model, so that the search procedure is definitely not "super-exponential".

Considering the topology of typical plants, and the corresponding SDG topology, it seems that much of the plant consists of straight-line propagation, without much branching. Most branching occurs within major equipment models. This suggests that,

[2] If the flow path template were the only case where multiple internal paths occurred, then it might be possible to discard the shortest path heuristic, if some means were provided to filter out the ambiguities. To date, we do not know how widespread multiple internal paths are, so the wisdom of making such a change is doubtful.

even if the complexity of search in the graph is exponential, the overall branching factor per arc should be quite low.

Some figures for average branching factor calculated from the arcs forming plant models of two example plants, are given in Table 4.2 below. The branching factor in both forwards and backwards directions has been calculated as follows. Firstly, the number of nodes in the SDG having at least one branch in the appropriate direction, is counted (this is the "number of nodes" figure). Then, the total number of branches offered from these nodes is counted, and divided by the number of nodes, to determine an "average branch factor" for the appropriate direction.

	Lawley Plant	Benzene Plant
Forwards Branch Factor:		
Number of Nodes	690	2662
Average Branch Factor	1.80	1.66
Backwards Branch Factor:		
Number of Nodes	639	2548
Average Branch Factor	1.94	1.73

Table 4.2 : SDG Branching Factors for Example Plants

These calculated figures seem to indicate that, if the search is exponential, the branching factor for search in either forwards or backwards directions is about 2. It seems likely that the complexity in the search that actually takes place during HAZOP is not actually so severe, because whereas these branching factors would imply quite a severe limitation on the size of the plants that can be analysed, such a limit has not been encountered so far.

It is also worth noting that the variables in the plant SDG form weakly connected sub-networks for propagating deviations between units, and are not inter-linked at every point. Indeed, the only points of contact between (say) temperature propagation and pressure propagation may be at major units where a significant unit operation occurs. For this reason, the average branching factors given above may not be representative of the SDG search required in HAZOP emulation.

The problem of complexity in AutoHAZID SDG search can be tackled in a number of ways:

- Particularly important, for reducing the potentially enormous branching factors which could make search much more difficult, are sensible conventions for modelling which eliminate unnecessary cross-linking between variables. If possible, branching fault paths should be limited to modelling phenomena within complex units, rather than being a commonplace feature of the fault propagation pathways throughout the plant model.
- The AutoHAZID HAZOP emulation algorithm was rewritten, to cut down on the amount of repeated search work that was being done with the old version (see Appendix B). The search for causes of HAZOP deviations is now a two-stage process: let L_I be the list of nodes corresponding to variables of interest in the HAZOP study. In a first stage, AutoHAZID expands paths for causes of deviations in the node, as far as the nearest other node also in L_I. When this has been done for each node in L_I, the program takes the partial paths produced by the first stage and combines them into full paths from faults to final deviations. This algorithm considerably reduces the search required for HAZOP.
- The shortest path heuristic can help to reduce the amount of work done in the second stage of the HAZOP search algorithm, and the number of resulting completed fault paths. This works by removing partial paths where they share the same starting point as other shorter partial paths for the deviation being examined. As discussed in Section 4.10, the shortest path heuristic is not a particularly sound rule of inference, but it does seem to work effectively and has been in operation for the whole time that AutoHAZID has been in development.
- The HAZOP search is usually exhaustive and finds all the paths in the SDG, no matter how long they are. AutoHAZID can also operate in a mode where a fixed limit to the length of the fault paths is prescribed. In this mode, as soon as a path reaches the specified number of arcs in length, the algorithm does not attempt to expand it any further. Good results can be obtained with this (non-rigorous) method, but there is a small possibility (in theory) that some relevant hazard scenario may be overlooked.

- The SDG can be pruned to remove arcs which are not required by the HAZOP. This reduces the number of arcs present and therefore reduces the time taken to look up nodes in the SDG. Under certain conditions, pruning the SDG can also cut the amount of search done, if it can be shown that such search will produce no results of interest to the HAZOP study requested. There may be no consequences of interest in a particular part of the graph, for instance, which may justify removing arcs from the SDG.

4.12 Concluding Remarks

The strengths of the SDG are related to its weaknesses. Computational efficiency is achieved by using a representation based in the middle ground of representational strength, between simple digraph models and some more highly structured model of causal mechanism in the physical plant. It is a weak but efficient representation.

Very frequently, the way an equipment model is constructed is the cause of the problems encountered with it. In these cases, all that may be required to side-step the problem is a rethink of the approach used in producing the model. This can only be done on a case-by-case basis and the evidence in favour of a large scale redesign of the system, to solve numerous problems of a fundamental nature, must be accumulated over some time, to justify such a redesign.

Fluid models will be used to focus the applicability of the output generated by the program. The problem is the quantity and paucity of output from the simple SDG model, where scenarios in reality may be valid only for specific conditions/circumstances in the plant. Additional expertise is needed, to improve the judgement of AutoHAZID by tempering the qualitative fault propagation with quantitative calculation or estimation. This may be achieved by links to the physical properties calculation packages, or making arcs in the SDG conditional in places.

The next chapter addresses the inherent limits of the purely qualitative approach and proposes a method for making use of quantitative information related to fluids in the plant, which is implemented in the fluid modelling system.

Chapter 5 : Conditionality in Fault Path Modelling and the Fluid Modelling System

Chapter 4 (in particular Sections 4.1, 4.3, 4.5, 4.9 and 4.10) has demonstrated that, for many important hazard identification problems, the qualitative SDG models of AutoHAZID are insufficient. This is an inherent limitation of the SDG, which allows the representation of only qualitative information in the AutoHAZID models.

This limitation is addressed in AutoHAZID using the fluid modelling system, which is described in this chapter. First of all, the issue of how to improve the results produced by AutoHAZID, is discussed, in Section 5.1. The approach chosen is to add more specific faults and consequences to the models in the SDG, and to control how these are reported in the HAZOP report by adding conditions to arcs, faults and consequences in the SDG. By verifying the conditions present in completed fault paths, using properties of fluids present in the plant, the validity of generated scenarios can be checked.

The fluid modelling system is described at length in Section 5.2, which explains the approach of fault path validation and the system of functions and predicates which implements this validation method. Section 5.2 also describes how the different subsystems making up the FMS are integrated.

An interesting application of the FMS is to monitor the quantitative limits on deviations in fault paths. This allows some scenarios to be ruled out because the deviations present can be demonstrated as not severe enough to cause the final consequence. This approach is illustrated in Section 5.3 using five case study problems. The chapter concludes with some overall comments on the FMS, problems encountered with it, and possible improvements for the future.

5.1 Improving on Fault Propagation

AutoHAZID uses "simple" fault propagation, where a fault is linked to a consequence by a linear strand of deviations, to formalise cause and effect in the development of a hazardous scenario. Real scenarios often do not match exactly with this model, so that the fault propagation method does not capture all details of the real situation. In such cases, careful analysis of the scenario is required, to ensure the most important features of the problem are captured in the model. An appropriate modelling methodology can help ensure completeness, as discussed in Section 3.5 and (later) in Section 6.4.

A difficult class of problems for the qualitative SDG system is where, at some stage, a combination of events or conditions is required for the scenario to develop. This "conjunction" of events corresponds to an "AND" gate in the fault tree for the development of the scenario. The basic SDG does not represent this sort of ("AND logic") step at all.[1]

If, for a recognised hazard scenario, no acceptable model can be constructed within the existing modelling system, one must consider what approach should be taken:

- Proceed with an unsatisfactory model. In this case, the hazard may be reported indiscriminately and the program may produce misleading output because it cannot apply the hazard model selectively enough.
- Abandon the new scenario and do not model it at all. This reduces the value of the results produced, because a hazard which may exist in some real plant cannot be identified by the HAZOP emulator.
- Enhance the model representation, by improving or replacing the SDG. This is a costly option, in terms of rewriting program code and equipment models. Forethought and planning are essential to avoid wasted effort and ensure an elegant and efficient solution to the problem. Often, new functionality can be added as an

[1] AND is sometimes presumed in modelling certain situations. For example, we may assume that alarms are ignored when identifying hazards and modelling their development.

optional feature, so that existing models can still be used. This approach reduces the risk associated with a change.

Some idea of how the SDG might be improved can be gained by analysing how existing models tend to fail when used for hazard identification. The usual signs of poor quality models are incorrect hazard identification and sparse reporting of interesting hazards in an otherwise uninteresting report, as discussed in Section 4.4.

Incorrect hazard identification, giving rise to an increased number of "false positive" results, may be due to:

- **Incorrect fault propagation arcs.** Where a particular arc in some equipment model can be identified as incorrect, the arc can be removed, or the equipment item can be remodelled in a different way. This sort of problem is detected by examining the HAZOP results critically and analysing the fault paths giving rise to suspect results. A number of tools provided in the AutoHAZID program itself can be used for this task.
- **Incorrect fault propagation paths that are locally sound.** Sometimes, one finds that every link in a fault propagation chain is locally valid, that each arc relates a variable to its neighbour in a valid way, but nevertheless the whole chain does not predict a real effect. This can occur because some higher level constraint, such as heat or mass balance, is not captured in the arcs concerned. Problems of this nature can be difficult to solve using localised causal relations, such as the arcs of the SDG, because the SDG does not carry much information between nodes.[2]
- **Indiscriminate reporting of hazards.** Some hazards can appear everywhere in a HAZOP report. This may be due to a fault or consequence being modelled as generally applicable, where it actually has a more limited scope in reality. In this case, a restriction/check on the applicability of the fault or consequence is needed.

[2] An example of a problem where the application of high level constraints resulted in the solution to an ambiguity problem, is discussed in Fanti *et al.* (1993). This was a case where local qualitative mass balances were not sufficient to unambiguously specify a system state, but higher level balance constraints solved the problem.

The most important issue to be addressed by any improvement to the SDG system is how to enrich the range of failure modes represented in equipment models. It must be possible to model highly specific faults and consequences within unit models, and to manipulate them so that they are only reported when relevant within the plant being examined. Therefore, the applicability of new faults and consequences should be made conditional on the context within the plant that makes them relevant.

The aim is to eliminate "blanket" reporting of hazards, by verifying the accuracy of fault propagation paths as far as possible. In this way, AutoHAZID can reduce the number of false or irrelevant hazards identified and it should become possible to model more interesting failure modes and hazards within the system. As a result, the number of interesting items in the HAZOP report should increase and its size should decrease, improving the richness and usefulness of the results produced.

Some terms will be used in the following discussion, which it may be helpful to define here:

- The objective is to enable AutoHAZID to produce highly focussed results, where all the hazardous scenarios reported are relevant and interesting in the context of the plant being studied.
- To do this, it is necessary to add more specific faults and consequences to the equipment models. Such faults and consequences provide more detail about the events concerned, compared to the generic faults and consequences often seen in AutoHAZID results. For example, one might consider reporting a "flammable leak to environment", rather than simply a "leak to environment".
- In order to prevent these more specific faults and consequences being reported indiscriminately, conditions are attached to faults, consequences and propagation arcs in the SDG. Such conditions must be satisfied (where present) for an arc to be valid in a fault path.
- Conditionality is the property possessed by arcs, faults and consequences which have conditions attached. Such arcs, faults and consequences can be referred to as conditional.

The factors of most use, in determining whether a hazardous scenario is feasible, are related to the types of fluids present. Luckily, information on the main fluids present in a plant is usually available in the process description for that plant.

Therefore, the first attempts to make SDG models in AutoHAZID conditional focussed on fluid-related factors, applying optional conditions to the faults and consequences in unit models. Using these conditions, the relevance of a fault or consequence could be checked when it was processed in a fault path. Once conditions had been applied to faults and consequences, it was a short step to allowing fault propagation between nodes to become conditional too.

Using the present "fluid modelling system" (FMS) to evaluate these conditions, scenarios in the basic SDG models can be tested during the HAZOP search, reducing ambiguity. The particular case of checking the magnitude of deviations in propagation chains, to reject infeasible chains, is discussed in Section 5.3.

In designing the FMS, care was taken that the library of qualitative equipment models could still be used in AutoHAZID without change. This means that conditions are optional - changes to models are made as and when new conditions are added to existing arcs, or new arcs are added. Also, the (highly efficient) graph search algorithm was not removed. It is used to produce fault paths in the SDG, which are then evaluated by the FMS. Conditions are evaluated whenever they are encountered in a fault path, and if any condition is found not to be valid, the fault path is removed. The HAZOP reports produced by AutoHAZID are more focussed as a result of this filtering.

This form of conditionality in the SDG is important for any hazard identification system which attempts to model potentially complex hazardous scenarios. The FMS, described in the next section, uses information about units in the plant model, fluid properties and quantitative data to verify the correctness of fault paths produced by search on the SDG.

5.2 The Fluid Modelling System

The earliest attempts at making the SDG conditional in AutoHAZID involved simple properties of the fluids present in the plant model. The names of fluid components were specified in lists associated with particular units in the plant, thereby identifying which fluids could be present where in the plant. These named fluid components corresponded to pure compounds for which the early AutoHAZID system could look up data in a "fluid model library".

The early fluid model library (which is still a subsystem within the current FMS) included a few properties which a compound may or may not be deemed to possess. For example, the consequence `'environmental contamination'` is relevant only if the fluid present in the equipment is toxic. Properties of the fluids in the system, such as toxicity and flammability, were defined in this early work and some consequences were made conditional on the fluid in the equipment item having a certain property. For instance, if no component of the fluid in a unit had the property `toxic`, then the consequence `'environmental contamination'` would not be reported within that unit.

This early system did not allow specification of where in a piece of equipment the given fluids were to be found, and it used a very simple algorithm for propagating information about expected fluids to other units. All fluid components in a unit were passed on to downstream units, which led to problems in heat exchangers, for instance - the program predicted that the shell and tube-side fluids would mix and that all downstream units would receive the same mixture. The present FMS associates fluids with ports in the equipment items, so that the fluids in the shell and tube sides of a heat exchanger are kept distinct unless an interface failure occurs.

The FMS is now quite a general-purpose rule system, which maintains information about currently applicable fluids at each point in a fault path, as well as allowing calculations to be included in rules. The sort of rules in the FMS include, but are not limited to, reasoning about numerical properties of the fluids present. Systems are included for dealing with logical operations, arithmetical comparisons and, most importantly, a number of different software systems for answering queries about fluids are integrated into one system.

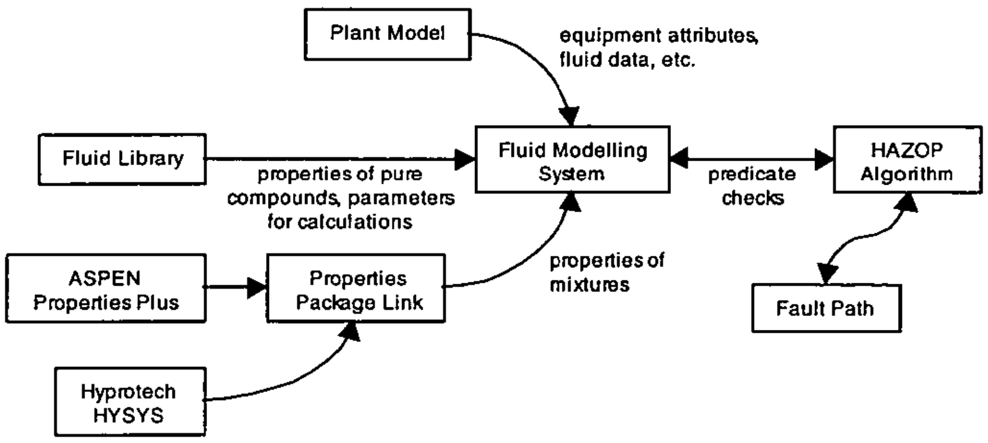


Figure 5.1 : Fluid Modelling System and associated Information Sources

A schematic view of the FMS subsystems and some of their associated data sources, is given above, in Figure 5.1. The various elements of the system will be described more fully in the sections which follow:

- Section 5.2.1 outlines the principle of fault path validation, which forms the basis of what the FMS does.
- The propagation, through the plant model, of user-supplied information about fluids is described in Section 5.2.2.
- Rules in the FMS make use of predicates and functions, which are described in Section 5.2.3.
- Section 5.2.4 outlines the types of information needed by the FMS to evaluate predicates and functions, including details of the "current fluids" in the plant.
- The integrated subsystems of the FMS are discussed in Section 5.2.5, which describes the evaluation of predicates and functions, as well as examining some operating system issues in the HAZID system.
- Section 5.2.6 describes the information stored in the fluid library, a precursor to the FMS which is still used as an information source on fluids.

- The calculation of fluid properties, by external packages and within AutoHAZID, is the subject of Section 5.2.7.
- The reactivity group-based system for detecting fluid compatibility problems has an interface in the FMS, which is described in Section 5.2.8.

5.2.1 Fault Path Validation

The chains of influence produced by SDG search during HAZOP emulation are known as "fault paths". They are validated by checking conditions attached to the faults, consequences and arcs, using calculations, qualitative and quantitative information. Rules are therefore defined to specify the checks to be performed.

The validation checks are activated in the HAZOP algorithm by the function which verifies completed paths produced by the search algorithm: `acceptable_path()`. The meaning of each condition is such that, if it is proven to be false, then the arc which contained the condition is no longer considered to be valid and the fault path containing that arc is removed. If the FMS cannot prove a condition to be false, even if this is due to a lack of data, then the condition is deemed to be true – this is to ensure that scenarios aren't rejected unless it is known for sure that they are not feasible.

It is also possible to associate a list of conditions (rather than a single condition) with a fault, consequence or arc, so that all conditions in the list must be satisfied for the fault, consequence or arc to be valid.

Validation proceeds by taking the fault path as a whole and evaluating the condition (if any) attached to the fault at the start of the path. If this condition fails, the fault path is rejected. Otherwise, each arc in the chain is examined in turn, and any conditions present are evaluated, until the last link in the chain is reached.

In general, the last arc in the chain need not be connected to a consequence – the same validation technique is used to check partially constructed paths during HAZOP emulation, and paths created by "causes of a deviation" queries raised by the user. If the last arc in the fault path does link to a consequence, however, then any condition on the consequence is evaluated as a final step in the validation check. If all these tests succeed, then the path is accepted, otherwise it is rejected.

5.2.2 Fluid Information and its Propagation

Information loaded into AutoHAZID from the plant description may include details of the intended fluids in the plant, either within individual equipment items or flowing between them. The system has been designed to respond in the absence of fluid information, but normally this information would be specified.

The fluid information is associated with ports, which may be defined as inputs to a unit, outputs from it, or internal locations within the unit. The following information may be given:

- "Amount" of fluid. For streams between units, this is the flowrate, in kg/hr; for internal ports it is the inventory of the fluid, in kg.
- Names of chemical components in the fluid and their mole fractions.
- Pressure, in bara.
- Temperature, in °C.

This information is presented to the program in `intendedFluids`, `portPressures` and `portTemperatures` slots in the plant model. `intendedFluids` slots provide information about the "amount" and composition of the fluid in question. Within the program, this information is stored in `Location` objects, one for each port in the unit where some information is known. The `Location` class is described in Appendix D. Any fields which are not known within the `Location` objects are given a special `undef_number` value.

Fluids do not have to be specified for every place in the plant model. A procedure known in AutoHAZID as "fluidisation" is used to infer, from the data given, other information about the fluids in the plant. By propagating information about fluids forwards in the plant wherever possible, using rules for managing incomplete data, the maximum use can be made of the information given, and data will then be available wherever the fluid identity has been inferred.

The connectivity of the plant, which determines where fluid can go and where it cannot, is defined in terms of `[unit,port]` locations linked by SDG arcs propagating the variable `composition`. This variable was chosen because it seemed that, of all the variables in the models, composition most closely mirrored the propagation of fluids themselves. In particular, composition is (usually) only propagated in one direction – the downstream direction of flow. The connectivity information extracted from the SDG is stored in a `Net` object.

When fluidisation finishes, `Location` objects corresponding to all the places in the plant where something is known about the fluids present are put into `info` slots with the name "`location`". This information is referred to in later analysis by the FMS.

A number of principles are observed when propagating fluids throughout the plant:

- Data may only be propagated between ports which are directly connected by a single link in the fluid connection network.
- Fluid propagation never overwrites the information specified in the plant model, so that information may only be propagated from `Location L1` to `Location L2` if the relevant property is known at `L1` and not known at `L2`. If properties are unknown, they are stored with the value `undef_number`.
- Propagation of flowrate information is considered separately from pressure, temperature, composition and component names. This is because flows can be added together at branch points, whereas the other properties cannot.
- Non-zero flowrates may be propagated directly downstream in unbranched lines.
- Flowrates in dead-end sections of the plant must be zero. If any non-zero flows are found in dead-end parts of the plant, they are reported and fluidisation fails. In this case, the fluid information is not propagated in the plant model at all. Units which comprise legitimate inlets or outlets for fluids in the plant are labelled in the unit

model library and checks are defined to decide whether a dead-end exists upstream or downstream of a given location.

- Flowrates can be summed at branches, so that if both inlet flows to a header are known, then the outlet flow is calculated. Similarly, if two of the flows at a divider are known, then the third is calculated. Whenever performing such a mass balance, the program checks for dead-end legs in the branch, assigning zero flowrates if appropriate and indicating an error if an impossible situation is found.
- Properties other than flow can be propagated to points immediately downstream in the plant (excluding places where two or more fluids are mixed together) if the relevant property is not known at the downstream point.
- Where two streams come together, for example at a header, if one of the inlet legs is a dead-end line upstream (with a zero flowrate) then all fluid properties may be propagated from the other inlet to the outlet.
- If both inlet legs of a header have a non-zero flowrate, then the only data which may be inferred for the outlet are the flow and the list of names of components. The latter is found by the union of the lists of components given at the inlets to the header. Suitable calculations, or calls to flowsheet simulator packages, could be used in the future to estimate the other properties of the fluid mixture.
- If an internal port in a unit is connected to an output port and there is some property (other than flow) which is present in the output port but absent in the internal port, then that information can be propagated to the internal port. A small weakness with this "fluid rule #1" is that there is no check for contradictory data in other output ports attached to the same internal port. Therefore, inconsistencies in data are not detected at such branchpoints and the first data found will be propagated. This problem is illustrated in Figure 5.2, for the outlet temperatures of a fluid leaving a vessel. Future improvement in this rule is quite straightforward.
- If, for a pair of two internal ports within the same unit, each port is directly linked to the other in a cyclical formation, then data for pressure and temperature which is known for only one location can be propagated to the other location. This rule is applicable for the ports `vap` and `liq` in Figure 5.2 if, when the temperature of `liq` has been determined, the temperature of `vap` remains unknown. In this case

the rule would assign the same temperature value to `vap` as to `liq`. This "fluid rule #2" can only be used where other propagation methods have failed.

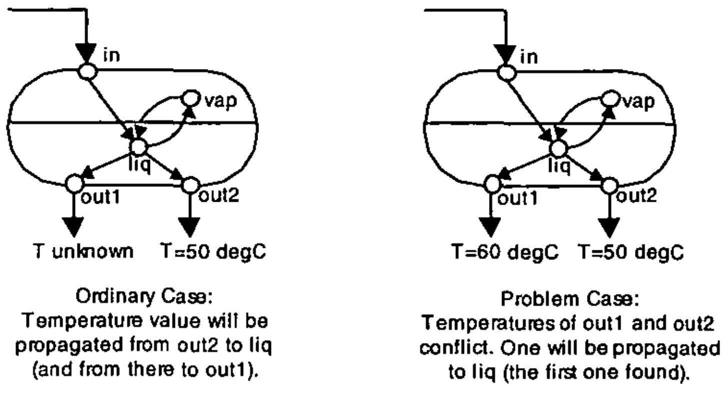

in
vap
liq
out1
out2
T unknown
T=50 degC
Ordinary Case: Temperature value will be propagated from out2 to liq (and from there to out1).
in
vap
liq
out1
out2
T=60 degC
T=50 degC
Problem Case: Temperatures of out1 and out2 conflict. One will be propagated to liq (the first one found).

Figure 5.2 : Inconsistent plant data cause problems for fluid rule #1

The principles outlined above seem fairly sound, and have produced good results in case study plants and units studied so far. However, there are areas where the default behaviour of the algorithm, when no data is given, could cause problems. Examples include the case where no discharge pressure is given for a pump, or where no outlet temperature is provided for a heat exchanger. In these cases, the inlet fluid data are propagated through the unit, because the algorithm presently makes no check that some expected data in the unit are missing.

5.2.3 Functions and Predicates

The validation tests introduced in Section 5.2.1 above rely on a system of predicate and function definitions in the fluid modelling system. These allow the FMS to integrate various different subsystems, used for deciding whether a condition is correct or for locating or calculating physical property information about the plant.

The term "predicate" is used here to describe a logical condition which evaluates to either `true` or `false`. The predicate has a name (sometimes referred to as its "functor") and a number of arguments (or parameters), which define information needed by the system in order to decide whether the predicate is true or not.

An example of a predicate is `flammable(Port)`, which is used to decide whether the fluid present at a given port in the plant model is flammable or not. Here, `Port` is a variable (symbols with initial capital letters are variables, as in the Prolog language) which can be given a value, such as `'out'`. When the arguments of the predicate are given values, the FMS can evaluate the condition and return an answer (`true` or `false`). Predicates may sometimes be defined without arguments, in which case the brackets are usually omitted.

The FMS also allows the definition of "functions". These look similar to predicates in that they involve a name and a list of arguments given in brackets, but they return values which may be of any type in general. Each function returns a particular data type, but this can be anything which fits in with the types defined for the `DObject` class. These types are listed in Appendix D and include constants, integer and real numbers, lists, strings and "structures", similar in form to predicate calls. The FMS functions allow the person defining predicates to do a limited amount of computation[3] using function calls within the predicate definition.

An example of an FMS function is `get_fluid(Port)`, which consults the plant model to find the fluid at the given port location and returns the data known about the fluid in a specific structure. The structure used corresponds to the data stored in the `Location` object class. Another example is `vapour_pressure(Fluid)`, which takes an argument in the same format as that returned from `get_fluid(Port)` and returns the vapour pressure of the fluid at its temperature and pressure (these data are provided within the `Fluid` argument).

Within the FMS, some special predicates and functions are defined which can be used in a shorthand form as "infix" operators. These correspond to the commonly used operators for arithmetic and logical operations and numerical comparisons, and can be used in between the items on which they operate. In addition to their infix form, each

[3] The computation possible within the FMS is limited in the sense that iterative loops and recursion are not permitted.

operator has an appropriate "longhand" form, using the convention that the name of the function or predicate starts with the prefix "op_".

Operators make the definitions of predicates and functions far more readable to the user than otherwise might be the case. They are listed in the table below, which gives the "infix" form, its "longhand" equivalent and the operator precedence which applies to that operator.

"Infix" operator	"Longhand form"	Operator Precedence	Description
*	op_mult	12	Arithmetic multiplication.
/	op_div	12	Arithmetic division.
+	op_add	10	Arithmetic addition.
-	op_sub	10	Arithmetic subtraction.
<	op_lt	8	Numerical 'less than'.
>	op_gt	8	Numerical 'greater than'.
<=	op_le	6	Numerical 'less than or equal to'.
>=	op_ge	6	Numerical 'greater than or equal to'.
==	op_eq	4	Test for equality. Requires that both arguments evaluate to the same value.
!=	op_ne	4	Test for inequality.
&&	op_and	3	Logical AND.
||	op_or	2	Logical OR.
=	op_assgn	1	Assignment of a term to a variable. The term on the right side of the operator is evaluated and its value is assigned to the variable on the left side.

Table 5.1 : "Infix" operators in the Fluid Model System

The precedence of an operator determines with what priority it binds to the terms on each side of it. An operator with a high precedence number is considered to bind to terms on its left and right sides before operators of lower precedence within the same formula. This idea (of precedence) is most familiar in connection with the addition and multiplication operators in algebra, where "3+5×6-5" is interpreted as "(3+(5×6))-5", for example.

The details of how competing operators are bound to their arguments when reading formulae into the program, as well as the processing of parentheses (brackets), are dealt with in the parsing codes developed for the program in newparse.cpp. These functions allow data compatible with the `DObject` class to be read directly from strings of characters, stored in `Str` objects.

The functions and predicates used in the arcs of the SDG are defined in the start of the unit model library, using `predicate()` and `function()` statements. These specify the name and arguments of the function/predicate as a "functional prototype" format, containing dummy variables for each of the arguments. Also specified is a type string, which maps the function or predicate that is being defined onto a specific system which is able to evaluate it:

- `"C"` – If the type string is the letter C, the function or predicate is defined within the AutoHAZID program. Thus, when it is evaluated, the query goes to a specific C++ function in the program which produces the appropriate result.
- `"V"` – If the type string is a V, the query is handled by the fluid rule system, developed in STOPHAZ by VTT. This has a separate handler function which maps these queries to rules in that subsystem of the FMS. Only predicates may be specified in this way.
- `"D"` – If the type string is D, then the function or predicate is defined in terms of other functions or predicates, and the definition is given following the type string. This definition takes the form of a list of functions or predicates to be evaluated, to determine the value of the function or predicate being defined.

The `function` and `predicate` statements in the unit model library are read into the program at start-up, and are stored in two lists for later reference by the FMS. Using these lists, the FMS can access the types and definitions of all known functions and predicates in the program. If a term, in either a unit model or a predicate definition, does not match with the "prototype" pattern stored for some item in these lists, then it cannot be evaluated as a FMS function or predicate.

A full record of the functions and predicates so far implemented in the fluid model system, is given in Appendix E, which attempts to give a very short summary of the items, and also classifies each of them into one of a number of groups:

1. Logical operations
2. Mathematical operations
3. General-purpose operations
4. Plant, fluid and fault path data access
5. Limit data access
6. Combining fluids (including compatibility checks)
7. Properties of single fluids
8. Consequence evaluation
9. Contamination
10. Design parameter checks
11. Miscellaneous physical checks
12. Leakage checks and limitations
13. Checks on VLE pressure limitations
14. Pressure deviation limits corresponding to resistance changes in flow paths

5.2.4 Information used in Fault Path Validation

In evaluating the predicates attached to the faults, consequences and arcs of a candidate fault path, the FMS uses two forms of information:

- The name of the predicate and values for its arguments are given in the condition as it appears in the unit model or in the fault path. These allow the form of the predicate appearing in the fault path to be matched against the definitions of known predicates stored in the program.
- A set of "context information" is also used in evaluation. This consists of data which are required so often that they are best supplied routinely by the FMS.

The same two types of information are also used to evaluate the FMS function calls which may appear in the definitions of type "D" predicates.

Since conditions are most often used to validate fault paths, the fault path object (class `FPath`, described in Appendix D) stores most of the context information needed for

FMS evaluation. The procedures for updating context information in `FPath` objects are also called from the code which validates the fault path objects:

- `FPath` stores a full list of the arcs in the propagation path. This allows access to the initial fault and final consequence, if required, during validation of any part of the path.
- The "current fluids" present at each point in the fault path are stored, as well as information on the limits of process variable deviations for those fluids. The latter information is used to solve the problems described in Section 5.3.
- Some information is stored on the classification, categorisation and ranking of the fault path. This information is calculated using methods and rules developed by Prof. Lees and Dr. Larkin within the STOPHAZ project.

In addition to the above "context" data, the name of the unit in which the condition currently being examined is resident, is also used. This data is not stored in the `FPath` object, as the `FPath` usually refers to a number of process units along its propagation path, and so cannot be readily associated with one single unit.

An important distinction in the FMS is between "nominal fluid data" and "current fluid data". The nominal fluids are the fluids in the plant under normal operation (*i.e.* in the absence of deviations). This information contains fluid data provided in the input model loaded into AutoHAZID, plus the information inferred by the "fluidisation" routine described in Section 5.2.2.

"Current fluid data" is a term used here to denote the conditions of fluids in the plant when a fault has occurred, *i.e.* at points along the fault path currently being examined. This information is derived from nominal fluid data, with property differences arising from contamination events or deviations in temperature and pressure, for example.

Fault path validation requires that the conditions at each link in the chain be evaluated in relation to fluids which are expected to be present at the relevant locations in the supposed fault scenario, rather than fluids which would be present there in normal operation. Thus, each `FPath` object maintains a list of `Location` objects to store this current fluid data. The current fluid data associated with ports can be examined or changed by the program during validation.

It is important to take account of the differences which may arise between nominal and current fluids during fault path validation, when determining how current fluids information propagates forwards in the plant. Differences may arise due to contamination events, or due to deviations in the values of process variables. AutoHAZID includes a prototype system to track the limits in numerical deviations of pressure and temperature during scenario development. This method is outlined in Section 5.3.

5.2.5 Integration of Fluid Model Subsystems

The fluid modelling system (FMS) provides a uniform way for AutoHAZID to make use of the various software subsystems developed by different partners in STOPHAZ, using predicate conditions on arcs in the SDG. Some of the queries handled by the FMS are directly related to fluids and their properties. Others relate to plant model data and some have a more general-purpose nature, providing the arithmetical and logical "glue" which allows complex checks to be formulated.

An additional complication is that AutoHAZID has been developed for use in both UNIX and Windows. Some parts of the system are not available in UNIX, and some external parts of the software system in a Windows environment may not be available at run-time, so the FMS must deal with this in producing the best available answer.

A sensible integration strategy should make the best use of available subsystems and data in answering fluid queries. If the FMS is not able to determine a predicate, it should default to returning an answer which enables HAZOP emulation to be completed, and only allows hazards to be rejected if they can be proven not to be feasible.

The subsystems involved in the FMS are outlined as follows:

- An important internal part of the FMS, implemented by C++ functions, is the set of general purpose operations in logic and arithmetic, including the operators described in Section 5.2.3. These allow convenient expression of the checks and evaluations needed to formulate FMS conditions.
- A number of properties of pure compounds are provided in the fluid library and read into AutoHAZID when it starts. This is the earliest version of the fluid model still in HAZID and is described in Section 5.2.6.
- Physical properties of mixtures and pure compounds are determined by calling on external packages such as Properties Plus or HYSYS, *via* a "Properties Package Link" (see Section 5.2.7).
- Alternatively, some properties of mixtures may be estimated by calculations within AutoHAZID, using data provided in the fluid library.
- The fluid rule system developed by VTT is an internal part of AutoHAZID, but was not developed at Loughborough. It is implemented as a subsystem for resolving predicate tests within the FMS.
- An external information source is used for the fluid compatibility checks developed by VTT, as outlined in Section 5.2.8. The data required is accessed through the functions of the database API and consists of a "reactivity group matrix", giving information about adverse reactions between fluid components.
- The internal model of the plant, constructed from the data read into AutoHAZID from plant descriptions and the unit model library, is an important source of information for resolving the FMS queries. It includes details of the fluids present in the plant and of the attributes of various units.

5.2.5.1 Outline of Function and Predicate Evaluation in the FMS

As noted above, the evaluation of a function or predicate in general relies on context information in addition to its arguments. Therefore, the C++ functions which evaluate these terms have a common list of arguments which communicates the context information between them. This common list is shown below for the function `evaluate()`, which is used to evaluate both functions and predicates:

```
DObject evaluate(
    const DObject& D1, BindList& BL1, FPath& FP1, const Str& UName)
```

In the above, the function or predicate to be evaluated is the argument `D1`. A list of variable bindings currently in force is given in `BL1` – the first thing that happens when a term is evaluated is that the bindings list is applied to `D1`. The `FPath` object `FP1` represents the fault path in which the function or predicate call occurs. It can be used to access the data on current fluids or on the arcs in the fault path. The contents of `FP1` may be changed by the evaluation, particularly the list of current fluids. Lastly, the argument `UName` gives the name of the unit in which the function or predicate is evaluated.

The "handler functions" which make up the system for evaluating FMS conditions, are outlined in Figure 5.3 below. The purpose of these functions is to determine the appropriate subsystem for resolving a query and to manage the call to that subsystem, providing arguments as required and handling returned values. The figure below shows only the relationships between the handler functions (in terms of which functions call which others) and omits the many functions which do the work of evaluating functions and predicates of the FMS.

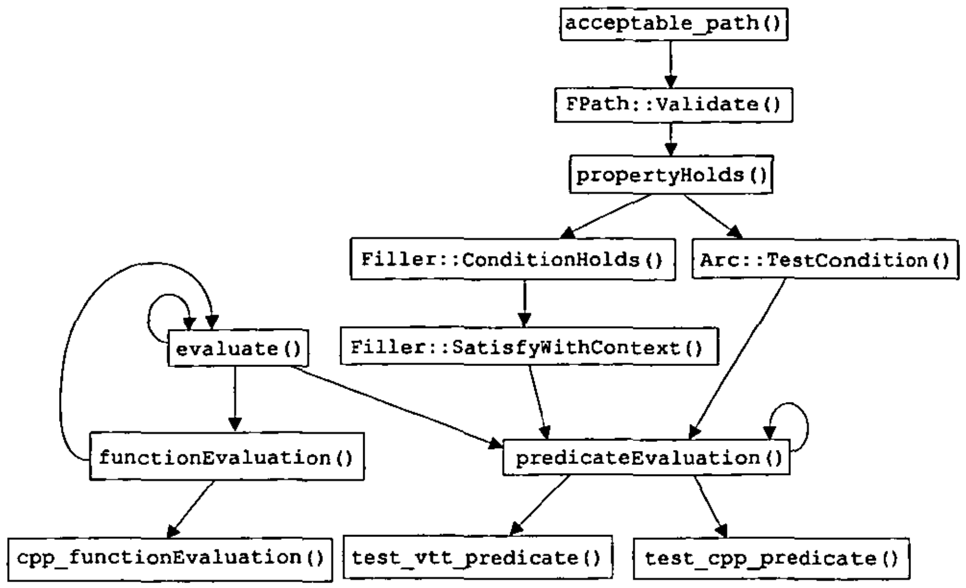


Figure 5.3 : Evaluation "Handler Functions" in the Fluid Modelling System

A brief summary of each of the main functions shown above, is given below:

- `acceptable_path()` – This is the function used to validate every one of the fault paths generated by graph search in the HAZOP algorithm.
- `predicateEvaluation()` – All types ("C", "V" and "D") of predicates are evaluated by this function. In the case of type "D" predicates, all the terms in the definition list for the predicate are tested, by recursively calling `predicateEvaluation()` – each evaluation must return `true` for the predicate to succeed.
- `test_cpp_predicate()` – The various predicates evaluated by C++ functions are handled by this function. Most of the C++ functions called are defined in the file `unitdata.cpp`.
- `test_vtt_predicate()` – This function deals with type "V" predicate queries passed to the VTT developed fluid rule system. The details of the processing that goes on in this subsystem are beyond the scope of the work described here, and will be described elsewhere by Perttu Heino of VTT (Heino, 1999).
- `evaluate()` – This is the general purpose evaluation function, which deals with evaluation of all types of intermediate FMS predicates and functions. It is called

by various C++ functions which evaluate type "C" functions and predicates, as well as the links shown in the figure above. Whenever an expression in the parameter list of some predicate or function requires evaluation, this is the function that is used. If it finds that a term cannot be evaluated as a function or a predicate, it returns the term unchanged.

- `functionEvaluation()` – This function manages the evaluation of FMS functions of types "C" and "D" (FMS functions of type "V" are not supported). In the case of a type "D" function, each term in the definition list of the function is evaluated in turn (by calls to `evaluate()`) and the return value of the function is the result of evaluating the final term.
- `cpp_functionEvaluation()` – FMS functions of type "C" are evaluated by this function. It manages calls to a number of C++ functions, defined in file `fns.cpp`.

The FMS is accessed at present from only two places. The first is the fault path validation code which operates during the HAZOP analysis of a plant model. This results in calls to the `predicateEvaluation()` function originating ultimately from the function `acceptable_path()`, as shown in Figure 5.3.

The second point of access to the FMS is a user option ("Evaluate a function/predicate") on the main menu in AutoHAZID, defined in the C++ function `opt_doEvaluation()`. This option requests a term from the user for the program to evaluate as a function or predicate, as well as an appropriate unit in whose context the term is to be evaluated. The original term, and its evaluation, are displayed to the user after evaluation has been attempted. This menu option makes use of the general FMS evaluator function, `evaluate()`.

Functions may be embedded in a predicate by appearing as values in the argument list of a predicate, or by appearing in the body of the predicate in an assignment or comparison statement, such as:

```
P = vapour_pressure(Fluid)
```

In the latter case, the function call appears as the second argument of the assignment operator (`op_assgn(P,vapour_pressure(Fluid))`), so the two cases are actually equivalent. Function evaluation therefore occurs when the arguments passed to a predicate are being evaluated.

5.2.5.2 Operating System Dependencies and Availability of Software Packages

AutoHAZID is written so that it compiles equally well for Windows and for UNIX. Wherever some part of the program needs to be different under Windows, compared to UNIX, "conditional compilation" selects the appropriate part of the code to compile. As far as functions and predicates in the FMS are concerned, however, the main issue is the availability of external software packages in Windows and UNIX.

Compatibility checks for fluid interactions (see Section 5.2.8) are not available in the UNIX version of AutoHAZID because the reactivity group table is present in the PC based database used to store plant descriptions from the Graphical Tool. Therefore, the UNIX version of AutoHAZID always produces a blank report in response to calls to the FMS function `compatibility_check(F1,F2)`. Compatibility checks are available for all versions of AutoHAZID under Windows.

The availability of an external package in which physical property calculations can be done (see Section 5.2.7) is determined at start-up when the program may attempt to link to a particular package as directed in its configuration file. The user is notified of whether a properties package was detected by the program and if a link was successfully made to it.

When a property package link is active in AutoHAZID, the function `physical_property_request()` attempts to evaluate queries using that package. If no link is present, or if an initial query to the external package fails, the function uses any appropriate C++ based routines in AutoHAZID to evaluate the query.

The availability of the properties package links is determined by the following considerations:

- If the operating system is UNIX, links to these packages do not exist in the current version of AutoHAZID.
- If the operating system is Windows 3.1, then the packages cannot be accessed because they rely on library functions accessed in 32 bit libraries, and Windows 3.1 is a 16 bit system.
- If the operating system is Windows NT or Windows 95, which are 32 bit systems, then the physical properties packages can be accessed from AutoHAZID, provided the following conditions are satisfied:
    - The user has one of the packages installed, HYSYS or Properties Plus.
    - All the libraries (`.DLL` files) required for the package are resident in the same directory as the AutoHAZID executable files (`HAZID7.EXE` and `HAZID.EXE`).
    - The configuration file, `hazpaths.dos`, is set up correctly, with the variable `PropPackageType` set to either `ASPEN` or `HYPRO` and the appropriate variable (`ASPEN_DLL` or `HYPRO_DLL`) set to point to the library file for the package which is to be used.

The system for deciding physical properties requests is discussed in Section 5.2.7.

5.2.6 Fluid Library Information

Physical data on pure compounds are stored in a fluid library file and read into the program at start-up. These data are stored in `Fluid` objects and can be accessed later, when required to answer a FMS query. Additionally, the fluid library is used to store parameters required for calculations to estimate certain physical properties, such as Antoine constants to estimate vapour pressure. A third use of the fluid library is to store data on reactivity groups needed by the compatibility checking code for determining unwanted fluid interactions (see Section 5.2.8).

Since the fluid library only contains information on specific pure compounds, it is of limited use when applied to determining accurate property values for mixtures. However, if appropriate "safe" assumptions are used in combining data on pure compounds, then good use can be made of the information available.

The data stored in the fluid library, for each pure compound, are:

- CAS Number.
- Average Molecular Weight, g/mole.
- Freezing Temperature, °C.
- Decomposition Temperature, °C.
- Flashpoint Temperature, °C.
- Autoignition Temperature, °C.
- Lower Flammability Limit, (%v/v).
- Toxicity Classification, measured on a scale of 0 to 3, where the classes have the following meanings:
    - 0 Non-toxic (*e.g.* air, water)
    - 1 Slightly toxic (*e.g.* nitrogen, which can asphyxiate)
    - 2 Toxic (*e.g.* toluene)
    - 3 Very toxic (*e.g.* benzene)
- Latent Heat at normal boiling point, J/mole.
- Boiling Temperature at atmospheric pressure, °C.
- List of three Antoine Constants for vapour pressure estimation.
- Liquid Density, kg/m^3.
- List of four constants for the evaluation of vapour heat capacity, J/mole.
- ERPG_3 value, a measure of toxicity for the Dow exposure index, mg/m^3.
- Liquid heat capacity, J/kg°C.
- List of four reactivity group codes, for use in the compatibility checking routines (see Section 5.2.8).

Some of the data in this list are used in calculations of physical properties which can be used as alternatives to the external packages discussed in the following section.

5.2.7 Physical Properties Calculations

During the STOPHAZ project, links from AutoHAZID to external packages were explored, to provide access to the physical properties data and calculations typically used in flowsheeting packages. Links to Aspentech's Properties Plus and Hyprotech's HYSYS packages, were explored. The link to Properties Plus was successfully demonstrated during the project.

The interface to the properties packages was specified by ASPEN, in conjunction with Loughborough University. ASPEN developed the library of functions which provides common access to the routines in individual calculation packages.

The following are the property calculations specified by ASPEN:

- Physical State (C)
- Average Molecular Weight (C)
- Boiling Temperature Range (C)
- Freezing Temperature (C)
- Vapour Pressure (C)
- Viscosity
- Density (C)
- Enthalpy
- Specific Heat (C)
- Latent Heat of Fusion
- Latent Heat of Evaporation (C)
- CAS Number
- Phase Temperatures (for the given pressure, these are the temperatures where changes of physical state will take place).
- Phase Pressures (for the given temperature, these are the pressures where changes of physical state will take place).
- Flashpoint Temperature

- Autoignition Temperature
- Lower Flammable Limit
- Upper Flammable Limit

Access to the physical properties packages is provided through FMS functions and predicates in the same way as for other properties. Some of these properties can be calculated either in external packages or in C++ functions relying on data in the fluid library. These are indicated by a (C) in the above list.

Calculations for various types of flash were also specified as part of the physical properties system. So far these have not been used within the FMS.

The fluid properties provided by the external packages allow better estimation of the properties of mixtures than is the case with the data provided in the fluid library, or in calculations carried out within AutoHAZID itself. It is also likely that the level of quality and consistency provided by using external data is better than using ad hoc properties based in the C++ code itself.

5.2.8 Compatibility Checks for Fluids

Unwanted interactions can occur within the plant, particularly when fluid compounds are mixed together, either deliberately or inadvertently. These sorts of interactions depend mostly on the nature of the fluids which come together and are not particularly affected by the process equipment in which they occur.[4] Therefore, the plant models represented by the SDG are not very useful for modelling the wide range of phenomena caused by such interactions.

Part of the STOPHAZ project involved building a software module within AutoHAZID for predicting the effects of unwanted interactions in the plant. To predict these effects requires knowledge of which compounds are present. This information is available through the fluid information in the plant model.

[4] Of course, the consequences of such fluid interactions may depend on where in the plant they occur.

Detecting interactions requires some knowledge of the effects of mixing chemical components together. An attempt to capture this knowledge was made in STOPHAZ, using a reactivity group tagging scheme for classifying chemical species, combined with a compatibility table method for predicting the effects of mixing species together.

Each chemical species in the fluid is associated with up to four numeric identifiers that label it as belonging to a certain group of chemicals, having certain properties. Members of the same reactivity group will tend to behave in similar ways when mixed with chemicals belonging to another particular group. This is the basis of the "compatibility table" which tabulates the reactivity group identifiers against each other and records a set of effects in each cell in the table, which are the consequences of mixing chemicals from the corresponding two groups together. An example of the type of compatibility table used is given in Figure 5.4 below. The effects recorded are taken from the following standard set of consequence types:

- heat generation caused by component interactions
- gas generation caused by component interactions
- toxic interaction between components
- flammable interaction between components
- explosive interaction between components
- violent polymerisation due to component interactions
- solubilisation of toxic substances due to component interactions
- possible unknown hazard due to component interactions

By examining the components of a fluid, one can predict the possible interactions which will occur due to the chemicals present. This is the basis of the compatibility checks carried out in the FMS whenever two fluids are considered to mix together in the HAZOP algorithm. The checks are carried out by the FMS function `compatibility_check`, which calls a function written by VTT. The VTT code consults a table of reactivity groups and produces a report consisting of a list of effects taken from the list above, each one associated with a pair of component names, identifying the species responsible for the interaction. This report object is added to a global report using the FMS function, `add_to_compat_report`, so that all the compatibility check results produced during HAZOP can be collected into a single report.

The collected report is appended to the end of the main HAZOP report, rather than integrating the results into the HAZOP table at the point where they were produced. This is because of the many problems of storing reported interactions in association with the fault path from which they originated, and reporting these clearly within the HAZOP table. The compatibility report declares the fluids which mixed (including their locations in the plant), the interactions produced by mixing and the fluid components responsible for those interactions, for each mixing event considered.

Reactivity Group No.	Reactivity Group Name																																									
1	Acids, Mineral, Non-oxidizing	1																																								
2	Acids, Mineral, Oxidizing		2																																							
3	Acids, Organic		G, H	3																																						
4	Alcohols and Glycols	H	H, F	H, P	4																																					
5	Aldehydes	H, P	H, F	H, P		5																																				
6	Amides	H	H, GT				6																																			
7	Amines, Aliphatic and Aromatic	H	H, GT	H		H		7																																		
8	Azo Compounds, Diazo Compounds and Hydrazines	H, G	H, GT	H, G	H, G	H			8																																	
9	Carbamates	H, G	H, GT						G, H	9																																
10	Caustics	H	H	H		H				H, G	10																															
11	Cyanides	GT, GF	GT, GF	GT, GF					G			11																														
12	Dithiocarbamates	H, GF, F	H, GF, F	H, GF, GT		GF, GT		U	H, G				12																													
13	Esters	H	H, F						H, G		H			13																												
14	Ethers	H	H, F												14																											
15	Fluorides, Inorganic	GT	GT	GT												15																										
16	Hydrocarbons, Aromatic		H, F														16																									
17	Halogenated Organics	H, GT	H, F, GT					H, GT	H, G		H, GF	H						17																								
18	Isocyanates	H, G	H, F, GT	H, G	H, P			H, P	H, G		H, P, G	H, G	U						18																							
19	Ketones	H	H, F						H, G		H	H								19																						
20	Mercaptans and Other Organic Sulfides	GT, GF	H, F, GT						H, G									H	H	H	20																					
21	Metals, Alkali and Alkaline Earth, Elemental	GF, H, F	GF, H, F	GF, H, F	GF, H, F	GF, H, F	GF, H	GF, H	GF, H	GF, H	GF, H	GF, H	GF, GT, H	GF, H				H, E	GF, H	GF, H	GF, H	21																				
22	Metals, Other Elemental & Alloys as Powders, Vapors or Sponges	GF, H, F	GF, H, F	GF					H, F, GT	U	GF, H							H, E	GF, H		H, GF, F		22																			
23	Metals, Other Elemental & Alloys as Sheets, Rods, Drops, Moldings, etc.	GF, H, F	GF, H, F						H, F, G									H, F						23																		
24	Metals and Metal Compounds, Toxic	S	S	S			S	S			S														24																	
25	Nitrides	GF, H	H, F, E	H, GF	GF, H, E	GF, H			U	H, G	U	GF, H	GF, H	GF, H				GF, H	U	GF, H	GF, H	E				25																
26	Nitriles	H, GT, GF	H, F, GT	H							U											H, P			S	GF, H	26															
27	Nitro Compounds, Organic		H, F, GT			H					H, E											H, GF, F				H, GF, E		27														
28	Hydrocarbons, Aliphatic, Unsaturated	H	H, F			H																	H, E						28													
29	Hydrocarbons, Aliphatic, Saturated		H, F																											29												
30	Peroxides and Hydroperoxides, Organic	H, G	H, E		H, F	H, G		H, GT	H, F, E	H, F, GT		H, E, GT	H, F, GT					H, E	H	E	H, F, GT	H, E	H, G		H, G	H, GF, E	H, F, GT		H, P		30											
31	Phenols and Cresols	H	H, F						H, G										H, F			GF, H				GF, H					H	31										
32	Organophosphates, Phosphothioates, Phosphodithioates	H, GT	H, GT						U		H, E											H									U		32									
33	Sulfides, Inorganic	GT, GF	H, F, GT	GT		H			E										H												H, GT			33								
34	Epoxides	H, P	H, P	H, P	H, P	U		H, P	H, P		H, P	H, P	U								H, P	H, P	H, P		H, P	H, P					H, P	H, P	U	H, P	34							
101	Combustible and Flammable Materials, Miscellaneous	H, G	H, F, GT																			H, G, F				H, GF, F					H, F, GT					101						
102	Explosives	H, E	H, E	H, E					H, E		H, E			H, E								H, E	H, E	H, E	E	E					H, E	H, E		H, E	H, E	H, E	102					
103	Polymerizable Compounds	P, H	P, H	P, H					P, H		P, H	P, H	U									P, H	P, H	P, H	P, H	P, H					P, H	P, H		P, H			H, E	103				
104	Oxidizing Agents, Strong	H, GT		H, GT	H, F	H, F	H, F, GT	H, F, GT	H, E	H, F, GT		H, E, GT	H, F, GT	H, F	H, F		H, F	H, GT	H, F, GT	H, F	H, F, GT	H, F, E	H, F, E	H, F		H, F, E	H, F, GT	H, E	H, F	H, F	H, G	H, F	H, F, GT	H, F, GT	H, F, G	H, F, G	H, E	H, F, GT	104			
105	Reducing Agents, Strong	H, GF	H, F, GT	H, GF	H, GF, F	GF, H, F	GF, H	H, GF	H, G				H, GT	H, F				H, E	GF, H	GF, H	GF, H						H, GF	H, E			H, E	GF, H	GT, GF, H		H	GF, H	H, E	H, F, GF	H, F, E	105		
106	Water and Mixtures Containing Water	H	H						G										H, G			GF, H	GF, H		S	GF, H								GT, GF						GF, GT	106	
107	Water Reactive Substances	EXTREMELY REACTIVE! DO NOT MIX WITH ANY CHEMICAL OR WASTE MATERIAL*																																								107
		1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	101	102	103	104	105	106	107

Reaction Code	Consequences
H	Heat generation
G	Innocuous and non-flammable gas generation
GT	Toxic gas generation
GF	Flammable gas generation
E	Explosion
P	Violent polymerization
S	Solubilization of toxic substances
U	May be hazardous but unknown

Figure 5.4 : Reactivity Matrix for Fluid Compatibility Tests

5.3 Reasoning using Numerical Limits on Deviations

Fault propagation often produces paths which are not credible, because the magnitude of deviation required to cause a final consequence cannot be realised within the scenario produced by the fault concerned. To tackle this problem, a method has been developed within the FMS to model the propagation of numerical limits on the size of deviations in process variables.

This means that maximum and minimum limits for deviations caused by certain faults are available for propagation through the fault path. Conditions can also be attached to deviation-consequence arcs, so that the magnitude of the deviation is checked against some limit, to test if it is severe enough to cause the consequence.

The aim is to capture some of the more usual commonsense rules which a human team would use in a conventional HAZOP study. An attempt to identify some of these rules has been made (by myself and Prof. Lees) in the meeting documented in Appendix F. The rules so far implemented in the FMS, for limiting the size of pressure and temperature deviations, are listed in full in the table given in Appendix E. A subset of these will be discussed in the following subsections.

In the FMS, `Location` objects are used to communicate information about current fluids in the plant during fault path validation. The system for maintaining information on numerical limits of deviations makes use of the `Notes` field of the `Location` object, to manipulate limit values using functions and predicates in the FMS, such as `get_max_temperature()`, `set_min_pressure()`, *etc.*

The following subsections illustrate how reasoning with numerical limits works in relation to a number of case study problems. These examples show possible strategies for implementing solutions to complex plant modelling problems in the FMS generally, not just in relation to numerical limits on deviations. It is important to note the way a semi-formal analysis of the scenario is used as a starting point for considering how that scenario could be formalised in the rule system.

5.3.1 Example 1 : Design Pressure for Pumps and other Units

High pressure can cause the casing of a pump to rupture, but the high pressure is only considered relevant if it rises above the design pressure of the pump. This can often only be achieved by specific causes, possibly including dead-heading the pump, which occurs when there is a complete blockage in the discharge side of the pump, corresponding to a *noFlow* deviation.

As an example of the use of design pressure checks in the models, consider the following arcs, taken from a pump model:

```
arc([deviation,[morePressure,out]],1,
    [consequence,['possible casing overpressure rupture',
    exceed_design_pressure(out)]]),

arc([out,noFlow],1,[out,pressure],
    assign_max_pressure(out,full_dh_pressure(in,out))),
```

The predicate `exceed_design_pressure(Port)` checks the maximum pressure for the given port against the maximum design pressure (in the attribute "`max_allowable_pressure`"), to see if the design pressure is exceeded. This check is used to validate the overpressure rupture consequence. A similar predicate, `exceed_design_vacuum(Port)` checks the minimum pressure of a unit against the minimum allowable design pressure, to check for the possibility of vacuum collapse. These two predicates can be used for any unit, not just pumps. It is a convention of the plant database that design pressures and temperatures are stored in the attributes `max_allowable_pressure`, `min_allowable_pressure`, `max_allowable_temperature` and `min_allowable_temperature`.

The arc linking *noFlow* to *pressure* represents the rise in pressure caused by completely blocking the pump discharge. The maximum pressure in this case is the dead-heading pressure of the pump, added to the operating pressure at the inlet, and this limit is set by the `assign_max_pressure()` predicate attached to the arc. When the two arcs are present in a fault path, validation succeeds only if this limit pressure is sufficient to exceed the pump's design pressure.

Note that, in the absence of information determining the size of a pressure deviation, it is necessary for AutoHAZID to report overpressure rupture as a potential consequence wherever `morePressure` could occur. Clearly, when there is no information available for the fault path on the size of the pressure deviation, the program must cautiously predict that the consequence could occur.

5.3.2 Example 2 : Atmospheric Pressure is (approximately) 1 bara

When a pressurised vessel leaks to atmosphere and the pressure inside it drops, the minimum pressure reached is about 1 bara. Similarly, when a vacuum system leaks and air goes in, the pressure inside it rises to a maximum of around 1 bara.

These observations are of course, quite trivial, but it was necessary to introduce limits on pressure deviations caused by leaks, to reduce the number of spurious results in the HAZOP report. Leaks are identified as causes of pressure deviations in many places in the HAZOP reports produced by AutoHAZID. Pressure deviations are also frequently associated with equipment damage (*e.g.* vessel rupture, vacuum collapse).

Therefore, unless pressure limits are considered and handled correctly, leaks out of a process can be quoted as causes of vacuum collapse in a vessel, and leaks into a vacuum system can be quoted as causes of overpressure rupture. In reality, unless the pressure deviation crosses one of the design limits of the system, no mechanical damage will actually be caused.

In order to prevent spurious output, 1 bara is therefore stated throughout the model libraries as the numerical limit on pressure deviations caused by leakage faults. When this information is propagated to a pressure damage consequence for the plant, the limit can be compared to the design pressure of the vessel (as described in Example 1 above) and the fault path can be found to be invalid.

Two predicates have been developed to deal with these features of leaks. They are `pressureLeak(Port)` and `vacuumLeak(Port)` shown below. These have been attached to leak faults throughout the library:

```
predicate(pressureLeak(Port),"D",
[  pressurised(Port),
   assign_min_pressure(Port,1.0)
]).

predicate(vacuumLeak(Port),"D",
[  vacuum(Port),
   assign_max_pressure(Port,1.0),
   % Put air into the system, too ...
   add_air_contamination(Port)
]).
```

Notice that the above predicates test that the process is under pressure (or vacuum) before they apply any limit to the pressure deviation. Therefore, the faults to which these predicates are attached will only be considered where the process operates under pressure or under vacuum respectively. Also, leakage into a vacuum system not only increases the pressure, it also contaminates the process with air (which will often be more significant, from a safety point of view, than the pressure change).

5.3.3 Example 3 : Pressure Limits When Valves Open

The flow path model uses the idea of flow path resistance to model blockages in pipes and the effects of a valve being opened or closed. Resistance therefore has an effect on the flow through the unit and the pressures at its inlet and outlet.

When a control valve fails open or closed, there will be certain limits on the pressure and flow deviations caused by the failure. If the valve fails closed, the upstream pressure will rise and the downstream one fall, but it is not very easy to determine limits for the pressures in this case, without using information from equipment attached upstream and downstream of the valve.

When the control valve fails to an open position, the resistance falls to a minimum of zero, and the flow rises to some maximum value which is not readily determined without analysing the overall flow system in some detail. The pressures also change in response to the valve opening – the upstream pressure drops and the downstream pressure rises. However, a change in the resistance of the valve flow path never causes a pressure reversal, so that limits can be stated for the pressure changes which occur.

The downstream pressure at the valve rises, and an upper bound for this variable is the maximum value of the upstream pressure. By a similar argument, the upstream pressure falls to a minimum value determined as the minimum value of the downstream pressure. In reality, for zero resistance, the pressures would equalise at some value between these two pressures, dependent on the overall context of the valve in the flow system.

This is illustrated in Figure 5.5 below, where the shaded areas delimit the possible pressure profiles in the case of the valve in a normal position (a) and fully opened (b). The error bars on valve inlet and outlet show the minimum and maximum pressures, which define the range over which the equalised pressure could exist in the fully open case.

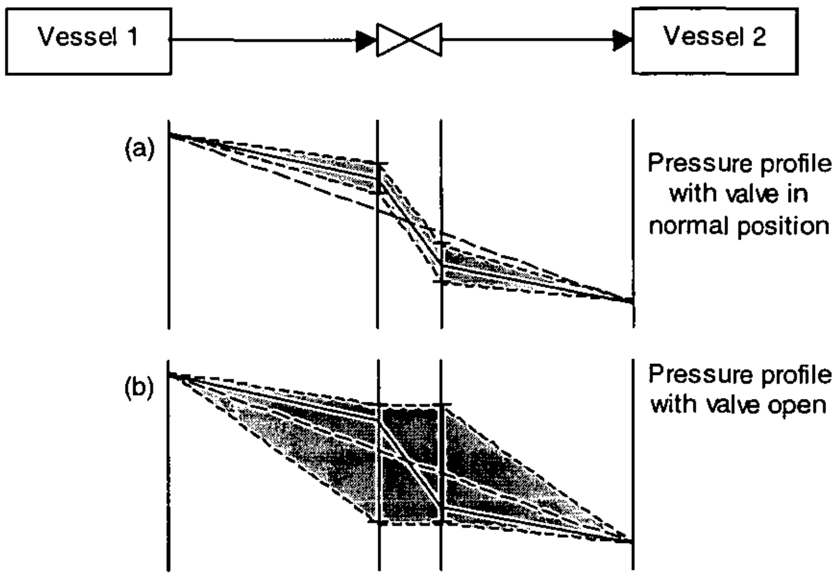

Vessel 1
Vessel 2
(a)
Pressure profile with valve in normal position
(b)
Pressure profile with valve open

Figure 5.5 : Pressure Profiles Around a Valve

It seems likely that this sort of reasoning about control valve failures can be applied in any flow path, wherever the resistance drops. Therefore, we can use the following two

FMS predicates to establish limits on pressure deviations resulting from changes in resistance within flow paths[5]:

```
/*
   Predicate to impose a limit on the pressure rise caused to a downstream
   port fluid by a change in the resistance of the flow port connected
   upstream to it. The max. pressure attainable when the resistance drops is
   the Max upstream pressure in the flow path, or the nominal upstream
   pressure, if there is no Max. value.

   This scenario corresponds to a valve opening full-bore, for instance.
*/

predicate(res_dsp_lim(USPort, DSPort), "D",
[  F1 = get_fluid(USPort),
   P1 = get_max_pressure(F1),
   P2 = cond((P1 == undef_number), get_pressure(F1), P1),
   assign_max_pressure(DSPort, P2)
]).

/*
   Predicate to impose a limit on the pressure drop caused to an upstream
   port fluid by a change in the resistance of the flow port connected
   downstream of it. The min pressure attainable when the resistance drops is
   the min downstream pressure in the flow path, or the nominal downstream
   pressure, if there is no min value.

   This scenario corresponds to a valve opening full-bore, for instance.
*/

predicate(res_usp_lim(USPort, DSPort), "D",
[  F1 = get_fluid(DSPort),
   P1 = get_min_pressure(F1),
   P2 = cond((P1 == undef_number), get_pressure(F1), P1),
   assign_min_pressure(USPort, P2)
]).
```

[5] Notes:

(a) The predicate names correspond (approximately) to "resistance determined downstream pressure limit" (for `res_dsp_lim`) and "resistance determined upstream pressure limit" (for `res_usp_lim`). Inventing short and descriptive names for predicates is often very difficult!

(b) The predicates include use of a "conditional" function, `cond(X, Y, Z)`, which tests the condition X; if X is true, `cond()` takes the value of Y and if false, the value of Z.

These predicates are attached to the arcs in the `flowpath` template, where there is a resistance effect on the appropriate pressure node (upstream or downstream), as shown in arcs 5 and 6 below:

```
% Flowpath from X to Z, where Y is used to label
% flow and resistance nodes :

template(flowpath(X,Y,Z),
   [
      % Propagation (flow path X->Z):

      arc([X,pressure],1,[Z,pressure]),          % (1)
      arc([Z,pressure],1,[X,pressure]),          % (2)
      arc([X,pressure],1,[Y,flow]),              % (3)
      arc([Z,pressure],-1,[Y,flow]),             % (4)
      arc([Y,resistance],1,[X,pressure], res_usp_lim(X,Z) ),        % (5)
      arc([Y,resistance],-1,[Z,pressure], res_dsp_lim(X,Z) ),       % (6)
      arc([Y,resistance],-1,[Y,flow]),           % (7)

      % Simple things for fluid flow :
      arc([X,temp],1,[Z,temp]),                            % (8)
      arc([X,composition],1,[Z,composition]),              % (9)
      arc([X,contamination],2,[Z,contamination]),          % (10)

      % Other things which happen by virtue of fluid flow. These arcs are
      % for propagating unintended phases, produced by phenomena elsewhere,
      % through the flow path :
      arc([X,solid],2,[Z,solid]),         % (11)
      arc([X,liquid],2,[Z,liquid]),       % (12)
      arc([X,gas],2,[Z,gas]),             % (13)
      arc([X,vapour],2,[Z,vapour])        % (14)
   ]
).
```

5.3.4 Example 4 : Methanol Cooler

This example (which is also discussed in McCoy and Rushton, 1997) relates to the methanol cooler shown in Figure 5.6 below, where hot methanol is cooled by water in a countercurrent shell and tube heat exchanger. The SDG model shown in Figure 5.7 correctly predicts that high flow or low temperature of the coolant causes a lower process fluid temperature. In the heat exchanger model this is linked to the possibility of the process fluid freezing. In this case, however, since the freezing point of methanol is -94°C, compared to 0°C for water, the cooling water will never succeed in freezing the methanol, because the water would have ceased to flow long before reaching the freezing point of methanol.

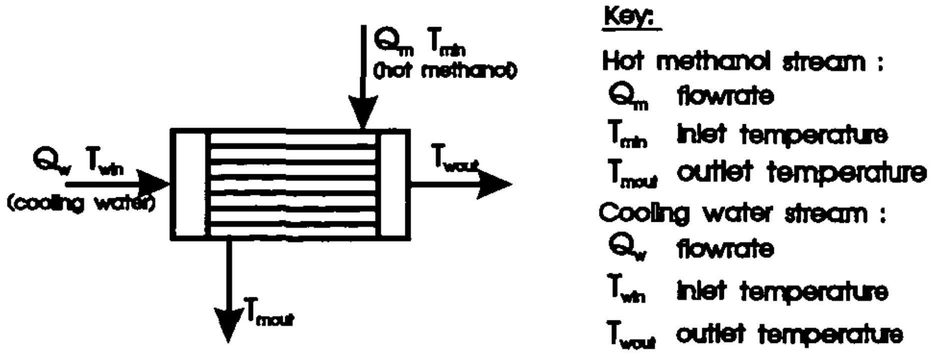

Q_m T_{min} (hot methanol)
Q_w T_{win} (cooling water)
T_{wout}
T_{mout}
Key:
Hot methanol stream :
Q_m flowrate
T_{min} inlet temperature
T_{mout} outlet temperature
Cooling water stream :
Q_w flowrate
T_{win} inlet temperature
T_{wout} outlet temperature

Figure 5.6 : Methanol Cooler and Associated Variables

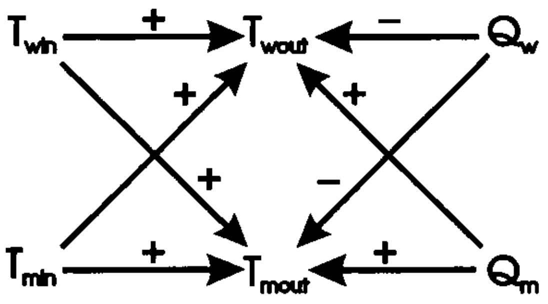


Figure 5.7 : Partial, Simplified SDG for Methanol Cooler

A solution to this problem is to enhance the SDG model of the heat exchanger with numerical information about the freezing points of the fluids present and rules for using this information. The consequence "process fluid freezes" is linked in the model to low temperature, T_{mout}. This is the coolest location for the methanol and is the place where it would start to freeze, if it became cold enough. Before deducing from the SDG that the fluid can freeze, the lower limit of T_{mout} must be evaluated and compared to the freezing point of the fluid. The test must be attached to the arc between T_{mout} and the consequence.

Two constraints govern the lower limit of T_{mout} in the arcs from T_{win} and Q_w. Firstly, cooling water must flow in order to reduce the methanol temperature. The cooling water will not flow at a temperature below its freezing point, so that the minimum water temperature at T_{win} is around 0°C. Secondly, in the cooler there is a constraint that the cooling water cannot cause the methanol temperature (T_{mout}) to fall below the value of T_{win}. From these two together, we can infer a minimum of 0°C for T_{mout}. These tests should be attached to the arcs from T_{win} to T_{mout} and Q_w to T_{mout}, and in conjunction with the test on the arc connecting T_{mout} to the freezing consequence, the consequence can be rejected as not possible.

The following two arcs model the effect of low temperature in a shell and tube exchanger causing the fluid to freeze:

```
arc([deviation,[lessTemp,tube]],1,
    [consequence,['freezing fluid blockage in tubes',
    fluid_can_freeze(tube)]]),

arc([deviation,[lessTemp,shell]],1,
    [consequence,['freezing fluid blockage in shell',
    fluid_can_freeze(shell)]])
```

The `fluid_can_freeze()` predicate above determines if the minimum temperature of the fluid at the given port is below its freezing point, defaulting to true if there is no minimum limit or no temperature is given for the fluid.

Unfortunately, the way heat transfer is currently modelled in the `shell_tube_exchanger` model (using the intermediate variable, `heatTransfer`) means that some of the links shown in Figure 5.7 above do not exist. Specifically, the $T_{win} \rightarrow T_{mout}$ and $Q_w \rightarrow T_{mout}$ arcs are absent. Therefore, it is impossible to implement the FMS conditions governing the ordering between temperatures on shell and tube side of the cooler, using the `shell_tube_exchanger` model.

However, in a suitable model which did possess the necessary temperature-temperature and flow-temperature links, the rules required to check freezing point information in the methanol-water case would look something like the arcs below:

```
arc([tube,temp],1,[shell,temp],
    assign_min_temperature(shell,get_min_temperature(tube)),

arc([tube,flow],-1,[shell,temp],
    assign_min_temperature(shell,freezing_temp(get_fluid(tube)))
```

In the above, the low temperature deviation in the tube is assumed to have been propagated to the exchanger with the necessary lower limit set at the freezing point of the fluid. Then, this limit is passed on to the shell-side fluid. In the second arc, the freezing point limit is imposed by the flow-temperature link. When fault propagation considers the freezing consequences for the shell-side (containing methanol), it discovers that the limit temperature for the shell-side fluid does not allow it to freeze, in the case of the methanol-water system. The ability of AutoHAZID to reject infeasible scenarios in such a plant has been demonstrated using a modified heat exchanger model.

5.3.5 Example 5 : Pressure Limits due to Vapour-Liquid Equilibrium

In a vessel containing liquid and vapour at the same time, there will be an equilibrium between the two fluids. If there are no inert gases present in the vapour space the pressure will be the vapour pressure of the liquid at the fluid temperature. In this case, one can determine limits on the pressure deviations expected for the vessel, resulting from deviations in the temperature of the liquid, if the temperature variations can be estimated.

The crucial condition for application of this limit calculation (for the upper limit of pressure) is that there should not be an appreciable partial pressure of inert gas in the vessel. Therefore, where nitrogen blanketing is used to maintain a non-flammable atmosphere, the calculation of vapour pressure is not so helpful, as the pressure of the nitrogen must be taken into account. Where inerts are effectively excluded, as may be the case in distillation, then the vapour pressure may be used.

The predicate `vle_pressure_limits()` can be used to calculate the pressure limits corresponding to temperature limits already determined, for a vapour-liquid system. It uses the predicates `vle_min_pressure_limit()` and `vle_max_pressure_limit()`:

```
/*
   Determine and assign the lower limit of vapour pressure to a vapour
   -liquid system represented by the fluids at the two ports given. Takes
   data from the liquid port L and determines its vapour pressure at its
   minimum temperature, assigning that value to the lower limit of pressure
   for the vapour port V :
*/

predicate(vle_min_pressure_limit(L,V), "D",
[
   F1 = get_fluid(L),
   (F1 != error),
   T1 = get_min_temperature(F1),
   P1 = cond((T1 == undef_number), undef_number, vp_at_given_temp(F1,T1)),
   assign_min_pressure(V,P1)
]).

/*
   Determine and assign the upper limit of vapour pressure to a vapour
   -liquid system represented by the fluids at the two ports given. Takes
   data from the liquid port L and determines its vapour pressure at its
   maximum temperature, assigning that value to the upper limit of pressure
   for the vapour port V :
*/
predicate(vle_max_pressure_limit(L,V), "D",
[  F1 = get_fluid(L),
   (F1 != error),
   T1 = get_max_temperature(F1),
   P1 = cond((T1 == undef_number), undef_number, vp_at_given_temp(F1,T1)),
   assign_max_pressure(V,P1)
]).

/*
   Predicate which establishes the limits on pressure due to vapour pressure
   in a system where liquid and vapour are in equilibrium :
   (L is the name of a liquid port, V is the name of a vapour port).

   It is assumed that the temperature of the system principally determines
   the vapour pressure. Calls on two subsidiary predicates, to establish
   lower and upper limits on the pressures.
*/

predicate(vle_pressure_limits(L,V),"D",
[  vle_min_pressure_limit(L,V),
   vle_max_pressure_limit(L,V)
]).
```

This predicate has been tested in models of storage vessels, but is not used in this context at the moment, because of the problem posed by inert gases. The predicate is typically attached to the arc connecting liquid temperature to pressure in the vapour space:

```
arc([liquid,temp],1,[vapour,pressure],vle_pressure_limits(liquid,vapour))
```

5.3.6 Managing Propagation of Information about Numerical Limits

As described above, information determining the limits on deviations is typically generated at one point in the plant, but may be used quite remotely, at a distant consequence, for example. It is vital that a coherent method is used to manage the propagation of this information, so that limits are not propagated to inappropriate places. Also, a workable strategy is required for dealing with cases where limit information is needed by a predicate, but is not available.

Where limits on variable deviations are requested but not available, the default behaviour should be to allow the condition on the arc or consequence concerned to succeed. The functions which access limit values of pressures, temperatures and compositions have been designed to return the value `undef_number` where the limit is not known, so that functions or predicates can detect this value. Absence of limit information is taken to imply that the deviation being considered is "unlimited", so that it should be assumed to be severe enough to cause any consequence it is linked to in the SDG.

Propagation of numerical limit information is at present limited to two simple rules for pressure and temperature deviations. These are:

1. Limits information is propagated forwards in arcs linking pressure to pressure or temperature to temperature.
2. Limits information is discarded when propagating to pressure or temperature from any other variable.

In due course, other rules could be developed to deal with other propagation variables (*e.g.* composition). The fluidisation heuristics mentioned in Section 5.2.2 are a possible source of guidance for this venture, although the correctness of rules needs to be assured within the system.

5.4 Conclusions

This chapter has described the basics of the fluid modelling system in AutoHAZID. On the whole, it seems that predicate conditions and fault path validation are good, general-purpose techniques for improving the SDG models. The model of SDG conditionality offered in the FMS is one that is suitably general to tackle a very large range of problems. What's more, as time goes on, there are fewer cases where new predicates need to be defined in terms of internal C++ functions (requiring program recompilation) and more cases where the new predicates can be defined in terms of already defined operations. This is an indication that the basic machinery is now in place to deliver big improvements to the models in AutoHAZID.

Many of the tests implemented in the FMS so far have had an impact by reducing the number of spurious results produced by AutoHAZID. This means that their contribution is, in some senses, an invisible one – they contribute to making the overall results more correct by controlling what is left out of the final HAZOP report. This development has been dictated by the need to remove obviously wrong hazards from the results during STOPHAZ, to attain a basic level of performance in AutoHAZID. In future, however, there should be more emphasis on the enrichment of models to include new, more interesting faults and consequences. If this is supported by the FMS, the quality of the HAZOP results can be maintained.

Clearly, the system is still in development, and some aspects of the fault path validation technique are still relatively primitive. The various rules, conventions and methods used for limit propagation are an example area where there is still much work to be done. I think that the most practical way to formulate these methods and conventions is by tackling real problems using the system as it is – this will identify to the developer where the weaknesses lie and how one may tackle them.

The approach used in the development of the FMS, of applying conditions to highly specific faults and consequences, seems to be well-justified, given the need for richer and more interesting scenarios to be identified in HAZOP emulation. This approach is one of the more important ideas behind the Fluid Modelling System. The other important or novel ideas in the work described here include the use of fault path validation and the propagation of fluid information through the plant model from data given in the input plant description.

The most interesting application of the FMS so far has been in the processing and propagation of limit information to verify propagation of deviations. This is probably one of the smartest prospective solutions to the problem of increasing the value of individual scenarios in the HAZOP report. It also uses methods which can be compared to the sort of naïve reasoning which might be used by participants in a conventional HAZOP.

The limits processing system in the FMS is still in a very early stage of development, and may need to be redesigned at some later date, in addition to the need to widen the scope of deviations treated to include (at least) composition. There are many areas like this within the AutoHAZID program and the FMS. Some of the possible areas for future improvement are mentioned in the next chapter, which discusses the thesis and the work on AutoHAZID as a whole.

Chapter 6 : Discussion and Future Work

This chapter discusses some of the issues raised by the preceding chapters and looks to possible future areas of work on AutoHAZID, and on hazard identification by computer more generally. The objective is also to record some thoughts about the subject which did not fit into the framework of the rest of the thesis.

First of all, a brief review is given of the strengths and weaknesses of AutoHAZID and the HAZID package, in Section 6.1. Then, Section 6.2 gives an overview of the main areas considered for future work, some of which are discussed at more length in Sections 6.3 to 6.9. Section 6.10 concludes the chapter with a recap of the topics covered.

6.1 Strengths and Weaknesses of HAZID

Some of the strengths of the HAZID package (including AutoHAZID as its central component), in comparison to other groups working on similar areas, are:

- Inclusion of a wide range of techniques related to hazard identification, in an integrated software environment. Examples include the fluid compatibility checks, the HAZOP emulation algorithm, fluid model system, consequence ranking, *etc.* No similar software package (as far as I am aware) tackles such a wide range of safety-related tasks.
- The large, hierarchically organised library of equipment models, which covers a wide variety of failure modes and a large number of equipment types. None of the other groups reviewed in Chapter 2 have attempted to model this range of equipment.
- The modular modelling approach using templates is quite novel, and allows repeated features of diverse models to be described concisely. This makes maintaining consistency in existing models easier and allows rapid prototyping of new models.

- A "Model Generation Tool" (MGT) for developing new, user-defined equipment models. This makes extensive use of templates, building whole models of vessels from components taken from the template library.
- Use of a "Fluid Modelling System" (FMS) to distinguish between feasible and infeasible scenarios. The rule-based system used to validate conditions on faults, consequences and propagation arcs is, as far as I know, unique in this field.[1]
- A promising prototype system within the FMS for handling numerical limits on propagated deviations of (so far) pressure and temperature. The aim of this system is to validate whether the deviations in a fault path are sufficient to cause the final consequence with which they are associated. Since this is a very novel approach within HAZOP emulation, I have not had time to develop the system completely.
- Ability of the system to model single mapping influences, using a new type of extension to the SDG, as discussed in Section 4.2. This method for extending the models was developed by myself and Dr. Rushton in response to problems recognised in HAZOP emulation results.
- Two-stage, breadth-first graph search algorithm used for identification of fault paths in the SDG. I developed the two-stage approach to prevent repetition in searching the graph.
- Compatibility checks between fluids which mix in the plant, to detect possible interactions and problems.
- Fully integrated access to physical properties data in the FMS, using external calculation packages, internally stored fluid data and calculations within AutoHAZID. These provide the numbers required for selective quantitative assessment of scenarios.
- The Graphical Tool and Database API allow entry of plant descriptions in a graphical format and their automatic transfer to AutoHAZID for HAZOP.
- A novel classification system has been developed for consequence types and ranking of consequences.

[1] It should be noted that conditions have been added to SDG models by other workers (*e.g.* in the "extended signed directed graphs" of Oyeleye and Kramer, 1988). However, I believe that the flexibility of the FMS rule based system used in AutoHAZID is a unique development in this field.

- Demonstration of a small set of "configuration rules", which detect design faults in the plant model and warn the user about them. While the rules are fairly elementary, their automation is probably quite new.
- Consideration of protections in the plant.

Some of the weaknesses in HAZID are:

- Input of the plant model into HAZID can be a problem, and will affect the future acceptance of the tool by industry. This problem is discussed in Section 6.3.
- The equipment models are not all at the same level of development or validation, so that some of the newer ideas, particularly in the FMS, have not been uniformly implemented in the models.
- Hazards still sometimes don't appear where expected in the AutoHAZID output, according to human experts in HAZOP.
- The efficiency of the program, in terms of slow execution speed or excessive memory requirements during graph search, remains a problem for large plant models.
- Many identified rules, models and scenarios have not been added to the libraries so far, due to time limitations or difficulties with knowledge representation.
- Qualitative ambiguity and computational complexity can be problems, as discussed in Chapter 4.
- AutoHAZID is not capable of modelling state-dependent plant behaviour, or temporal sequences of events, so that its ability to tackle batch plants, or abnormal states of continuous ones, is quite limited. This problem is discussed in Section 6.5.
- The single fault assumption, as discussed in Section 4.3, limits AutoHAZID to considering a limited range of possible scenarios (those with a simple, linear development sequence). However, it should be noted that this is actually how HAZOP is usually carried out, so the HAZOP emulation method is sound in this respect.

- Recursive calls between functions and predicates in the FMS are not prevented at the moment. This could give rise to problems of infinite recursion in FMS calculations, at some future stage.
- Debugging and testing of functions and predicates in the FMS is difficult at present, because there is no debugging utility.
- Comparing HAZOP results files for the same plant model, to find differences, must be done by eye, which is a tedious and error-prone procedure.

6.2 Future Work

This section briefly mentions some possible areas of work to improve HAZOP emulation. Some items tackle the problems identified above. Others extend the functions of HAZID to cover activities previously seen as out of scope for the tool. A few topics are discussed in greater depth in the sections following this one.

Some of the future work items are quite trivial changes and are outlined in Appendix G. In addition to these "trivial" changes to the existing system, a number of larger pieces of work were not completed during the project due to time limits:

- The equipment and template models in the HAZID libraries are not all at the same level of development. For industrial acceptance of a HAZOP emulation tool, consistent levels of performance have to be produced, so quality assurance of the expertise present in models is very important. Therefore, the equipment models must be examined to determine a core of functionality which can be expected of every one of them. Then, in a second sweep, the models can be systematically upgraded so that they all meet the minimum requirement. Using this method will ensure that the new features which have been selectively added to some models during a "test" phase get disseminated to all other appropriate models in the library. It will also help to document the features of the package and to locate areas for improvement, new rules to add, *etc.*
- A large quantity of information, comment and expertise was collected from process industry users during the STOPHAZ project (STOPHAZ, 1997a). In addition to the feedback on test cases, output from modelling seminars and other

information collected during the development of HAZID, two other parts of STOPHAZ produced results. CHOPIN investigated how to improve the development of operating instructions prior to HAZOP. ELDER was developed as a hypertext resource, containing safety-related design advice for engineers to use when developing process designs from PFD to P&ID stage. Systematic use should be made of these information sources, to enrich models by adding new failure modes, for example.

- Related to the previous point, wider use should be made of the fluid modelling system, using quantitative rules and landmark values, *etc.* for fault path validation. The integrated links to the properties packages should also be fully utilised.
- Further use should be made of flags and filters to improve the way the results of HAZOP emulation are presented.
- In principle, any weaknesses in templates, equipment models and FMS rules should be tackled by a systematic methodology for model improvement. This area of development is discussed in Section 6.4.
- To move HAZID forward to market, success must be demonstrated with a very large plant model, if possible a "live" example of an industrial plant design. Program efficiency is less an issue here than the quality of output produced, compared to conventional HAZOP studies carried out on the same plant. The range of equipment in the model libraries would need to be widened as a result of the trial. Issues of information management in evaluating a large plant design have not been explored within STOPHAZ, so these will probably be discovered in such a trial.
- So far, the links to external physical properties packages have been demonstrated, in practice, for only a subset of the functions specified in the link to ASPEN Properties Plus. It would be good to demonstrate access to the full range of calculations in HYSYS as well as Properties Plus, to show the generality of this particular part of HAZID. Work on this would consist of debugging some problems in the interface between the external packages and AutoHAZID.

Clearly, progress in the above work areas would significantly improve the performance of HAZOP emulation across the board. By encoding a broader range of expertise in models developed to a consistent depth, the quality of output from HAZID can be made far more consistent.

The next group of future work topics require quite significant effort, in software design and analysis. Some of these involve optimising the user interfaces to the software tools in HAZID, as well as encouraging closer integration and further development of the functions demonstrated as "proof of concept" in STOPHAZ:

- AutoHAZID itself is largely text-based in the current version of HAZID. While there is nothing inherently wrong about this, some parts of the user interface could be improved, and it is natural nowadays to expect a graphical user interface (GUI) to any commercial software package. Therefore, the user interface of HAZID should be redesigned, with a view to optimising the input of plant data, user interaction with the HAZOP emulator, and viewing output reports.
- A properly designed graphical interface to the model generation tool (MGT) would also help, by reducing the repetition of user input typical in the question and answer session carried out at present. The MGT should also be integrated with the design of icons for the Graphical Tool and tools to define the attribute data of new units for storage in the Database API. In short, a fully-fledged model development workbench should be developed.
- The Graphical Tool GUI should be redesigned, to make it easier to specify properties of fluids, component chemicals, *etc.*
- In entering models into the MGT or other model development tool, it would be helpful to be able to use different representations, to suit the user's past experience. Functional equations, SDG arcs and truth tables are examples of qualitative representations that are equivalent, and so could be used as alternative input formats for models.
- Redevelopment of the interface to HAZID should be carried out in conjunction with a critical appraisal of the features to be implemented in the tool, and a more object-oriented reimplementation of the system. Clearly, many "expert" features of the STOPHAZ prototypes were put in as proof of concept only. There needs to be a full functional specification for any features developed to a commercial stage.

- In the longer term, HAZID may form part of an integrated safety software environment, combining tools for maintaining checklists, emulating FMEA, HAZOP, sneak analysis, performing routine calculations for water hammer, vent sizing, *etc*. The experience gained so far in integrating the parts of HAZID would be quite valuable in building such an over-arching system.

A number of new features could be added to HAZID, to extend its functionality beyond HAZOP, or to support the HAZOP emulation done at present:

- A debugging environment for AutoHAZID and the FMS, to allow the developer of new equipment models, functions and predicates to test these without having to construct demonstration plant models and do HAZOPs on these.
- Preliminary check of the plant design to detect the unwanted reactions and inherent problems in the plant, before HAZOP emulation. The check could take place when the plant model is fluidised, to examine every case where fluids are detected to be mixing.
- Preliminary checks to identify sneak flows, where fluids may be unintentionally discharged through vents or drains due to errors in plant operation, for instance.
- In addition to the tabular report produced during HAZOP emulation, HAZID should also produce a concise summary of equipment and fluids in the plant. This summary would remind the user of the plant structure and likely resident hazards.
- The interface to HAZID could be changed, so that it operates as an interactive browser for fault paths, instead of a "batch mode" HAZOP emulator, as mentioned in Section 4.7.
- A utility is required, so that results sets can be compared, to quickly identify differences between HAZOP reports. This requires a way of saving results in files so that the fault-deviation-consequence structure is retained. Such a file format would also help in developing other means of presenting results.
- Selective quantitative simulation could be considered for certain hazardous scenarios, to validate their feasibility or to estimate the seriousness of consequences. Such an approach may use flowsheeting packages, or implement the sort of mathematical programming simulation described by Purdue.

- Links to external HAZAN software and selective hazard analysis could also be considered, possibly making use of fault tree analysis to estimate the likelihood and magnitude of identified hazards.
- Non-process propagation of faults can be important in escalation of faults, as discussed in Section 6.6. Some effort should therefore be spent examining how to model the human factors issues inherent in operating procedures, as well as the escalation of scenarios by the "domino effect".

The various rule-based systems contained within AutoHAZID should also be improved or re-examined in future work:

- During plant fluidisation, when a pump is encountered, the program does not check that a discharge pressure is given. If no value is given, the inlet pressure value is propagated straight through the unit. The same is true for temperatures in heat exchangers. A similar policy is used when propagating limit information on pressures and temperatures, which may not be entirely safe. There should be a warning for these conditions, instead of the program silently propagating values through the unit. These problems are due to the fact that the models do not define the function of equipment items. One idea which may be useful is that of "fluid breakpoints", as mentioned in Paper 9 of McCoy *et al.* A breakpoint is a point where a stream undergoes some sort of change, such as a change in pressure, temperature or composition. The concept of breakpoints, defined for certain variables in the model of the equipment, may be a good way of representing those variables whose values should be specified in the plant model. For example, a pump is designed to raise pressure, so that its outlet is a breakpoint for pressure. The aim of HAZOP is to examine the causes of deviation from intended operation. If full equipment specification data is represented in equipment models, HAZOP emulation can be extended to consider more than just deviation of process variables.
- In the fluidisation routine, the fluid rule #1 does not include a check for conflicting information where a number of output ports are attached to the same internal port (*e.g.* where two different outlet temperatures are given for outlets from the same chamber of a vessel). It just finds the first output port that has data

which can be transferred and propagates this data. There should be a check for such conflicts in the input data, possibly before any fluidisation or application of fluid rule #1.

- The set of rules given in Section 5.3.6, used to propagate information about the limits of deviations, should be expanded. In particular, these rules should be extended to cover other variables (such as composition), as well as pressure and temperature, which are the only deviations whose limits are monitored so far.
- An ad hoc rule has been used to decide ambiguous causal influences operating in a feedback loop, as outlined in Section 4.10, so that the shortest path is not always used to determine the fault paths in these parts of the graph. The need for such rules should be reviewed, with a view to justifying the approach theoretically, or doing something more general to prevent incorrect fault paths propagating through loops. The issues of loops and other topological features of the plant and the SDG, are discussed further in Section 6.7.
- Similarly, an ad hoc rule is used to disallow reverse flow propagation in faulty units, as described in Section 4.3. The issue of how to control reasoning through unhealthy units should be examined in detail, as these sorts of problems are likely to be quite common.
- The set of configuration rules, for detecting design faults in the plant model, could be extended in the future. These sort of rules are useful, but are not best reported in a HAZOP report format – a separate section of the HAZID report should be devoted to such problems detected in the plant.

Some other possible areas of future work include:

- The model of fault propagation used in HAZOP emulation can be extended to include the idea of generic faults and consequences, as described in Section 6.8.
- The HAZOP algorithm should be optimised, to reduce the number of repeat validation checks carried out during fault path generation. As outlined in Section 6.9, a new object class for fault paths is needed, to allow the results of fault path validation (current fluids, deviation limits, *etc.*) to be stored with the fault path.

- Another area for optimisation is the use of graph pruning. By removing parts of the SDG which are not required, the speed of search could be increased.
- The treatment of chemical interactions and reactions, whether intended reactions or not, should be improved, and this facility should be more widely used in equipment models.
- Reverse propagation of temperature and concentration deviations, under conditions where reverse flow is occurring, should be modelled, The sort of scenario where reverse flow takes hot material to an upstream location, causing a problem related to *highTemp*, rather than *revFlow*, has never been satisfactorily treated in AutoHAZID so far. It might be possible to deal with this by propagating composition and temperature values upstream in *revFlow* propagation chains, so long as a link from *revFlow* to *temp* (or *composition*) is made in the upstream model.
- The representation of instrument systems and protective devices in the plant model should be improved.
- Consider abandoning the shortest path heuristic for graph search, accepting that multiple paths will be generated. The relevance of competing fault paths could be determined by comparing the strength of their causal links in some way, as discussed in Section 4.10.
- The single fault assumption, as discussed in Section 4.3, should be challenged, with a view to modelling more complex scenarios than is now possible with AutoHAZID.
- The process-based approach to qualitative modelling, as used by Forbus (Section 2.2.4) and the group at Pennsylvania (Section 2.3.4) should be revisited. The main problem with this approach was perceived to be computational complexity, which it may be possible to avoid by careful formulation of the models and the inference methods used on them. Certainly, the power of a system capable of representing phenomena in a plant, and reasoning about changes in their activation over time, is worth having. The histories idea of Hayes (1979), discussed in Section 2.2.3, could be useful in taming the complexity problems in this type of model.

- Potentially the biggest improvement to the equipment modelling system would be to introduce a representation capable of handling landmark values and state-dependent behaviour, if possible including temporal reasoning within fault paths. With such capability, modelling the plant in off-normal or alternative operational states (start-up, shutdown, maintenance, batch, *etc.*) would be possible. This type of improvement is discussed in Section 6.5.

6.3 Access to Plant Descriptions

One of the most critical success factors for a commercial HAZOP emulator will be ease of use, in respect of the input and output interfaces. Because the tool is intended to support hazard identification, potentially at a late design stage, one cannot expect users to struggle with a difficult interface to access the benefits of HAZOP emulation.

The effort required to input plant descriptions to HAZID is quite considerable at present, especially for larger plants. This problem has been improved significantly during the STOPHAZ project using the "intelligent CAD" interface of the Graphical Tool, developed by TXT. Nevertheless, if any re-typing or re-entering of plant details is needed, the input task quickly becomes unviable for larger plants.

User companies often have a CAD representation of the plant design in some electronic format already, before a HAZOP emulator is used. The ideal situation would be where a representation of the plant P&IDs can be read into HAZID, possibly *via* some neutral file format. This requires that there is some "intelligent CAD" system in place, so that the equipment items in the plant correspond to objects on the drawing. Otherwise, one has to consider how to recognise the plant components from the line segments and arcs used to draw them.

The main problem at present and into the near future is likely to be the proliferation of non-standard file formats for structured CAD data, where each format is proprietary to a particular CAD program. Communication between diverse software packages is the aim of the initiative known as STEP. Ultimately, STEP-compliant file formats will be defined for the exchange of process plant information, so that any program able to read in and write out data in STEP format will be able to communicate with a large number of other programs with the same capability. So far, STEP has not been developed to this stage, so "seamless data exchange" between software is still some way off.

Future work in developing HAZID should investigate the options for intelligent CAD on the market, and look at the possibility of automatic transfer of P&IDs from the CAD system to HAZID. It is important to make sure that the effort of building such interface software is well spent — the file format considered must be technically capable of transferring the required data into HAZID and the associated CAD package(s) must be widely used in industry. Proof of the viability of HAZID on industrial scale plant designs would greatly improve its long-term prospects of success.

An alternative strategy is to shift the focus of automatic hazard identification to an earlier stage of design, namely flowsheeting. At this stage, the user is likely to be using a graphical interface to a flowsheeting package for sorting out the overall mass and heat flows in the plant. Therefore, much of the basic process information is available at this stage, such as the main unit operations and materials involved, together with flowrates, temperatures and pressures. Clearly, transfer of electronic information is still an issue, but the level of detail is less with this option, and re-entering the flowsheet may be less of a headache. As discussed in Section 4.8, the current HAZID models are not suitable for analysis of flowsheets, but it may be worthwhile developing a new set – advantages include early hazard identification and a reduced volume of results for the user to look through.

6.4 Methodology Issues in Unit and Fluid Modelling Systems

To encourage the development of a range of models whose quality is assured to be of a certain level, a procedure should be set up to govern how models are created, maintained and documented. Following the procedure should ensure that a minimum level of competence is achieved in the models produced. This section addresses some issues related to such a modelling methodology, from a general point of view, rather than with reference to AutoHAZID.

Methodology has been mentioned before now, in Section 3.5, where the development of the flow path template model was used to illustrate a method for development and documentation of new models. Section 6.4.1 offers a view of the general modelling process, which can be used as the basis of developing models in the way illustrated by Section 3.5. Section 6.4.2 gives guidelines for the sort of documentation that should be provided by the model designer, so that the new model is comprehensible to other workers, who may need to modify it at a later stage. Section 6.4.3 looks at how pointers for model improvement can be identified, and is therefore quite strongly linked to Section 3.5.7, which discussed the knowledge elicitation techniques used in STOPHAZ.

Additional possible sources of information for model development include the following, which were not used systematically during the development of HAZID:

- Characteristic failure modes of equipment, as identified by other techniques, such as FMEA.
- Codes and Standards for best practice design.
- The advice in the STOPHAZ ELDER tool, which was designed as a repository of information about safe design.
- Other sources, such as standardised incident reports, could be used. These often include analyses of the causal principles behind accidents, and are therefore useful for identifying the mechanism of the incident. A good example of this type of expertise is the Accident Database package published by the Institution of Chemical Engineers (1997).

In addition to the advice offered here, Paper 9 of McCoy *et al.* (1998) contains some suggestions for methodologies to be followed in processing HAZOP results into formal qualitative equipment models. Such methods are needed to make the best use of information from modelling seminars and other meetings, where experts are questioned about the expertise they use in hazard identification.

6.4.1 A General Approach to Model Building

This subsection presents a general view of the process of building formal models of equipment or phenomena. Although the emphasis during development of this methodology has been on qualitative models for HAZOP emulation, there is no reason why such an approach could not also be used for other types of model or application. The aim of the methodology is to build robust and maintainable models, in which all assumptions, restrictions and dependencies are clearly stated.

The view of the modelling process adopted here is presented in Figure 6.1, where the equipment or phenomenon model is a formal representation which can be manipulated using mathematical or other symbolic means. The model must represent some portion of the real world in such a way that the behaviour predicted by the model, when used in simulation, is similar to that which would be observed in reality.

The designer determines the development of the model, as illustrated schematically in Figure 6.1. The first task is to define a "system boundary" around that part of the real world which is to be modelled, effectively cutting off the "system" from the rest of the world. This is shown as a process of "restriction", and determines the scope of the model's applicability.

The next step is for the designer to form an understanding of the functioning of the system. This can be seen as a process of "abstraction", producing an "internal mental model" in the designer's head. It can be very useful if the designer writes down what they understand about the system at this stage, even if it is not possible to state this very precisely, as this can be used as the basis of a later structured investigation of the problem.

The process of "formalisation" consists of translating as much as possible of the internal mental model into the formal language of the model system. The formal model so produced can then be used in simulation and any weaknesses of the model can be addressed at this stage, possibly introducing extra restrictions or generalisations of the model.

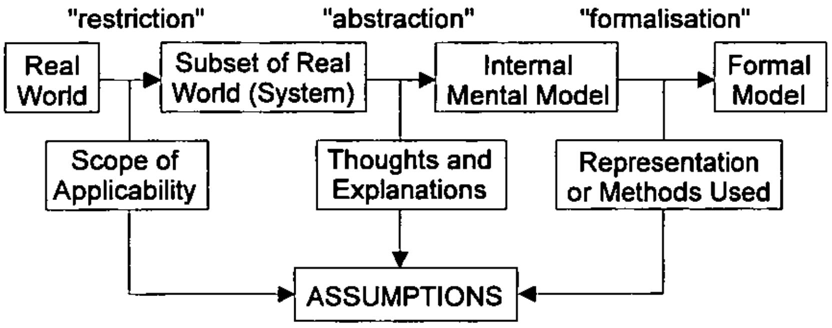


Figure 6.1 : The Modelling Process

The above procedure can be seen as a generally applicable method for model building, whether the final model is qualitative or quantitative in nature. The product of the modelling process is not just the formal model, containing the symbols and rules of the final implementation of the model. Just as important for defining a model is the set of assumptions which govern the system, or range of systems, for which the model is applicable. It is also important to give an explanation of what the designer understood about the system and how they went about formalising that internal understanding.

In any case, if enough information is presented in the assumptions (description) of a model, it should be possible to reproduce the formal model from scratch. Therefore, a good aim is to state as much as possible of the reasoning, assumptions, restrictions, *etc.*, while the model is being constructed. This is a difficult task, as a lot of knowledge seems to be “given”, or “obvious” in the design exercise, leading to poor documentation of such knowledge. It might also be difficult to ensure that known deficiencies and problems are documented, but this information is vital for future development of models, as well as for signalling known weak areas.

The control of changes to models, once built, should be carefully examined, as even small changes can have wide-ranging effects on the performance of the model. Above all, it is unwise to “tinker” with individual rules without first examining whether any of the assumptions of the model are affected. Such tinkering frequently occurs when there are small problems with the results produced by the model and there is a temptation to go in and do a "quick fix".

The process of model development as described conceptually above does not address the question of how to get started on a particular problem. Typically the brief for a problem may be as complex or ill-defined as "model flow and pressure propagation in a chemical plant" (see Section 3.5). When given an open-ended problem like this, the best approach is to target a single fairly well-defined system which captures the most commonly observed types of behaviour in the problem area. This target definition is an activity in the "restriction" part of Figure 6.1, and gives rise to a number of scope-limiting assumptions, which should be documented at this stage.

By concentrating attention on a well-understood instance of the phenomenon or item which needs to be modelled, the models will more likely be correct and well-populated by known assumptions, and will hopefully be re-usable in a wide variety of situations. This approach should also prove economical in quickly producing models to be used as "base models" for further development. Such development is made by varying the assumptions used in a base model, so that the new model becomes either more general, or applicable to a different problem area. Clear statement of model assumptions is vital for this process.

The ultimate goal (in developing from a base model) might be elimination of restricting assumptions, giving a fully general model for the phenomenon being studied, but it need not be. Some of the "base" assumptions in a model may be harder to eliminate than others. Whereas some assumptions are made for the sake of agreeing conventions for the models, others may be made to render the problem tractable or understandable, and so could be more closely tied to the nature of the model itself. An example of the latter might be the assumption, in the flow path model developed in Section 3.5, that no work is done on the fluid in the flow path. It is much more complicated to model a fluid where shaft work is involved, than in the simple flow path model.

6.4.2 Unit Model Documentation

For a knowledge-based system to be acceptable to industry, all models need to be developed to a consistent level, and the assumptions made during this modelling must be documented. As a minimum standard of documentation, the following types of information should be provided, where appropriate, for any template or equipment model:

- **SCOPE OF MODEL**
  - Give the common name of the entity to be modelled and a basic description of its function(s).
  - State any known subtypes of the entity modelled, and indicate whether they are modelled.
  - State any known entities which the modelled entity is a subtype of.
  - Give some impression of how general/specific the model is.
  - Describe the known internal features/subcomponents of the real object and state if they are modelled/not modelled.
  - State any other features known but not modelled.
  - Define how connections are made to other models.
  - Describe the context/applicability of the model.
- **DESCRIPTION OF MODEL**
  - Give details of the component parts of the model:
    - Ports, for connection to other units, or for definition of internal locations.
    - Chambers, as separate spaces within the equipment.
    - Other structures (packing, *etc.*).
    - Fluids present, where these can be stated without presupposing the context of the model in a plant.
    - Materials of construction, if appropriate.
    - Phenomena operating within the model.
    - What variables are relevant to the model.
  - Connections between parts of the model, and to other modelled entities:
    - Internally, between ports.

        - To other units.
        - Between variables in the model.
        - Failure modes and hazards, with their associated deviations.
    - Define any state dependent behaviours in the unit and any attribute-conditional subtypes which could be defined to model them.
    - Fluid model system dependencies.
    - Higher order modelling decisions or conventions (*e.g.* causal hierarchy).
    - List modelling principles/assumptions.
    - State how well developed the model is, any known deficiencies, problems, *etc.*
- **FORMAL DEFINITION OF MODEL**
    - Name of model.
    - Parent of model.
    - Known child models.
    - Specify ports and internal connections.
    - Attributes relevant to model subtypes.
    - Reference to libraries where defined/used.
    - Text of the SDG arcs in the model.
- **OTHER INFORMATION**
    - Change history, names of authors, *etc.*
    - Supporting analysis for modelling, *e.g.* truth tables, methods used, *etc.*
    - Schematic line diagram of unit, with ports. Should show internal connections between ports, if appropriate.
    - Bitmap icon for equipment type.
    - Schematic diagram of parts of SDG model.

The documentation should allow a complete understanding of how the model is built, functionally, and how it compares to the equipment it is designed to mimic. Providing this level of documentation would make the job of extending existing models, and developing new ones, much more straightforward. It would also provide an assurance of quality in the model libraries, which is bound to be a critical factor in determining industrial acceptance of any system like HAZID in the longer term.

6.4.3 Improving Model Performance

In the same way that equipment models in the HAZID unit model library benefit from the use of a sound development methodology, it is important to use sound methods for identifying, developing and maintaining rules within the FMS. So far, little work has been done on the methodology of FMS development.

As with unit models, any improvement policy should combine methods to tackle both "false negatives" and "false positives", with respect to the results of HAZOP emulation. False negatives are scenarios not present in the results, which should be, whereas false positives are identified scenarios which are not interesting, or not feasible.

To enrich the fluid modelling system, so that it represents a wider scope of real problems (eliminating false negatives), "brainstorming" techniques can be used to identify candidates for new fluid rules. This approach can be used in addition to the method of criticising results produced by HAZOP emulation on case study plants. An example of this sort of "brainstorming" was attempted by myself and Prof. Lees, to try to identify rules governing limits on pressure and temperature deviations. The minutes of our meeting are reproduced as Appendix F and can be seen as an information resource, containing ideas for further development in the FMS.

To tackle the false positives in the HAZOP results, a methodology needs to be adopted for identifying problem areas and for formulating and implementing solutions to them. This sort of activity concentrates on criticism of the results of HAZOP analyses and might include the following elements:

- The starting point is a result (fault–consequence pairing) which does not make sense in some way. Therefore, this is a "false positive" which should be removed.
- First, the fault path(s) giving rise to the result should be examined carefully, to find out where the weak or incorrect link is.
- If the fault or consequence is not valid in the specific case identified, an FMS condition could be added, to restrict the applicability of the item.

- If some arc in the path is clearly not a feasible influence in the model, then it should be removed. However, it is important to determine that the arc is genuinely incorrect, and wasn't put into the model for some other specific reason.
- Where there is no obviously wrong link, each component of the fault path must be examined, to see where there is a gap between model and reality. If a weak link can be identified, this is a candidate position for applying a conditional rule. Identifying this point requires a good understanding of the hazardous scenario identified. Such an understanding should be documented, so that the basis for modelling the scenario is understood at a later date.
- Possible strategies for dealing with the model weakness include use of new or different variables for propagation, use of single mapping influences, as described in Section 4.2, or adding propagation conditions to arcs.
- To add new conditions to the arcs in the graph, one must consider what information is required to decide the new condition and whether that information is present locally or needs to be propagated somehow. Using fault propagation, faults cause local effects which may be propagated *via* deviations to remote locations, where a susceptibility to some deviation gives rise to a consequence. Maintaining the local nature of these events embodies the "no function in structure" principle and ensures that the equipment models developed are usable in many different contexts.
- Once any fluid rule has been created, the rationale for its development should be documented. Such documentation should include an explanation of the real-world problem it is designed to solve, as well as the information it uses and any assumptions it makes about the plant data available in the system.

6.5 Modelling State-Dependent Behaviour and Temporal Sequences

A very significant improvement to the AutoHAZID modelling system would be to develop a representation capable of handling landmark values and state-dependent behaviour, if possible including temporal reasoning within fault paths. With such a capability, modelling the plant in off-normal or alternative operational states (start-up, shutdown, maintenance, batch and semi-batch, *etc.*) would be possible.

The references to state-dependent behaviour mentioned in this thesis, which may be of use when considering how to tackle the subject, are:

- De Kleer and Brown (1984) discuss the issue of state-based models and their relationship to causal reasoning.
- In the work published by Purdue University, Srinivasan and Venkatasubramanian (1996) discuss a method for using Petri nets and digraphs for modelling the progress of a batch processing recipe.
- The work of the group at Pennsylvania University, as reviewed in Section 2.3.4, illustrates a process-based approach to simulation, which relies on model rebuilding in response to state changes. It may also provide pointers to the types of ambiguity and complexity problems to be tackled when building state-dependent simulators.

There are at least two big issues to tackle within a representation which is to handle the state-dependent behaviour of plant components. One is the state-dependency issue – how to represent the fact that parts of the model change when the state changes. The other is how to determine what state transitions are possible when simulating the model behaviour.

The former problem can be tackled using rules of the form: "if equipment is in state1 then use model_section1", or some equivalent. That is, the use of each different section of the model would depend on the state the equipment was in. Such a system could be implemented using the rules of the FMS, by attaching state-dependent conditions to the relevant SDG arcs in the equipment models.

The latter problem, that of determining legal state transitions, can be tackled by defining the applicability of a state transition in a number of ways:

- A state is dependent on a certain variable being within a range, defined by landmark values of that variable. The state is only valid when the variable is within the landmark values.

- State transitions may be caused by faults, which effectively change the model of the equipment item.
- State changes can also be caused by operator actions, such as opening or closing valves, switching machines on or off, *etc.*
- Alternatively, no cause can be sought for the state change – it may be assumed to occur spontaneously, or at least one may not be interested in the cause of it.

In certain cases, the above definitions of state applicability may be muddied by the possibility that a state transition is not guaranteed by the cause given. A probability may be associated with a statement like: "if the control valve fails closed, then a change to state1 may be caused". In this case, both possibilities (*i.e.* change or no change) should be followed up, and computational complexity becomes a problem if this sort of "forking" occurs too often.

States should be defined, either in relation to individual equipment items (*e.g.* "pumpJ1 is running"), or in terms of a certain number of global conditions which may affect many units in the plant (*e.g.* "electric power is failed"). Using the latter type of state-dependence, some types of common-mode failures could be examined, and systematic "what-if?" studies could be carried out on the plant to see how it would respond in the event of a power or cooling water failure, for example. The constraints imposed by operating instructions (or safety interlocks) on the states of valves in the plant, may also be represented by this sort of global constraint.

It should be noted that allowing some of the above types of state transition to occur, outside the immediate causal pathway of the fault path being considered, amounts to relaxing the single fault assumption. The result is that the fault paths are no longer simple or linear, as before. An example is: "the flow into the tank increases and, because the level control loop is in manual state, the tank overfills". The operator leaving a control loop in manual is not an immediate cause of the tank overfill, but is a plausible state of affairs for the plant when that event is caused by the increased flow.

It is important, therefore, to address the single fault assumption in the context of this type of state-dependent behaviour. A certain number of state changes may be plausible, but a large number of independent and coincident events of this nature are highly unlikely. One might imagine relaxing the single fault assumption slightly, to allow a limited number of additional state changes in a fault path. The ambiguity introduced to the SDG by allowing equipment state changes may be tamed using this sort of method. However, the logic used in arguing that events are independent, and therefore unlikely to occur together, could be rather difficult to formalise.

The present FMS rule system could, in principle, be used to implement state-dependency in equipment models. A number of attributes would be defined, giving the states of each equipment item in the plant, and a smaller number of "global states" for the plant as a whole, as mentioned above. These state attributes would be accessible by functions of the FMS.

State-dependent parts of models would be expressed with conditions, dependent on the state attributes, attached to the relevant parts of the SDG model. Some parts of this "attachment" could be automated, so that the model builder would not have to explicitly code these "activating conditions" into models. They would be added by the system in response to the relevant syntax (*e.g.* defining state-dependent blocks of arcs) in the model library.

HAZOP search would operate as it does at present, generating fault paths for later validation by the FMS. Therefore, arcs belonging to all states of the equipment would be treated as equally valid in the search (this would certainly cause complexity problems!). Only at the validation stage would infeasible paths be rejected, including those where the states of equipment were found to be inconsistent with one another. During validation, legal state transitions would be allowed, as discussed above, subject to some limit on the number of simultaneous "failure" events. The current states of equipment items in the fault path (and elsewhere) would have to be recorded by the FMS as the validation proceeded, in much the same way that "current fluids" are tracked by the FMS at present.

It may be that the suggested solution above (using the FMS) is flawed, and that the simulation of state-dependent processes requires some new system to be developed. I feel that the biggest problem, after designing an adequate representation for the state-dependent models, will be the complexity introduced by the state changes in the system. Finding means to localise the effects of these changes and manage the "single fault assumption" (or its successor, the "maximum N faults assumption") may be the key to tackling this problem.

6.6 Non-Process Propagation of Faults

AutoHAZID concentrates on modelling fault propagation using an almost entirely process-based view of propagation – deviations cause other deviations by virtue of the interconnection of process equipment *via* streams between them. "Real World" propagation of hazards can also occur by other means, due to the other types of connections present in the plant. Connections between components in the plant can be viewed as types of constraint in the model. The types of connections/constraints present in a real plant include the following:

- Process streams connect one equipment item to another. These are well-modelled at present.
- Signal connections from sensors to controllers to control valves constitute (in part) the control and protective systems in the plant, which further constrain its behaviour. Instruments, trips, relief devices and control loops are represented to a limited extent in AutoHAZID – improvement is possible in this area.
- Physical proximity and spatial layout are often important factors in the escalation of hazardous scenarios, where the "domino effect" comes into play. An example is where an explosion in one part of a plant causes a missile to be propelled through a pipeline, or into a vessel in another part of the plant. The two damaged pieces of the plant may be entirely unrelated, from a process viewpoint, so that such factors may be overlooked in a study of the plant design.
- A further level of constraint is that imposed by the operating procedures of the plant. These "soft constraints" rely on the operators following the instructions and impose restrictions on the possible states of the plant, defining some of these

states as more probable than others. Clearly, errors in following instructions are possible. It may be possible to model the ways that such mistakes occur, and use this as the basis of hazard identification. It may also be possible to analyse interventions directed at correcting disturbances in the plant, using such models.

It is possible to consider a HAZOP emulation tool being used to identify possible "domino effect" scenarios, or hazards caused by human error in relation to the operating instructions. What is needed in either case is a means of representing the necessary information (plant layout details or draft operating instructions), and then an inference procedure which allows systematic checking of the proposed design.

It seems that future work to identify the "domino effects" in a plant could make use of the work of Hayes (1979) on histories, as discussed in Section 2.2.3, to govern the range of possible interactions between equipment items.

6.7 Loops, Plant Topology and Higher Level Constraints

Some of the problems encountered with HAZOP emulation have been related to the presence of loops in the plant model, and the inability of the system to model high level constraints in the SDG. This type of problem has been mentioned briefly in Section 4.9 in connection with qualitative ambiguity. Modelling higher level constraints, spanning a number of process units, can reduce ambiguity in predicted behaviour.

An example is given in Figure 6.2, where a spill-back line returns part of the liquid pumped from a vessel back into that vessel. Changing the flow in the spill-back line can itself have no effect on the level in the tank, unless the net flow out of the loop changes. This constraint is not captured by the SDG, but could be detected by suitable analysis of the plant topology.

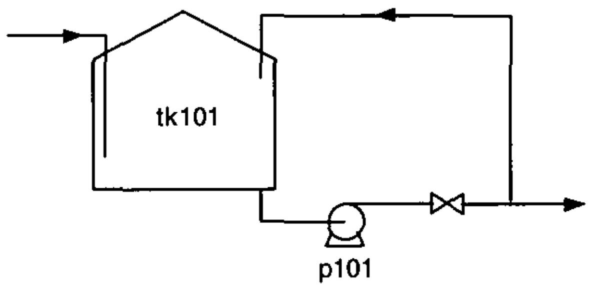


Figure 6.2 : Mass Balance Problem with Spill-back Loop

There should be a concerted effort to identify cases where high level constraints are required, and to capture those constraints by analysing the topology of the SDG or of the plant itself. Care must be taken, however, to be sure that the constraints introduced are generally applicable, in all plants containing the relevant structures.

In the particular case of feedback control loops, the system can be made to deduce certain features of the loop from the SDG arcs and the plant topology, such as the controlled variable in the loop. This data can be confirmed to the user, and used to reason about possible failure modes of the loop, and their effects on the plant.

6.8 An Extended Representation for Fault Propagation

The fault paths in AutoHAZID so far have been entirely linear. An initial fault is linked to a final consequence *via* a sequence of deviations. Faults must appear at the start of a fault path and consequences may only appear at the end of fault paths. There is no scope for faults or consequences to appear as intermediate events in the chain.

Firstly, this limitation should be removed: faults and consequences should be modelled as equivalent events, from the point of view of fault propagation. There should be no problem with consequence events being linked to further deviations or consequences through escalation of the hazard. A typical example is where some initial failure causes a valve or other component to become blocked, which then gives rise to further variable deviations and (possibly) to another consequence. In HAZOP emulation at the moment, the blockage must be modelled as two separate events (one fault and one consequence), whereas it should be represented as a single event.

Also, the way faults and consequences are modelled at present ignores the similarity between the same events occurring in different equipment items. The "leak to environment" fault in a pump is entirely disconnected from the same fault in a storage tank, from the point of view of the modelling system. This means that when such faults or consequences are changed, they must be changed everywhere in the unit model library.

A more sensible system would treat faults and consequences as model entities, instances of which are used in equipment models. A library of event types, analogous to the current library of equipment models, could be constructed. In such a library of event types, a change to the event model would imply that all instances of that event, in equipment models and templates, would be changed.

If faults and consequences were modelled in this way, as fully fledged objects in the model system, the next step would be to model the relationships between similar (generic or specific) events. During the STOPHAZ project, Prof. Lees developed the idea of consequence classification and evaluation (discussed in Paper 5 of McCoy *et al.*, 1998, and in Section 3.3.8). Using this idea, a number of basic types of consequence are defined, and each specific consequence may be classified as an instance of a number of different types. Future work in modelling could treat events as instances of generic types in this way, so that only the most general events would be present in the SDG models. Specific consequences and faults would be modelled as instances of the generic types in the SDG models.

Under such an interpretation, fault propagation would take place in two dimensions (see Figure 6.3 below) instead of the linear, one-dimensional propagation used at present. An initial, specific fault occurs, which is an instance of some more generic fault type. The generic fault type is linked by a number of variable deviations, in the SDG, to a generic consequence event. The generic consequence is realised in the plant by an instance of a more specific consequence type. Clearly, this type of scheme may involve more complicated model building, and possible extensions to the SDG search algorithm, compared to the current models in HAZID.

$$\begin{tikzcd}
\text{fault (generic)} \arrow[r] & \text{deviation} \arrow[r] & \text{deviation} \arrow[r] & \text{deviation} \arrow[r] & \text{consequence (generic)} \arrow[d] \\
\text{fault (specific)} \arrow[u] & & & & \text{consequence (specific)}
\end{tikzcd}$$

Figure 6.3 : Alternative Fault Propagation Model

6.9 Optimisation of the HAZOP Algorithm and Fluid Modelling System

The speed of the program is quite drastically reduced by the execution of the fault path validation technique, particularly the parts of the system which maintain the deviation limit information in the fault path.

Part of the reason for this is repeated search. When the plant model is loaded, AutoHAZID compiles a set of lookup tables for the alarms and indicators on the plant, giving the causes by which those devices are activated. This involves calling the search algorithm for each of the deviations related to the alarms and indicators, which negates many of the advantages of two-stage search. It also involves search which is repeated at a later stage, when the HAZOP is performed. Therefore, this task of compiling lookup tables for the instruments is inefficient, and should be done when the causes of all the HAZOPed deviations have been determined by HAZOP.

Also, the fault path information is stored in such a way that the results of fault path validation (such as the current fluid lists), for partially completed fault paths, are not available for reuse later on in the search algorithm. The `Scenario` objects used for storing the search data do not allow storage of this data. The result of this representational shortcoming is that there is some repeated validation in the algorithm, at least doubling the work done. Specifically, when partial fault paths are joined together producing longer paths, the whole long path has to be re-validated and when consequences are added to the fault paths at the end of the HAZOP search phase, all the fault paths have to be validated once again.

This is a strong argument for changing the data structures used in the HAZOP algorithm, so that fault paths and partial fault paths can be represented as objects which record all the context information generated by validation, including current fluids. The validation of these paths could be updated whenever they were extended, with minimal effort, and the fault path objects would be copied whenever necessary, so that repeat validation of the same partial paths could be avoided.

6.10 Conclusions

This chapter has discussed the strengths and weaknesses of the HAZID approach to hazard identification, and outlined a number of areas of possible work to improve HAZOP emulation in the future. A small number of these topics have been discussed at length – I hope that the sketches offered by Sections 6.3 to 6.9 are sufficient to allow another person to continue the work done on HAZID and, in particular, on its Fluid Modelling System.

The seven areas of future work discussed in detail were:

1. Access to Plant Descriptions
2. Methodology Issues in Unit and Fluid Modelling Systems
3. Modelling State-Dependent Behaviour and Temporal Sequences
4. Non-Process Propagation of Faults
5. Loops, Plant Topology and Higher Level Constraints
6. An Extended Representation for Fault Propagation
7. Optimisation of the HAZOP Algorithm and Fluid Modelling System

The main areas of concern reflected in these headings are:

- Improving the representational strength of models used.
- Management of large volumes of information, in the form of models encapsulating expert knowledge.
- Optimisation of program performance.
- Developing interfaces to external systems.

These summarised concerns seem representative of the sorts of problems which need to be tackled, to gain an even more acceptable level of performance from a model-based hazard identifier, such as AutoHAZID. The next chapter attempts to summarise the conclusions that may be drawn from the work presented in the thesis.

Chapter 7 : Conclusions

The automation of HAZOP analysis, using qualitative plant models for process simulation, is motivated by the prospect of saving some of the time and money traditionally spent in HAZOP studies conducted by teams. The AutoHAZID computer program was developed in the STOPHAZ project to emulate HAZOP, using qualitative reasoning methods.

This thesis has described how qualitative reasoning can be successfully applied to hazard identification by emulation of HAZOP. It has also demonstrated, however, that purely qualitative models are not sufficient to provide the accuracy required in reported hazards. Checks based on quantitative information are needed to prevent spurious identification of hazards.

The qualitative model system in HAZID proved to be a highly efficient way of modelling fault propagation in the majority of simple hazard scenarios. However, there were some problems with the method, as outlined in Chapter 4 and summarised below:

- Indiscriminate reporting of hazards and repetition in HAZOP reports.
- Qualitative ambiguity, leading to undecidable influences in the SDG and to problems with computational complexity.
- The SDG only represents two types of deviations in process variables, which is a problem for flow, for instance.
- The "shortest path heuristic", used in the graph searching algorithm at the heart of HAZOP emulation in HAZID, is not theoretically sound.
- The SDG model of an equipment item does not change when that equipment fails, so that it is possible to reason through unhealthy equipment, with erroneous results.

- Single mapping influences in the plant are not represented in the SDG as originally formulated.

An important method used to tackle many of these problems was by using quantitative information, typically concerning the fluids in the plant, implemented in the Fluid Modelling System (FMS). The FMS was described in Chapter 5 and is summarised briefly below:

- The FMS verifies the feasibility of fault-consequence scenarios produced by the (qualitative) HAZOP search algorithm.
- It does this by evaluating (optional) conditions attached to the fault, the consequence and the propagation arcs that link fault to consequence in a scenario. If any condition in the chain fails, the scenario is suppressed.
- The FMS conditions are implemented by a system of predicates and functions, which use information on the fluids in the plant, and their properties.
- A number of sources of information are integrated by the FMS in providing the rule-based checks. These sources include information provided in the plant model on fluids present, their temperatures and pressures, as well as internal and external program modules for determining physical property values.
- The FMS also does some reasoning about the limits of process variable deviations in scenarios, and their ability to cause the consequences they are linked to.

The choice of fault propagation as a model for scenario development was a good one, despite the consequent limitation of HAZOP emulation to single fault, single consequence scenarios. Once the capability to conduct practically useful HAZOP emulation studies on real industrial problems has been demonstrated, the model of scenario development may be widened to include more complicated constraints between events.

The SDG is a very useful formalism for building models of equipment suitable for representing fault propagation. It allows the causal links between variables to be stated in a quite natural way. Search on the SDG is also probably the most efficient model for inference which could have been chosen.

The frame-based models in AutoHAZID make use of inheritance and are organised into a hierarchy of types within the unit model library. The definition of equipment models in this way facilitates the easy construction of plant models with a minimum of externally supplied information. Maintenance of the unit model library is eased by the hierarchical nature of the model frames, and by use of template models, which cut down on the number of arcs in the unit models by modelling commonly observed features of equipment models. Proliferation of unit models in the library, to cover multiple subtypes of more general models, is reduced by the use of attribute-conditional model sections in the more general model frames. These factors all contribute to making the model library easy to use when creating plant models or adding new unit models.

Despite the success of the qualitative SDG based approach to modelling hazardous scenarios, there are problems which cannot be solved using just qualitative fault propagation. Such problems are related to dependencies which are not represented in the qualitative graph models. For example, the linear model of fault propagation in AutoHAZID does not allow for simultaneous events to be modelled (*i.e.* no "AND" logic). Also, there is no representation of the dependency of scenarios on the properties of plant fluids, in the simple SDG.

The FMS was introduced as a means of adding dependencies outside the immediate scope of linear propagation of process variable deviations. It allows properties of the fluids in the plant (as well as other plant information) to be used in the evaluation of conditions which allow the verification of fault paths. The model of fault path verification used in the FMS mimics some features of scenario development in the real plant. In order for a deviation to cause a consequence, it must have a sufficient magnitude, for instance.

In formulating conditions for the FMS, the modeller is given the option of making use of external physical properties packages to determine fluid property values, or of using information resources within the AutoHAZID program itself. This demonstrates the versatility of the integrated HAZID package, which also provides access to plant descriptions prepared in the Graphical Tool.

Due to the application of the FMS, the focus of HAZOP results produced by AutoHAZID was improved and the quantity of irrelevant output was reduced. This added significantly to the value of the HAZOP emulation results.

Quite separately from the development of the FMS, an innovative new extension to the SDG was developed, to model single mapping influences, where the usual dual mapping SDG arcs are not sufficient to capture the real influences in some equipment. This extension (using code numbers to represent the single mapping influences) seems to be the most specific enhancement possible within the framework of the SDG – any further change would require a more radical change to the model system.

The experience of developing the "flow path" modelling technique, for fluid flow and pressure propagation, was particularly valuable. A number of methodological issues were highlighted by this effort, including the use of the "causal hierarchy" idea for controlling and simplifying the scope of permitted influences between variables. It is likely that this approach to solving modelling problems could be used elsewhere.

None of the research groups reviewed in Chapter 2 have tackled the HAZOP emulation problem as comprehensively as we have at Loughborough. It appears that we have a program capable of making use of a wider range of equipment to study much larger case study plants. However, there are still problem areas in this domain, as discussed in Chapter 6. A few of these are summarised below:

- There is no means at present to model state-dependent behaviour and temporal sequences of events.
- Non-process aspects of the plant model are not represented well. The constraints imposed by operating instructions, instrument systems, and spatial relationships between equipment (for domino effect prediction), could all be modelled.

- The topology of SDG models, and that of the plant itself, can be examined to extract information about higher level constraints in the plant (*e.g.* mass balance constraints). This could help tackle ambiguity problems in HAZOP emulation.
- The representation of fault propagation could be extended, in terms of making fault and consequence events equivalent in the SDG, and allowing a taxonomy of such events. The latter measure could simplify equipment models greatly.
- The use of ad hoc rules, outside the equipment and fluid modelling systems, should be re-examined. Examples are the rules to prevent propagating reverse flow deviations through leaking units, or to prevent anomalous influences being reported in feedback loops.
- For industrial acceptability, all model development should be carried out using a methodology which ensures consistent model quality and documentation.

Solving the problems above, related to representation of all aspects of the plant and its behaviour, will significantly widen the scope of hazards which can be identified.

The most immediate problem for the future use of HAZOP emulation is (automated) access to plant descriptions. Software links to existing CAD or intelligent CAD packages must be defined (possibly using STEP file transfer) in order to make the use of a HAZOP emulator worthwhile.

In conclusion, HAZOP emulation by computer is potentially worthwhile, and the qualitative approach is the right one for basic modelling of fault propagation. Qualitative reasoning is an efficient form of simulation which mimics human-like thought processes. However, there are unavoidable problems with a purely qualitative approach, which cannot be solved without the use of some quantitative information.

Such information should not rely on numerical simulation of the process, because this requires too much numerical data. Verifying hazard scenarios, by testing fluid-dependent conditions attached to the qualitative models in the hazard identifier, seems to tackle the problem at an appropriate level of detail.

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Appendix A : Outline of the AutoHAZID Package

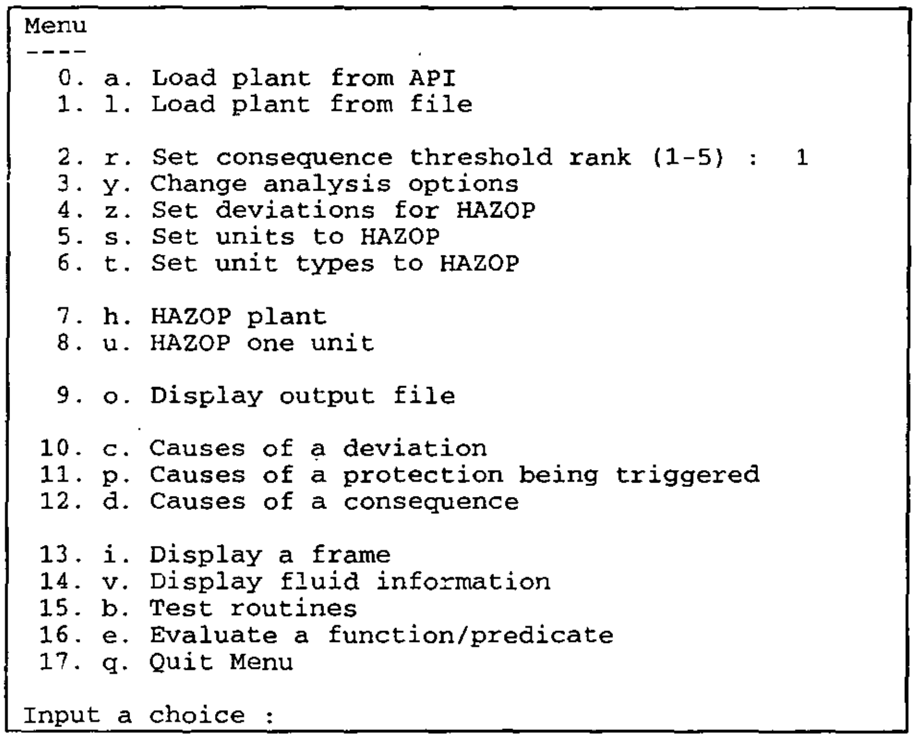
AutoHAZID is a text-based program which is embedded, for the purposes of a Windows-based implementation, in a very simple Windows graphical user interface. Nevertheless, the main interface between the user and the program is by interaction with a text-based menu system, and the program can still be used as a (separately compiled) UNIX application. This appendix outlines the start-up procedure for the HAZID program and the options available on the program's main menu, and finally gives a sample of the type of output produced by HAZOP emulation.

A.1 Program Start-up

This section outlines the start up procedure of AutoHAZID, placing emphasis on the Windows version of the program. Double clicking on the AutoHAZID icon starts up a "wrapper" program, which displays a window with just two menus and two menu items ("Start HAZID" and "Exit"). This program only configures a link to the API database used in HAZID and allows the user to start the AutoHAZID program proper.

As an alternative to starting AutoHAZID in this way, a number of command line options can be used. These have been designed mainly for use with the UNIX version of the program but are available in all versions. They allow the user to specify that the program should perform certain tasks in a "non-interactive" mode before starting the program's main menu. The command line options are not discussed further here, but are documented in the Advanced User Options Section of the AutoHAZID documentation (STOPHAZ Project, 1997b, Appendix 4).

Start-up continues as follows. After initialising the text menus and the Windows interface, AutoHAZID reads the configuration settings file, `hazpaths.dos`. This allows some optional aspects of the program configuration to be specified, as well as giving the names of files to be read into the program, directories in which to store HAZOP results, *etc.* Other files read in during the start-up phase give information on translations of model names between the API and the unit model library, details of permitted deviation names in the SDG and details of standard consequence types. Details of which variables in the plant model are considered to propagate upstream and downstream between connected units are set up by a "hard-wired" routine in the program itself. The program then attempts to make a link to the physical properties package specified in the configuration file. Next it reads in the template library, the unit model library and the fluid library files, using the parser, and sets up a list of `Fluid` objects for storing the information from the fluid library. The main menu for interaction with the user is then started. The main menu appears as in Figure A.1 below.



```
Menu
----
  0. a. Load plant from API
  1. l. Load plant from file

  2. r. Set consequence threshold rank (1-5) :  1
  3. y. Change analysis options
  4. z. Set deviations for HAZOP
  5. s. Set units to HAZOP
  6. t. Set unit types to HAZOP

  7. h. HAZOP plant
  8. u. HAZOP one unit

  9. o. Display output file

 10. c. Causes of a deviation
 11. p. Causes of a protection being triggered
 12. d. Causes of a consequence

 13. i. Display a frame
 14. v. Display fluid information
 15. b. Test routines
 16. e. Evaluate a function/predicate
 17. q. Quit Menu

Input a choice :
```

Figure A.1 : AutoHAZID Main Menu

The main options available from this menu are described in the following sections. The options are selected by typing either the number or the letter listed, in response to the "Input a choice :" prompt.

A.2 Load Plant from API or Text File

In the Windows implementation of AutoHAZID, there are two options for loading a plant description into the program: from the Database API or from a manually keyed text file. The UNIX version of the program only offers the latter option.

If the user elects to load a plant description from the API, the first action of the program is to remove from memory details of any previously loaded plant. It then asks the user to choose a plant description from the list of those available in the database. The next step is for the program to read all the data in the database associated with this plant and write the information to a text file in the same format as would be required for a keyed-in plant description. Once the file has been produced, it is read back into AutoHAZID through the parser, and various internal data are initialised as in the case below, where a plant model is read from a file.

If the option to load a plant description from a text file is chosen, the user is prompted to give the name of the file (the existence of which is verified); then the details of any previous plant description are removed from memory. The file is read into the program through the parser and the various data structures associated with the plant model are initialised. Initialisation includes connecting units to one another within the plant model, checking that mandatory port connections have been made, preparing lists of information concerned with splitting the plant up into "lines" for HAZOP, checking protection devices, *etc.* The SDG model of the plant is constructed and indexed for efficient access at this point, and the information on the fluids present in the plant is propagated throughout the plant model.

A.3 HAZOP Analysis of Whole Plant or Single Unit

Once a plant model has been loaded into AutoHAZID, a HAZOP study can be carried out on it. From the main menu, the user can choose to perform a full HAZOP on the whole plant model, or to HAZOP only one unit, in the sense that only the deviations belonging to that unit will be examined for causes and consequences.

In the "HAZOP plant" option, the whole plant is examined, subject to the scope settings described in Section A.4. These allow the user to choose which units, unit types or deviations to include in the analysis.

When the user chooses to run a HAZOP on the whole plant, the program first asks for an output file name (which must not exist already in the results directory) and then asks the user if they wish to define the order in which units are examined. If the user does not want to order the units, the program will do this automatically, using its own breakdown of the plant into flow lines. Manually choosing the order of units requires that the user type the identifying numbers of units, which are indicated by AutoHAZID in a list, in the user's preferred order. When the order of units has been decided, the program goes on to perform a HAZOP analysis of the plant, printing results to the specified file when it has finished. An example of the type of results file typically produced by HAZOP emulation is given in Section A.8 of this appendix.

The "HAZOP one unit" option is simpler, in that it asks for a unit name and a file name to send the results to, then goes on to examine the named unit and print the results to the named output file. The menu option "Display output file" can be used in the Windows version of AutoHAZID to display the results produced by HAZOP emulation, or the text file can be examined using any text editor or similar program.

Some details of the processing that goes on in the HAZOP algorithm arc given in Appendix B.

A.4 Scope of HAZOP

AutoHAZID allows the user to set up a restricted scope for the units and/or deviations to be examined in the HAZOP analysis. Options are presented for the user to choose which units, unit types or deviations will be examined in the HAZOP which is subsequently initiated as described in Section A.3 above. This is implemented in three "toggle menus", which allow the user to switch on or off different options in the lists given.

A.5 Flags for Reporting and Filtering

A number of features of the HAZOP analysis and reporting procedure are controlled by flags which may be manipulated by the user. These are present in the "Set consequence threshold" item on the main menu and in the "Change analysis options" sub-menu, accessible from the main menu:

- Set consequence threshold. This option allows for consequences below the given severity threshold to be eliminated from the results set produced by HAZOP. Each of the consequences in the unit models has an associated consequence severity ranking, in the range 1 to 5, where 1 is least severe and 5 is most severe.

In the "Change analysis options" sub-menu the following choices can be made:

- Display faults with no consequences. If this reporting option is on, then faults not associated with any consequence will be reported in the HAZOP report. This increases the size of the report significantly.
- Display consequences with no causes. If on, this reporting option will leave in the report all consequences found linked to a deviation, including those which were not associated with any cause found by fault propagation.
- Filter out repeat faults. When many similar faults are reported as causes of the same deviation, the repetition can be distracting. Therefore, it is possible to remove all but one of the similar faults in the results, incidentally modifying the fault description by adding "etc." to it. If this filtering option is switched on, the program will eliminate repetitions of faults with the same descriptor string, belonging to units in the same "line", with the same unit type.
- Filter out repeat fault-consequence pairs. This is a reporting option to remove repetitions of scenarios, which otherwise may be reported for a number of different deviations.
- Display protections present. This option controls whether the program will look for (and report) any protective devices in association with scenarios it identifies.

- Only display faults with no protections. When the "Display protections" option is turned on, this option controls whether scenarios which have protections associated with them will be reported.
- Use fluid model defaults. This is a switch for de-activating the fluid modelling system, so that certain queries will return default answers.

Section 4.4 also discusses the above features for filtering and reporting, in the context of the methods used in AutoHAZID to improve on the unfiltered output from fault propagation.

A.6 "Causes-Of" Options

Three options are provided in AutoHAZID to allow the user to request explanations of HAZOP results from the program. These give a way for the human user to look directly at the fault paths generated by the machine, to see if there is some problem or unappreciated feature in the HAZOP results as produced. The options are:

- Causes of a deviation. The user identifies a variable deviation to the program, which then performs a search to find all faults which cause the deviation. It displays the fault paths in order of length.
- Causes of a protection being triggered. For a plant in which there are some protective units, this option is used to find fault paths which will cause those protections to operate. The user chooses a protection in the plant and the program displays the fault paths it finds, in order of length.
- Causes of a consequence. The user chooses one of the defined consequences for a unit in the plant model and the program then searches for fault paths leading to that consequence. It displays the fault paths in order of length.

A.7 Other Options

A few options are available on the AutoHAZID menu which have been used mainly for testing the program and accessing information about the plant or models within it. These are not present in the released versions of the program, but are nevertheless quite useful sometimes:

- Display frame. This allows the user to see the information in the program on particular unit models or instances of those models in the plant.
- Display fluid information. This option allows the information on fluids present in the plant to be displayed, either for the whole plant model or for a single particular unit in the plant.
- Test routines. Used during program development, this option may be attached to any function which needs to be tested in isolation from the mainstream activities of AutoHAZID. At the moment, this option activates a simple function to analyse the forwards and backwards branching factors of the plant SDG in memory at the time.
- Evaluate function or predicate. This option provides access to the functions and predicates of the fluid modelling system (see Chapter 5). The user types an item to be evaluated and a "context" unit for the query, and the program activates an FMS query to evaluate the item.

A.8 Example of HAZOP Report produced by AutoHAZID

The text below gives an example of the type of output produced by HAZOP emulation by AutoHAZID. It is an output file produced for the water separator example cited by Lawley (1974).

```
Report for FULL PLANT HAZOP.

HAZOP started at     Sun Mar 07 11:47:34 1999

HAZOP completed at   Sun Mar 07 11:51:41 1999

                  -------------------------------------------

Library Used    :    library2

Plant Used      :    plants\lawley.pl
Results File    :    results\lawley.txt
Templates File  :    tlib
Fluids File     :    fluidlib


Flag Settings Used

display faults with no consequences          NO
display consequences with no causes          NO
filter out repeat faults                     YES
filter out repeat fault-conseq pairs         YES
display protections present                  NO
only display faults with no protections      YES
consequence rank threshold set at            1

                  -------------------------------------------

-----------------------------------------------------------------------------
|DEVIATION      |CAUSE                                 |CONSEQUENCE       | |
-----------------------------------------------------------------------------
|heatExchanger1 |tail1 leak to environment,            |toxic release 2,  | |
|moreFlow tubeIn|heatExchanger1 leak to environment    |fire/explosion risk 2| |
-----------------------------------------------------------------------------
|heatExchanger1 |dummyHead3 high temp upstream         |tube overtemperature| |
|moreTemp tubeIn|                                      |rupture 3         | |
-----------------------------------------------------------------------------
|heatExchanger1 |valve2 leak to environment,           |toxic release 2,  | |
|lessFlow       |flowControlValve1 leak to environment |fire/explosion risk 2| |
|shellIn        |                                      |                  | |
-----------------------------------------------------------------------------
|heatExchanger1 |tail2 leak to environment,            |fire/explosion risk | |
|moreFlow       |heatExchanger1 leak to environment    |2,  toxic release 2 | |
|shellIn        |                                      |                  | |
-----------------------------------------------------------------------------
|heatExchanger1 |bufferTank1 moreTemp topLiquid,       |shell overtemperature| |
|moreTemp       |pumpJ2 external fire                  |rupture 2         | |
|shellIn        |                                      |                  | |
-----------------------------------------------------------------------------
|heatExchanger1 |pumpJ2 leak to environment            |fire/explosion risk | |
|moreComposition|                                      |2,  toxic release 2 | |
|shellIn        |                                      |                  | |
-----------------------------------------------------------------------------
|heatExchanger1 |dummyHead3 high pressure upstream,    |tube overpressure | |
|morePressure   |tail1 high pressure downstream        |rupture 3         | |
|tube           |                                      |                  | |
-----------------------------------------------------------------------------
|heatExchanger1 |flowControlValve1 control failure - open, |freezing fluid | |
|lessTemp tube  |heatExchanger1 (etc) leak to environment, |blockage in tubes 3 | |
|               |heatExchanger1 tube rupture,          |                  | |
|               |pumpJ2 morePressure out,              |                  | |
|               |heatExchanger1 interface failure,     |                  | |
|               |tail2 leak to environment,            |                  | |
|               |dummyHead3 low temp upstream,         |                  | |
|               |dummyHead3 low pressure upstream,     |                  | |
|               |tail2 low pressure downstream,        |                  | |
```

	tail1 complete blockage downstream, heatExchanger1 tube blockage, flowControlValve1 passes when no flow is desired, dummyHead3 no flow upstream, bufferTank1 lessTemp topLiquid, tail1 high pressure downstream			
heatExchanger1 morePressure shell	pumpJ2 morePressure out, tail2 high pressure downstream	shell overpressure rupture 2		
heatExchanger1 lessTemp shell	flowControlValve1 control failure - open, heatExchanger1 (etc) leak to environment, heatExchanger1 fouling, dummyHead3 low pressure upstream, heatExchanger1 tube rupture, dummyHead3 no flow upstream, tail2 low pressure downstream, tail2 leak to environment, tail1 complete blockage downstream, flowControlValve1 passes when no flow is desired, tail1 high pressure downstream, heatExchanger1 tube blockage, pumpJ2 morePressure out, bufferTank1 lessTemp topLiquid, bufferTank1 lessLevel topLiquid, dummyHead3 low temp upstream	freezing fluid blockage in shell 3		
heatExchanger1 maintenance	heatExchanger1 no drains available	inadequate isolation and drainage 2		
dummyHead3 lessFlow out	dummyHead3 leak to environment	fire/explosion risk 2, toxic release 2		
dummyHead3 revFlow out	tail1 high pressure downstream, dummyHead3 low pressure upstream, heatExchanger1 tube rupture	possible upstream contamination 3		
tail1 noFlow in	dummyHead3 no flow upstream, tail1 complete blockage downstream, heatExchanger1 tube blockage	loss of production/revenue 2		
bufferTank1 lessFlow in1	halfMileLine leak to environment, valve4 (etc) leak to environment, valve5 leak to environment, levelControlValve leak to environment, valve1 leak to environment	toxic release 2, fire/explosion risk 2		
bufferTank1 moreFlow in1	levelControlValve control failure - open, bufferTank1 lessPressure vapour, pumpJ1 morePressure out, valve5 opened or passing, levelControlValve passes when no flow is desired	incomplete phase separation 3		
bufferTank1 morePressure in1	bufferTank1 unacceptable equipments in vent lines	inadequate pressure relief on vessel 5		
bufferTank1 lessFlow in2	pressCntrlValve2 leak to environment	toxic release 2		
bufferTank1 moreFlow out1	pumpJ2 leak to environment, bufferTank1 morePressure vapour, bufferTank1 lessLevel topLiquid, bufferTank1 moreLevel topLiquid	incomplete phase separation 3		
bufferTank1 moreFlow out2	pressCntrlValve1 leak to environment	fire/explosion risk 2, toxic release 2		
bufferTank1 moreFlow out3	valve6 leak to environment	non-hazardous release 1		
bufferTank1 lessPressure vapour	bufferTank1 vapour leak to environment	flammable vapour release 2, vessel depressurisation 2, toxic vapour release 2		

	pressCntrlValve1 control failure - open, pressCntrlValve2 control failure - closed, bufferTank1 lessTemp topLiquid, pressCntrlValve1 (etc) leak to environment, pressCntrlValve2 (etc) leak to environment, dummyHead2 low pressure upstream, pressCntrlValve1 passes when no flow is desired	vessel depressurisation 2	
bufferTank1 morePressure vapour	pressCntrlValve2 control failure - open, pressCntrlValve1 control failure - closed, pressCntrlValve2 passes when no flow is desired, bufferTank1 moreTemp topLiquid, dummyHead2 high pressure upstream, tail3 incorrect sizing	possible overpressure rupture 2	
bufferTank1 moreTemp vapour	dummyHead2 high temp upstream, bufferTank1 external fire, bufferTank1 moreTemp topLiquid	design temp exceeded - structural weakening 2	
bufferTank1 moreLiquid vapour	levelControlValve control failure - open, bufferTank1 moreLevel topLiquid, levelControlValve passes when no flow is desired, bufferTank1 lessPressure vapour, pumpJ1 morePressure out, valve5 opened or passing	liquid droplet entrainment 3	
bufferTank1 moreTemp topLiquid	pumpJ1 external fire, bufferTank1 external fire, dummyHead1 high temp upstream, halfMileLine external fire	design temp exceeded - structural weakening 2	
bufferTank1 contamination topLiquid	dummyHead1 upstream contamination, pumpJ1 ingress of lubricant or seal fluid into pump	liquid contents contaminated 3	
bufferTank1 lessLevel topLiquid	bufferTank1 liquid leak to environment	gas breakthrough 3, toxic liquid release 2, flammable liquid release 2	
	levelControlValve fails closed, levelControlValve control failure - closed, valve5 (etc) leak to environment, pumpJ2 leak to environment, bufferTank1 liquid leak to environment, valve6 (etc) leak to environment, bufferTank1 morePressure vapour, valve1 partly closed, valve4 (etc) leak to environment, valve1 (etc) leak to environment, valve4 (etc) closed, pumpJ1 noFlow out, pumpJ1 lessPressure out, levelControlValve (etc) leak to environment, valve3 (etc) partly closed, halfMileLine (etc) leak to environment, halfMileLine blockage, valve1 closed, pumpJ1 revFlow out, dummyHead1 low composition upstream	gas breakthrough 3	
bufferTank1 moreLevel topLiquid	levelControlValve control failure - open, bufferTank1 lessPressure vapour, pumpJ1 morePressure out, valve5 opened or passing, levelControlValve passes when no flow is desired	vessel overfilling 2	
	valve6 partly closed, pumpJ2 noFlow in, tail4 high pressure, pumpJ2 revFlow out,	liquid droplet entrainment 3, vessel overfilling 2	

	dummyHead1 high composition upstream, valve6 closed			
bufferTank1 lessTemp botLiquid	bufferTank1 lessTemp topLiquid	freezing fluid in sump - blockage of drain outlet 2		
bufferTank1 lessLevel botLiquid	dummyHead1 low composition upstream, bufferTank1 liquid leak to environment, valve6 (etc) leak to environment, bufferTank1 morePressure vapour	incorrect liquid out 3		
	bufferTank1 lessPressure vapour, bufferTank1 moreLevel topLiquid, bufferTank1 lessLevel topLiquid	incorrect liquid out 3, gas breakthrough 3		
bufferTank1 maintenance	bufferTank1 no vents available	inadequate isolation and drainage 2		
dummyHead2 lessFlow out	dummyHead2 leak to environment	toxic release 2		
dummyHead2 revFlow out	dummyHead2 low pressure upstream	possible upstream contamination 3		
tail4 moreFlow in	tail4 leak to environment	possible treatment system overload 3, non-hazardous release 1		
	bufferTank1 moreLevel topLiquid, bufferTank1 morePressure vapour	possible treatment system overload 3		
tail4 morePressure in	bufferTank1 moreLevel topLiquid, bufferTank1 morePressure vapour	possible drain system overpressure 2		
tail3 moreFlow in	pressCntrlValve1 control failure - open, tail3 incorrect sizing, bufferTank1 morePressure vapour, pressCntrlValve1 passes when no flow is desired	fire hazard at outlet 3, toxic hazard at outlet 3		
tail3 revFlow in	pressCntrlValve1 leak to environment	fire/explosion risk 4		
tail3 moreComposition in	dummyHead1 high composition upstream, dummyHead2 high composition upstream	toxic hazard at outlet 3, fire hazard at outlet 3		
tail3 contamination in	dummyHead2 upstream contamination	environmental contamination 3		
pumpJ2 revFlow in	tail2 high pressure downstream, pumpJ2 loss of drive, pumpJ2 incorrect pump setup/installation	possible suction piping overpressure 2, seal failure due to reverse impeller rotation 2		
pumpJ2 lessPressure in	bufferTank1 lessLevel topLiquid, pumpJ2 leak to environment, bufferTank1 lessPressure vapour	cavitation - possible mechanical damage 3		
pumpJ2 lessTemp in	bufferTank1 lessTemp topLiquid	seal failure - freezing of seal fluids 2		
pumpJ2 moreGas in	bufferTank1 lessLevel topLiquid	vapour lock 3, pump damage - increased vibration 3, bearing overheat - loss of lubrication 3		
pumpJ2 moreVapour in	bufferTank1 moreTemp topLiquid, pumpJ2 external fire	cavitation - possible mechanical damage 3		
pumpJ2 moreFlow out	bufferTank1 morePressure vapour, pumpJ2 lessPressure out	possible motor overload or trip 3		
pumpJ2 noFlow out	flowControlValve1 fails closed, valve2 closed,	possible seal overtemperature 2,		

	tail2 complete blockage downstream, heatExchanger1 shell blockage	possible pump casing overtemperature 2
pumpJ2 morePressure out	flowControlValve1 control failure - closed, pumpJ2 pressure surge at startup or shut-down, bufferTank1 morePressure vapour, pumpJ2 noFlow out, tail2 high pressure downstream, valve2 partly closed	possible seal overpressure 2, possible pump casing or delivery pipework overpressure 2
pumpJ2 moreTemp out	bufferTank1 moreTemp topLiquid, pumpJ2 external fire	possible pump casing overtemperature 2, possible seal overtemperature 2
pumpJ2 maintenance	pumpJ2 no drains available	inadequate isolation and drainage 2
pumpJ2 startup	pumpJ2 no pressure sensor on pump delivery	cannot monitor pressure development at start-up 4
tail2 noFlow in	flowControlValve1 fails closed, valve2 closed, heatExchanger1 shell blockage, tail2 complete blockage downstream, pumpJ2 noFlow out	loss of production/revenue 2
pumpJ1 lessFlow in	valve7 (etc) leak to environment	fire/explosion risk 2, toxic release 2
pumpJ1 moreFlow in	pumpJ1 leak to environment	fire/explosion risk 2, toxic release 2
pumpJ1 noFlow in	dummyHead1 no flow upstream, valve7 closed	dry running - possible pump rupture 2
pumpJ1 revFlow in	valve7 leak to environment, pumpJ1 incorrect pump setup/installation, dummyHead1 low pressure upstream, pumpJ1 loss of drive	possible suction piping overpressure 2, seal failure due to reverse impeller rotation 2
pumpJ1 lessPressure in	valve7 (etc) leak to environment, pumpJ1 leak to environment, dummyHead1 low pressure upstream, valve7 partly closed, valve8 opened or passing	cavitation - possible mechanical damage 3
pumpJ1 morePressure in	pumpJ1 unit can be locked in	potential for liquid lock in and damage to unit by thermal expansion 3
pumpJ1 lessTemp in	dummyHead1 low temp upstream	seal failure - freezing of seal fluids 2
pumpJ1 moreVapour in	dummyHead1 high temp upstream, pumpJ1 external fire	cavitation - possible mechanical damage 3
pumpJ1 moreFlow out	dummyHead1 high pressure upstream, pumpJ1 lessPressure out	possible motor overload or trip 3
pumpJ1 noFlow out	levelControlValve fails closed, valve1 closed, valve4 (etc) closed, halfMileLine blockage	possible pump casing overtemperature 2, possible seal overtemperature 2
pumpJ1 morePressure out	levelControlValve control failure - closed, valve4 (etc) partly closed, pumpJ1 noFlow out, pumpJ1 pressure surge at startup or shut-down, valve1 partly closed, dummyHead1 high pressure upstream	possible seal overpressure 2, possible pump casing or delivery pipework overpressure 2

pumpJ1 moreTemp out	dummyHead1 high temp upstream, pumpJ1 external fire	possible pump casing overtemperature 2, possible seal overtemperature 2	
pumpJ1 maintenance	pumpJ1 no vents available	inadequate isolation and drainage 2	
pumpJ1 startup	pumpJ1 no pressure sensor on pump delivery	cannot monitor pressure development at start-up 4	
halfMileLine morePressure in	halfMileLine unit can be locked in	potential for liquid lock in and damage to unit by thermal expansion 3	
	levelControlValve control failure - closed, pumpJ1 morePressure out, valve4 (etc) partly closed	possible overpressure rupture or leakage 3	
halfMileLine moreTemp out	dummyHead1 high temp upstream, halfMileLine external fire, pumpJ1 external fire	design temp exceeded 2	
halfMileLine maintenance	halfMileLine no drains available	inadequate isolation and drainage 2	
dummyHead1 lessFlow out	dummyHead1 leak to environment	toxic release 2, fire/explosion risk 2	
dummyHead1 revFlow out	pumpJ1 loss of drive, dummyHead1 low pressure upstream, pumpJ1 incorrect pump setup/installation	possible upstream contamination 3	
tail5 moreFlow in	tail5 leak to environment	possible treatment system overload 3, fire/explosion risk 2, toxic release 2	
	valve8 opened or passing	possible treatment system overload 3	
tail5 morePressure in	valve8 opened or passing, tail5 blockage - frozen fluid	possible drain system overpressure 2	

Appendix B : Improved Algorithm for HAZOP Search

This appendix briefly describes the HAZOP algorithm used in AutoHAZID, which was developed to reduce the amount of repeated search which took place in an earlier version. The approach to graph search outlined here may be of general interest for applications other than HAZOP emulation. Firstly, the "traditional" way of modelling the HAZOP study, which forms the basis of the older HAZOP algorithm in AutoHAZID, is outlined. Then, some disadvantages of this method are identified and a more efficient method is suggested.

The purpose of the HAZOP emulation algorithm in HAZID is to imitate the procedure followed by a conventional HAZOP study team in examining the design of a plant, and to produce a table of results in a similar format, using the headings of "deviation", "cause", "consequence" and "protection".

Therefore, the algorithm must examine every deviation of a process variable in the plant model and find faults which could cause that deviation. It must also report consequences of the deviation and consequences of any faults which cause the deviation, as well as the presence of any protective devices which could prevent, or reduce the impact of, the hazardous scenarios found.

From this definition, which closely mirrors the definition of the conventional HAZOP study procedure, the HAZOP algorithm is shown in Figure B.1 below.

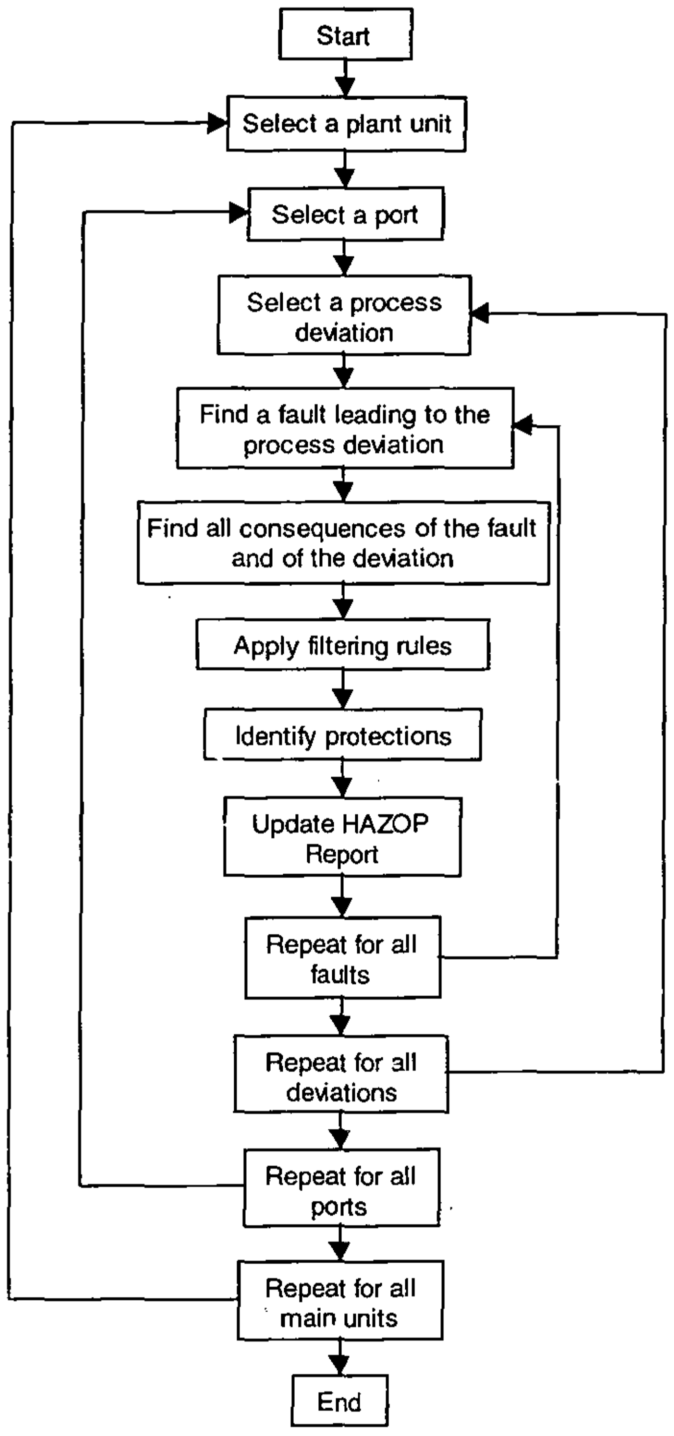

Start
Select a plant unit
Select a port
Select a process deviation
Find a fault leading to the process deviation
Find all consequences of the fault and of the deviation
Apply filtering rules
Identify protections
Update HAZOP Report
Repeat for all faults
Repeat for all deviations
Repeat for all ports
Repeat for all main units
End

Figure B.1 : "Traditional" HAZOP Algorithm

The procedure outlined in Figure B.1 is centred around the analysis of separate deviations. Firstly the deviation is formulated from a unit, port and deviation guide word applied to a process variable. Then the causes of the deviation are found by searching the SDG, giving a list of the fault paths leading to the deviation. Then the consequences of the deviation and of the faults are added to the results set. Results are filtered and protections added to the results for the deviation. This deviation is then added to the results set. The whole procedure is repeated for every appropriate deviation in the plant.

Because it requires the use of graph search, finding the causes of a deviation is the most costly step in the procedure. Each deviation is associated with a node in the SDG. To find the causes of the deviation, all the paths leading to a change in that node must be found. Then, all paths which do not give rise to the deviation under examination are discarded. This is very wasteful if the HAZOP procedure must actually examine both deviations of the SDG node in due course.

Another source of wasted search effort becomes apparent when considering how the deviations in the HAZOP report may chain together and cause one another. If the causes of deviation D1 have already been established in the HAZOP and, when searching for causes of another deviation D2, D1 is found to be a cause of D2, then the search procedure illustrated above will repeat the search which was done to find the causes of D1. In cases where the whole plant is to be HAZOPed, this is a large source of repeated search effort, which could be avoided with a little more intelligence on the part of the search algorithm.

The HAZOP search algorithm currently used in AutoHAZID is more "intelligent" than the "traditional" algorithm shown above. When finding the causes of a deviation, the new HAZOP emulation approach takes account of other "HAZOPed" deviations and avoids repeating the search for causes of those deviations. The new algorithm proceeds as follows:

- Compile a list of the deviations which need to be "HAZOPed". The content of the list depends on how the user has chosen to have the study performed.
- From the deviation list, compose a list of the SDG nodes which correspond to the deviations (this list is shorter than the list of deviations).

- Search for the causes of any effect on the nodes in this list, using graph search in the SDG. This is a two-stage graph search procedure, which produces a list of fault propagation paths for each node in the list:
    - The first stage of the search involves searching backwards from a subject node, expanding lists of paths backwards, either to originating faults or as far as the first other node also found to be in the list of subject nodes being examined. A number of completed paths will be formed, from a fault to a node, but a number of partial fault paths will also be formed, leading from one "HAZOPed" node to another.
    - The second stage of the search "knits together" the partial paths produced in the previous stage, to form lists of completed paths. Therefore, if there is a partial path linking node N1 to node N2, then all the causes of N1 will be used to compose new paths which end in N2. This second stage search is an iterative procedure, but it avoids a lot of the repeated search inherent in earlier versions of the search algorithm.
- Partition the results of the search into the paths which give rise to each of the deviations in the original deviation list. For each node, paths will usually be produced with both "direct" and "reverse" influences; these usually correspond to "less" and "more" deviations of some process variable in the plant.
- Identify the consequences of the deviations and the faults which cause them, and add information about any protections which operate, putting all these results into lists suitable for transfer to HazRes result objects, prior to formatting and filtering.
- Transfer the results just prepared into new HazRes objects, adding the results of the configuration checking rules.

The function which starts up HAZOP emulation and deals with the collection of results, preparation of deviation lists, different options for analysis, *etc.*, is `PerformFullHazop()`. The function which coordinates the emulation procedure to do a HAZOP on a list of deviations is `full_hazop2()`. The structure of these functions is outlined in Figure B.2 and Figure B.3 below.

The algorithm described here has the effect of cutting down the HAZOP time required for the Lawley case study plant, from 12 minutes to about 4 minutes. These figures should be treated with caution, however, as the former was obtained for the summer 1996 version of AutoHAZID and the latter with the January 1999 version. Differences between the two versions might be significant in favour of a better or a worse speed-up factor.

Also relevant to speed-up considerations is the note produced by Dr. Larkin after the change to the algorithm, which showed that the dependency of run-time on size of plant was much more severe for the old algorithm than the new one (Larkin, 1996).

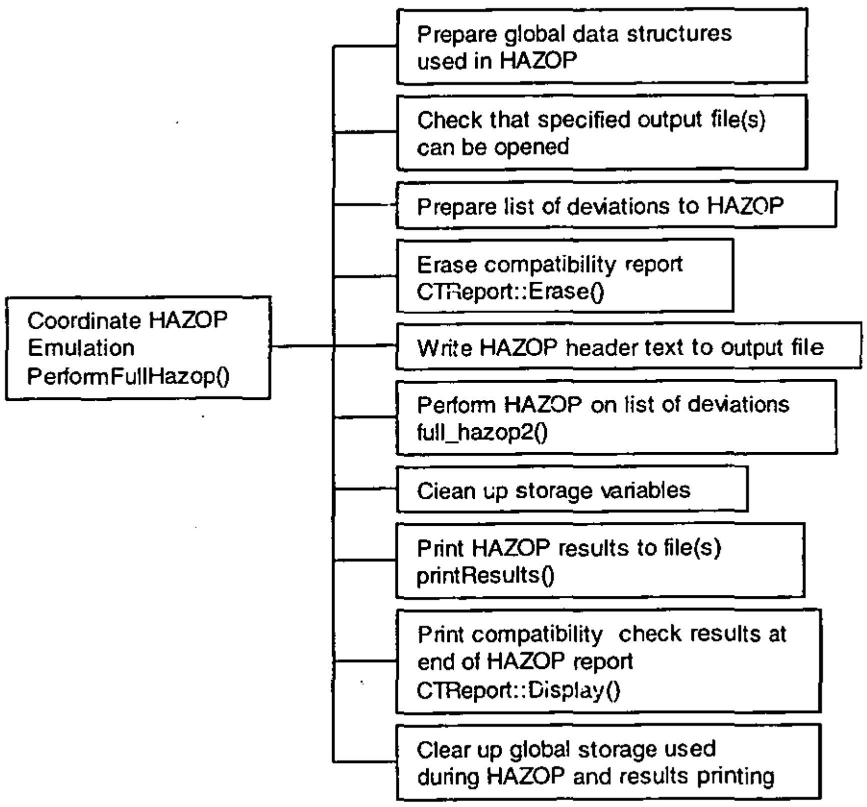

Coordinate HAZOP Emulation PerformFullHazop()
Prepare global data structures used in HAZOP
Check that specified output file(s) can be opened
Prepare list of deviations to HAZOP
Erase compatibility report CTReport::Erase()
Write HAZOP header text to output file
Perform HAZOP on list of deviations full_hazop2()
Clean up storage variables
Print HAZOP results to file(s) printResults()
Print compatibility check results at end of HAZOP report CTReport::Display()
Clear up global storage used during HAZOP and results printing

Figure B.2 : The HAZOP coordinating function, PerformFullHazop()

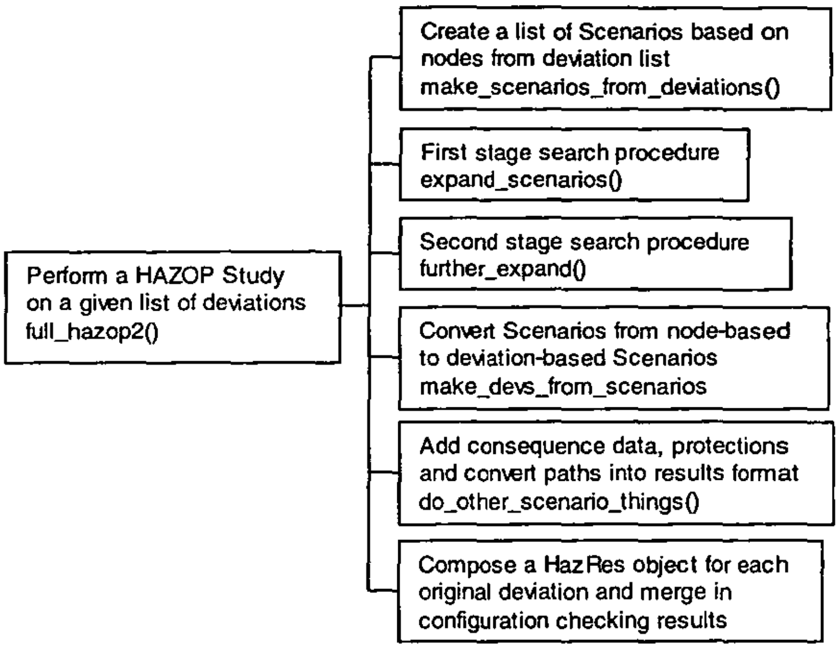

Perform a HAZOP Study on a given list of deviations full_hazop2()
Create a list of Scenarios based on nodes from deviation list make_scenarios_from_deviations()
First stage search procedure expand_scenarios()
Second stage search procedure further_expand()
Convert Scenarios from node-based to deviation-based Scenarios make_devs_from_scenarios
Add consequence data, protections and convert paths into results format do_other_scenario_things()
Compose a HazRes object for each original deviation and merge in configuration checking results

Figure B.3 : The new HAZOP emulation algorithm, full_hazop2()

Appendix C : Flow and Pressure Modelling in Dividers and Headers

The flow path models for flow and pressure propagation presented in Chapter 3 rely on the assumption that the flow path in which flow is considered to occur has only one inlet port and one outlet. For equipment in which that assumption is not valid, the appropriate qualitative model is somewhat more tricky to develop, because of the inherent ambiguity in the mass balance equation (*e.g.* $Q_{in} = Q_{out1} + Q_{out2}$), for a qualitative model. This appendix considers the models of flow and pressure propagation for "tee-pieces": pipes which either split an input flow (dividers), or join multiple flows together (headers). Two of the simplest models are considered here.

Both models contain four locations (ports) where pressure is defined. The divider model has one inlet (*in*), one internal port (*self*) and two outlet ports (*out1* and *out2*). The header model has two inlet ports (*in1* and *in2*), one internal port (*self*) and one outlet port (*out*).

The divider and header models do not contain faults or consequences, just the arcs governing fault propagation through them. There are not many interesting things that can go wrong with a tee-piece, which cannot also occur in other equipment types.

The parts of each model which deal with pressure deviation propagation and the flow deviations *lessFlow* and *moreFlow* are constructed by putting three flow path models together and removing the nodes for resistance in each flow path. Resistance nodes are used in modelling blockages and other faults, so they are not needed.

In use, the flow path models seem to predict accurately most of the expected behaviour of a "tee-piece", with respect to propagation of pressure and the flow deviations, *lessFlow* and *moreFlow*. However, as was the case for unbranched flow paths, *noFlow* and *revFlow* cause significant problems in dividers and headers. No flow is considered in Section C.2 and reverse flow in Section C.3.

A number of possible definitions for the model of a tee-piece are possible. In the divider model presented below, an attempt has been made to make the model as general as possible, so that both legs of the divider are considered to be usually carrying fluid flows. This may not always be the case for actual dividers, where one or both of the legs may be connected to a "blocking" component, such as a closed valve. Such a situation may be best handled by a check on the configuration of the component in the plant model, followed by selection of an appropriate, simpler, model for the divider. AutoHAZID uses this approach.

Another possible complication for building models of general tee-piece components is that controllers may constrain the actual behaviours of the flows and/or pressures in the plant. Typically, in the case of a real divider, some control system would control either the flowrate into the divider, or the pressure near it. It turns out that the deviations possible in the two constrained cases are subsets of those for the unconstrained case. Therefore, the general divider model is suitable for all cases where a control loop is in operation, but will over-predict deviations in these cases.

C.1 Development of divider Model

The latest divider model is shown in Figure C.1 below, including the arcs for modelling *noFlow* and *revFlow*, which are discussed in Sections C.2 and C.3.

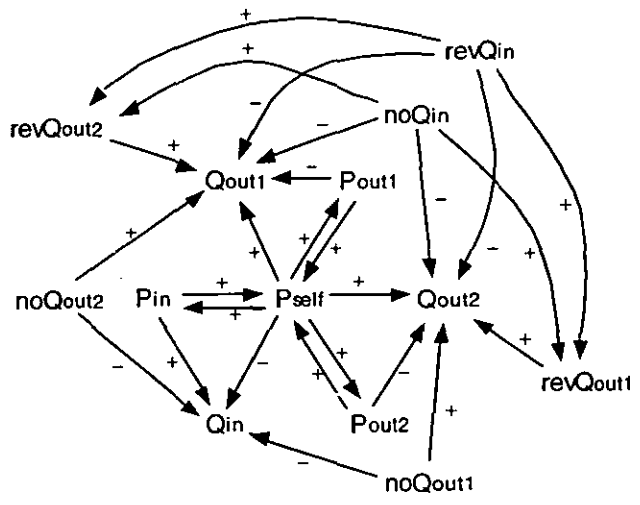


Figure C.1 : Pressure and Flow Propagation Model for a divider

The assumptions used in the above divider model are as follows:

- Flow and pressure are modelled in the unit by considering the flows between, and pressures at, four locations: one inlet port (*in*), one internal location (*self*), and two outlet ports (*out1* and *out2*). *in* is considered to be connected to *self*, and *self* is considered to be connected to both *out1* and *out2*.
- The divider unit is filled with a single phase fluid (either liquid or vapour) and enclosed by rigid walls.
- Density changes in the fluid are not modelled, so that the fluid is assumed to be incompressible, within the scope of the model.
- Fluid in the flow path is considered to normally flow from *in*, *via self*, to *out1* and to *out2*. Therefore, no flow and reverse flow are exceptions to this condition, which require separate consideration in the model. Also, none of the inlet or outlet legs of the divider is considered to be blocked, or attached to a closed or blocked component.

- The flows and pressures in the unit are not constrained by any control system, so that the divider provides modelling for an unconstrained, general case.
- Pressure deviations are allowed to propagate freely from any inlet or outlet to any other port in the unit, upstream or downstream.
- Flow deviations (*lessFlow* and *moreFlow*) are not propagated – they are only generated locally, for each part of the divider.
- The causal hierarchy described in Section 3.5.4 is considered to operate in the divider unit.
- The relevant variables are P and Q, representing pressure and flow. Resistance, R, is not used in this model. *noFlow* and *revFlow* are also present as deviations.
- There is no significant height difference between the locations *in, out1* and *out2*, so that static head is the same everywhere within the unit.
- No shaft work is done on the fluid within the flow path.
- The fluid does not exchange significant quantities of heat with its surroundings.
- Within the SDG model, the shortest path between two nodes determines what the appropriate influence is between those nodes.
- The driving force for flow is pressure difference, which is not represented explicitly in the model. As in the unbranching flow path model presented in Section 3.5.5, upstream pressures have a direct effect on flow, and downstream pressures have a reverse effect.
- Deviations in pressure within the divider are considered never to be sufficient to cause the flow to reverse in the flow path.

C.2 Modelling *noFlow* for the divider

In the unbranched flow path model, *noFlow* was simply propagated between the inlet and outlet, without linkage to other variables in the flow path model. For a divider, however, it is reasonable to expect blockage of one leg to cause deviations in flow and pressure in the other legs.

Unfortunately, it is not possible to put arcs into the model to represent the pressure changes caused by *noFlow* in one of the legs of the divider, because of the effect this has on the flow variable in the same leg as the blockage - the deviation *lessFlow* would be predicted at the same time as the deviation *noFlow* in an outlet leg, for example.

Therefore, the model in Figure C.1 only links *noFlow* to deviations in flow throughout the unit, and to reverse flow in the outlet legs. It may well be the case, however, that the fault which is the root cause of *noFlow* also causes a pressure change, so that these same effects will be propagated independently.

Note that, due to the interpretation of *noFlow* as a blockage event, *noFlow* in any one of the legs of the divider does not imply *noFlow* in either of the other legs - because there is a split in the flow path, fluid is not necessarily blocked by any single blockage.

C.3 Modelling *revFlow* for the divider

As with the unbranched flow path model, pressure is not linked to reverse flow in a divider. This means that the real effect of *lessPressure* in one of the outlets causing *revFlow* in the other outlet is missed in the model presented in Figure C.1, but to put the necessary arc in to achieve this effect would mean that a whole host of other spurious predictions would appear.

The effects that are represented by the *revFlow* model for a divider, are those of *revFlow* on the outlet flows from the unit, and the possible effects of *revFlow* in the inlet port on *revFlow* in the two outlet ports. Reverse flow of fluid in one of the outlets causing a possible reduction in the inlet flow to the divider is not explicitly represented because of the difficulties this would cause. However, the initial fault causing reverse flow should include an effect on pressure, which can propagate to the divider and cause the necessary flow deviations. This underlines the importance once again of using consistent methods for developing failure modes information for equipment in the plant model system.

One further area in which the model fails to represent a recognised real effect, is that the possible reverse flow effect in the inlet, caused by *revFlow* in either outlet leg, is not represented. Again, the problem is that the arcs needed for these links would create so many incorrect additional predictions, that the change was judged not worth putting in.

It may be possible in future to circumvent the problems with determining consistent flow deviations in the legs of the divider, by using quantitative information on pressure deviation limits.

C.4 Development of header Model

The header unit is modelled in the same way as the divider, and the header model produced (Figure C.2 below) is analogous to the divider model presented above.

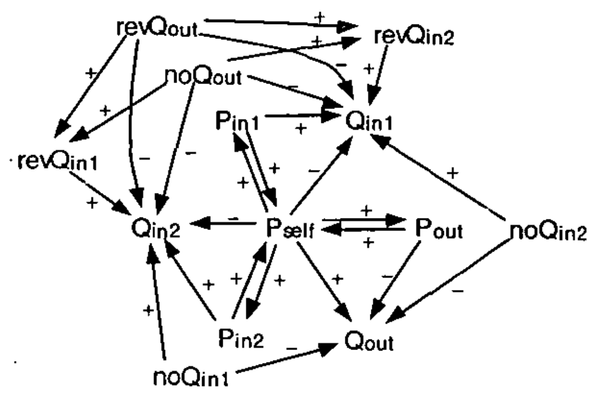


Figure C.2 : Pressure and Flow Propagation Model for a header

The assumptions used in the header model are similar to those for a divider:

- Flow and pressure are modelled in the unit by considering the flows between, and pressures at, four locations: two inlet ports (*in1* and *in2*), one internal location (*self*), and one outlet port (*out*). *in1* and *in2* are considered to be connected to *self*, and *self* is considered to be connected to *out*.
- The header unit is filled with a single phase fluid (either liquid or vapour) and enclosed by rigid walls.

- Density changes in the fluid are not modelled, so that the fluid is assumed to be incompressible, within the scope of the model.
- Fluid in the flow path is considered to normally flow from *in1* and *in2*, *via self*, to *out*. Therefore, no flow and reverse flow are exceptions to this condition, which require separate consideration in the model. Also, none of the inlet or outlet legs of the header is considered to be blocked, or attached to a closed or blocked component.
- The flows and pressures in the unit are not constrained by any control system, so that the header provides modelling for an unconstrained, general case.
- Pressure deviations are allowed to propagate freely from any inlet or outlet to any other in the unit, upstream or downstream.
- Flow deviations (*lessFlow* and *moreFlow*) are not propagated – they are only generated locally, for each flow path.
- The causal hierarchy described in Section 3.5.4 is considered to operate in the header unit.
- The relevant variables are P and Q, representing pressure and flow. Resistance, R, is not used in this model. *noFlow* and *revFlow* are also present as deviations.
- There is no significant height difference between the locations *in1*, *in2* and *out*, so that static head is the same everywhere within the unit.
- No shaft work is done on the fluid within the flow path.
- The fluid does not exchange significant quantities of heat with its surroundings.
- Within the SDG model, the shortest path between two nodes determines what the appropriate influence is between those nodes.
- The driving force for flow is pressure difference, which is not represented explicitly in the model. As in the unbranching flow path model presented in Section 3.5.5, upstream pressures have a direct effect on flow, and downstream pressures have a reverse effect.
- Deviations in pressure within the header are considered never to be sufficient to cause the flow to reverse in the flow path.

Appendix D : Object Types in AutoHAZID

The purpose of this appendix is to give a brief explanation of some of the more useful C++ object classes developed during the STOPHAZ project, for use in the AutoHAZID program. The information presented is technical in nature, describing some of the internal details of the Str, DObject, Location and FPath classes. Further information on all technical aspects of the program can be found in the STOPHAZ project deliverables (STOPHAZ Project, 1997a), or by reference to the source code of the appropriate object classes.

Many of the ideas (coding "idioms") used in the classes described below were inspired by "Advanced C++" by Coplien (1992).

Storing character strings with Str

The Str class is an object class which provides a simpler string handling system than that provided by the usual method in C, which is to consider strings as arrays of characters and access them using character pointers. Some of the better features of the C system are kept, such as accessing individual characters using the square bracket array subscript notation, but the functions available to this class allow a much more intuitive use of character strings.

Str is the class which will be used by programmers, whereas the StRep class supports Str in what it does (see Figure D.1 below). For this reason, StRep functions and data cannot be accessed from outside the scope of the Str and StRep functions.

Str is a reference counted class which uses the StRep class to maintain the storage of the characters and a count of the number of Str objects which share the same StRep object pointer. Str objects themselves can thus be created, copied from others and destroyed more quickly, and using less storage, than would be the case if the characters were stored and allocated for each Str object.

Any number of Str objects can share the same characters using this reference counting method. The StRep object maintains a count of the number of objects which contain a pointer to it. When this count falls to zero the StRep object is destroyed, recovering its own storage and that of the characters in the string. When a Str object is destroyed, only the Str is recovered, unless the count for its StRep object goes to zero.

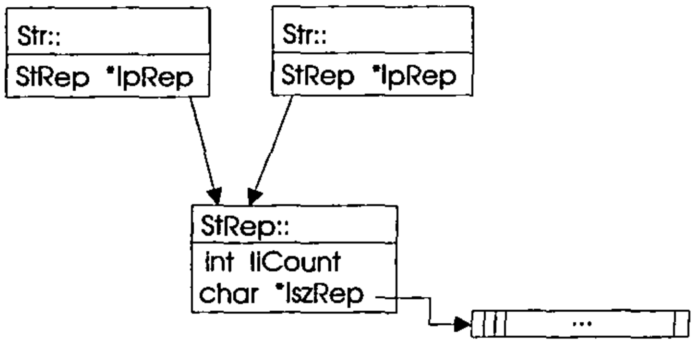


Figure D.1 : Many Strs can share the same characters using StRep objects

Summary Features of the Str class:

- Initialisation from the following types: `Str`, `char*`, `char`, `int` and `double`.
- Conversion to the following types: `char*` (should be used with caution).
- Assignment, copying, construction and destruction without the need to worry about assigning memory.
- Output to streams using the `Display()` function and left shift operator.
- Input from streams using the right shift operator and the `ReadLine()` function.
- Uses integer indexing scheme similar to that used by C arrays, with subscripts running from 0 to (length – 1). Use of array subscript notation (square brackets) in reading single characters in the string. Users of this class should be aware that using an index outside the legal range for a Str object will cause an error or warning.
- Concatenation of `Str` with `Str` or `char*` type character string, uses the functions `Append()` and `Prepend()`.
- Comparison of strings is possible using the equality and inequality operators which are overloaded for this class. Also, an equivalent to the `strcmp()` function is provided in the form of `Compare()`.

- Various "sub-string" operations are defined for splitting up strings. These are modelled on equivalent operations in the BASIC language: `Left(int)`, `Right(int)`, `Mid(int, int)`, `ToRight(int)`, `After(int)`.
- Searching for occurrences of strings within a `Str` is provided by the `Find()` function.
- Conversion to and recognition of numbers is provided in the functions `IsInteger(int&)` and `IsDouble(double&)`.
- Conversion to upper and lower case characters is provided by `ToUpper()` and `ToLower()`, respectively.

DObject

The DObject class is designed to offer many of the symbolic manipulation and pattern matching features of the clauses found in Prolog. This class can store data of many different types and forms quite transparently and can be used to develop prototype applications relatively quickly. However, one concern which may arise from the widespread use of this class is the efficiency of the programs which result.

The motivation for developing this class was that there are many different data types in the AutoHAZID system and there are some areas of the program where a flexible "untyped" data object would be of great use in making the operation of the program more powerful. Examples include the system which is used to represent the rules belonging to the fluid model system, which should allow quite complex structures to be put together to represent rules. Also, the representation of plant models in the system should provide the ability to store new slots and their values in Frame objects, without requiring too many changes to the parser and other code in the system. DObjects here allow the definition of a generalised slot type which stores a list of DObjects as its values.

The DObject class allows objects to be of several types, which are implemented *via* a type field in the object, rather than using some other method (such as C++ based inheritance). The types are enumerated in the enum type DObType, which is declared in the file `dobtype.h`. The types are as listed in Table D.1 below.

Type	Description
Atom	"Constant symbols", as in Prolog. These should start with a lower case letter and include no spaces. Alternatively, they may be enclosed in single quotes (*e.g.* `constant_symbol` or `'flammable atmosphere'`).
Integer	Integer constant values.
Real	Real number values, implemented using double precision floating point numbers in C++.
Variable	Variable symbols, as in Prolog. The variable name should start with an upper case letter or an underscore character (*e.g.* `UnitName` or `_variable125`).
Structure	Similar in form to a predicate term in Prolog. An identifier which has the same format as an Atom, followed by a list of terms (each of which may be an object of one of the types listed here), separated by commas and enclosed in round brackets (*e.g.* `equals(4, plus(2,2))`).
StrType	Strings of characters, enclosed in double quotes (*e.g.* `"hello world"`).
ListType	Lists of terms, which may be any of the types listed here) separated by commas and enclosed in square brackets (*e.g.* `[a,b,[4,5.02],Var1]`).

Table D.1 : Data types stored in the DObject class

With a class which allows this sort of flexibility in the range of information it can store, it is possible to build programs which perform quite powerful symbolic operations, such as pattern matching. This feature is built into the DObject class, in the form of the `UnifyMatch()` function, which allows one DObject to be matched against another, making allowances for variables in each term.

The DObject class is a reference counted class, using the DObRep class to store the data which it manipulates. The DObRep class remains invisible to the user, hidden behind the public interface of the DObject class. The data which are stored include the following (which may not all be in use at any one time):

- A string giving the "name" of the DObject, used for Atom, Variable, Structure and StrType objects.
- An integer value for the DObject, used only for Integer type DObjects.
- A double precision floating point number value, used for the Real type.

- A DObList (list of DObjects) which comprises the argument list of a Structure type DObject, or the list elements of a ListType DObject.

The relevant files for defining and implementing the DObject class are: `dobject.h`, `dobject.cpp`, `dobrep.h`, `dobrep.cpp`, `doblist.h`, `doblist.cpp`, `dobtype.h`, `newparse.h`, and `newparse.cpp`. The Binding class is also closely related to the DObject class and must be present for any of the advanced matching functions of DObject to be used.

The main features of the DObject class are:

- The usual set of constructors, destructor and assignment definitions are provided so that DObjects can be declared, assigned and copied, destroyed and passed as function arguments, just as if they were a built-in type of the C++ language, such as `int` or `double`.
- Other constructors allow the programmer to initialise DObjects of any type given in Table D.1, by providing the data needed to set up the new object.
- The DObject type can be automatically assigned or constructed from a Str object, using parsing code implemented in the file `newparse.cpp`. It can also be converted back to Str form, using a conversion operator defined for that purpose.
- Read and write access to the data members of the DObject is provided by a set of member functions, which include functions to read or change specific elements of a ListType or Structure DObject and to add new elements to a Structure or ListType.
- Two functions are provided for displaying the contents of the DObject. The function `Display()` simply prints the contents of the object out to a single line on the output stream given, while the `Pretty()` function prints the DObject out to the output stream on multiple lines if needed, making sure that the length of each line is not greater than a given number of characters.
- The function `ExactMatch()` allows the programmer to compare DObjects together where every part of one object must match the other one exactly.

- `UnifyMatch()` is a function which allows a less rigorous matching process to take place, known as "unification matching". This means that the two terms must be formally identical, in such a way that all the non-variable components must match exactly between the two objects, but variables may be allowed to match single terms in the other DObject, subject to the provision that the variable bindings produced are not inconsistent. The procedure therefore produces a yes/no answer saying whether the match succeeded, plus a list of variable bindings generated by the match. This is a very powerful symbolic technique, widely used in Prolog.
- `DoBinding()` and `DoAllBindings()` are used in `UnifyMatch()` to perform variable binding substitutions on a DObject.
- `MakeVarsDistinct()` is also used in `UnifyMatch()` and ensures that any variable names in a DObject are not also used in another DObject to which it is to be matched, which would cause confusion. In the case where variables have to be renamed, `UniqueVariableName()` is used to generate a variable name which has never so far been used.
- `VariablesUsed()` is used to find out the names of the variables used in the DObject, and `Grounded()` simply tests if the list so produced is empty. These are both support functions for `UnifyMatch()`.
- The DObject and DObRep classes both use customised memory management primitives, `new` and `delete`, which use a simple first-fit allocation routine.

A number of functions of the BindList class are particularly useful in supporting the unification matching of DObjects. These are:

- The function `BindList::AddBinding()` attempts to add a new Binding to the list currently stored, whilst maintaining the integrity of the Bindings already in the table. The arguments to this function are DObjects giving the variable and its value to be added to the table.
    - If the variable is not so far in the BindList, then the new binding can be added.

    - If the variable is in the BindList and the value of the new Binding does not unify with the value in the BindList already, then the Binding is not added and the function fails.
    - If a unification match succeeds, then the variable bindings produced by the match are added to the BindList by a recursive call to `AddBinding()`. If all bindings are inserted properly, the function succeeds, otherwise it fails.
- `BindList::CollapseBindings()` is a function which attempts to simplify the variable Bindings in the list by reducing chains of variables. This does not reduce the number of elements in the BindList, but converts the values of any which can be so reduced to constants where this is possible.
- The function `BindList::LookupBinding()` retrieves the value recorded for a variable, if there is one in the BindList.
- `BindList::ResolveFinalValue()` gets a value for a variable from the BindList, converting it to a non-variable term, if this is possible.

Location

The Location class stores, and allows for the manipulation of, information concerning fluids at particular places in the plant (characterised by a `[unit,port]` pair). The checks and predicates of the fluid modelling system rely on objects of this class to communicate information about fluids.

The Location object is a reference counted object class which uses the LocRep class to carry the data for any number of copy Locations. The implementation of reference counting is similar to the method used for the Str class. The relevant source code files for these classes are `location.h`, `location.cpp`, `locrep.h` and `locrep.cpp`.

The specific data stored in the LocRep object (on behalf of Location objects) are:

- Strs indicating the relevant unit and port names for the Location.
- A Str object indicating the type of the process port to which the Location refers:
    - "I" indicates that it is an input port of the unit.
    - "O" indicates that it is an output port of the unit.
    - "U" indicates that it is an internal (`unitports`) port in the unit.
- Numerical values for the temperature of the fluid (in °C), its pressure (in bar abs) and its quantity (in kg inventory for internal ports, or kg/hr flow rate for input and output ports).
- A list of names of chemical components of the fluid, and a corresponding list of compositions (mole fraction values) for the fluid components. There is also an integer value for each component, to store flags concerning the component, such as whether it is a contaminant or not.
- A DObList list of DObjects is provided to record miscellaneous information (notes) on behalf of the fluid modelling system. This is mostly used to record the limits of deviations of process variables during validation of the fault paths uncovered in the HAZOP search.

The main user-accessible features of the Location class are:

- The usual set of constructors, destructor and assignment definitions are provided so that Location objects can be declared, assigned and copied, destroyed and passed as function arguments, just as if they were a built-in type of the C++ language, such as `int` or `double`.
- Location objects can be converted to or from appropriate DObject Structures. The form used is: `location(Unit,Port,Type,Temperature,Pressure, Quantity,[[Component1,Composition1,Flags1],..],Notes)`
- Functions are provided to allow the class user to read the data stored in the Location object. These are: `UnitName()`, `PortName()`, `PortType()`, `Pressure()`, `Temperature()`, `Quantity()`, `NoComps()`, `CompName()`, `CompValue()`, `CompFlags()`. The last three require an

integer index of the component in the Location, between 0 and (NoComps()-1). This can be found from the name using the function FindCompIndex().

- Similar functions are defined to change the values of the data stored in the object, or to give them "undefined" values. These are: SetUnitName(), SetPortName(), SetPortType(), SetPressure(), SetTemperature(), SetQuantity(), UnSetTemperature(), UnSetPressure() and UnSetQuantity().
- Components of the fluid can be added to or removed from the Location using the functions AddComponent() and RemComponent().
- The flags which indicate whether a component is a contaminant or not can be changed using the functions SetContaminantFlag() and ResetContaminantFlag(), or read using the function IsContaminant().
- The Display() function can be used to output a representation of the information in the Location to an output stream. This is the same function used by the left shift operator, '<<'. The function Describe(), which uses DescriptionString(), produces a more intelligible format for all the information except for the "notes" field.
- Two functions are provided to compare Locations for equality. The equality operator, '==', tests all the fields, so that numerical data, unit, port and component data must match between two Locations. A less strict comparison is the function SamePlace(), which tests to see if the unit and port fields of the two Locations are the same.
- A number of functions are provided to read, add, remove, search through and change the contents of the notes in the Location. These are: GetNotes(), SetNotes(), AddNote(), RemNote(), RemMatchingNotes(), FindMatchingNotes() and HasNotes().
- The function Mixture() takes two Locations and produces a new Location corresponding to mixing together the fluids from each one. The two Location objects need not refer to the same place in the plant, but the resulting mixture

object is defined at the same place as the "host" object which initiated the function call.

FPath

The FPath class is used in the validation of fault paths which is performed during the HAZOP search algorithm and elsewhere when the program searches for the causes of some deviation. The FPath represents the path to be validated, along with data such as the list of fluids relating to that path, and various classification data generated by the validation process.

The data stored in this object type are as follows:

- A List of pointers to Arcs, defining the path which is the subject of the FPath.
- A List of currently defined fluids, in Location objects, which defines the necessary information about fluids relevant to the nodes visited along the fault path.
- Fields to store information concerning the classification and ranking of the consequences of the fault path (see Section 3.3.8). These are:
    - An importance number, between 0 and 5.
    - A consequence rank number, between 0 and 5.
    - A category for the consequence of the path, taken from the list ('none', 'haz', 'op' and 'haz_op').
    - A bit field of up to 16 bits, encoding whether the consequence of the FPath is a member of the various standard classes of consequences.

The main features of this class are as follows:

- The usual constructors, destructor and assignment are defined in order to make the type into a "concrete class". The FPath can also be initialised from a List of Arc pointers, which represents the fault path.
- FPath objects can be compared for equality using the '==' operator.
- FPath objects can be printed to an output stream using the function `Display()`.

- The current fluid list belonging to the FPath can be accessed (for reading or changing) using the function `Fluids()`.
- The List of Arc pointers which makes up the path in the FPath object can be accessed (for reading or changing) using the function `Path()`.
- The last Filler in the path can be referenced using the `EndOfPath()` member function.
- The steps in the fault path represented by the FPath object can be checked using the fluid modelling system, with the function `Validate()`. This function performs all the necessary tests on the links in the fault propagation chain, and maintains the necessary information on the numerical limits of deviations, as described in Chapter 5. It makes particular use of the external function `propertyHolds()` and the private member functions `Fwd_Limits()` and `RemoveLimits()`.

Appendix E : Table of Functions and Predicates in the Fluid Modelling System

This appendix provides a complete listing of the functions and predicates developed for the fluid modelling system described in Chapter 5. The columns in Table E.1 give the following information:

- **Prototype:** An indication of the prototype (*i.e.* name and list of arguments) for the function or predicate.
- **P/F:** A flag indicating whether the item is a function ("F") or predicate ("P").
- **Imp?:** An indication of whether the function or predicate has been fully implemented in the FMS ("Y" indicates that the item has been implemented and tested in AutoHAZID).
- **Used?:** Indicates whether the item is actually used in the FMS.
- **System:** This shows whether the item is implemented in a C++ function ("C"), defined in terms of other items ("D"), or corresponds to a rule in the VTT fluid rule system ("V").
- **Group:** This is the group of the FMS in which the function or predicate is considered to belong. The groups are listed below.
- **Description:** A short description of what the predicate is supposed to test, or what the function is supposed to evaluate.

Functions and predicates in the FMS are considered to belong to one of a number of groups, covering the type of activity that it deals with. The complete list of groups is:

1. Logical operations
2. Mathematical operations
3. General-purpose operations
4. Plant, fluid and fault path data access
5. Limit data access
6. Combining fluids (including compatibility checks)
7. Properties of single fluids

8. Consequence evaluation
9. Contamination
10. Design parameter checks
11. Miscellaneous physical checks
12. Leakage checks and limitations
13. Checks on VLE pressure limitations
14. Pressure deviation limits corresponding to resistance changes in flow paths

Table E.1 : Functions and Predicates in the Fluid Modelling System

Prototype	P/F	Imp?	Used?	System	Group	Description
GROUP 1: LOGICAL OPERATIONS						
true	P	Y	Y	C	1	Logical constant.
false	P	Y	Y	C	1	Logical constant.
op_and(T1,T2)	P	Y	Y	C	1	Logical AND operator. Also valid as infix operator "&&".
op_or(T1,T2)	P	Y	Y	C	1	Logical OR operator. Also valid as infix operator "||".
not(T1)	P	Y	Y	C	1	Logical NOT operator.
GROUP 2: MATHEMATICAL OPERATIONS						
op_add(T1,T2)	F	Y	Y	C	2	Addition of numerical values. Also valid as infix operator "+". Multiple arguments possible.
op_mult(T1,T2)	F	Y	Y	C	2	Multiplication of numerical values. Also valid as infix operator "*". Multiple arguments possible.
op_sub(T1,T2)	F	Y	Y	C	2	Subtraction of numerical values. Also valid as infix operator "-".
op_div(T1,T2)	F	Y	Y	C	2	Division of numerical values. Also valid as infix operator "/".
power(Base, Exponent)	F	Y	N	C	2	Exponentiation of numerical values.

Prototype	P/F	Imp?	Used?	System	Group	Description
op_ge(T1,T2)	P	Y	Y	C	2	Comparison: "greater than or equal to". For numerical values of T1 and T2. Also valid as infix operator ">=".
op_le(T1,T2)	P	Y	Y	C	2	Comparison: "less than or equal to". For numerical values of T1 and T2. Also valid as infix operator "<=".
op_lt(T1,T2)	P	Y	Y	C	2	Comparison: "less than". For numerical values of T1 and T2. Also valid as infix operator "<".
op_gt(T1,T2)	P	Y	Y	C	2	Comparison: "greater than". For numerical values of T1 and T2. Also valid as infix operator ">".
GROUP 3: GENERAL PURPOSE OPERATIONS						
op_ne(T1,T2)	P	Y	Y	C	3	Comparison: "not equals". For any type of value for T1 and T2. Also valid as infix operator "!=".
op_eq(T1,T2)	P	Y	Y	C	3	Comparison: "equals". For any type of value for T1 and T2. Also valid as infix operator "==".
op_assgn (T1,T2)	P	Y	Y	C	3	Assignment of the value of T2 to variable T1. Also valid as infix operator "=". T1 must be an unbound variable before this predicate is called, and will be a bound one afterwards.
undef_number	F	Y	Y	C	3	A function (with no arguments) which returns the special constant value for undefined numbers.
grounded(T1)	P	Y	N	C	3	Test the term T1 and fail if it contains any ungrounded variables.
unify_match (T1,T2)	F	Y	N	C	3	Unification match of terms T1 and T2. Returns false if the match was not possible, or a list of variable bindings of the form: [[XVar,XVal],[YVar,YVal],...].

Prototype	P/F	Imp?	Used?	System	Group	Description
get_binding (BList,Var)	F	Y	N	C	3	Look for the value of Var as given in the binding list BList. Format of BList is as for return from unify_match().
list_length(L)	F	Y	N	C	3	Returns the length of the list L.
list_element (L1,I1)	F	Y	N	C	3	Returns the term in the list L1 at position I1, where (0 <= I1 < list_length(L1)). Returns 'error' if the index is not good for L1.
list_append (L1,T1)	F	Y	N	C	3	Appends the item T1 to the end of the list L1. Returns the new list L1.
list_prepend (L1,T1)	F	Y	N	C	3	Puts the item T1 in at the start of the list L1. Returns the new list L1.
list_insert_after(L1,POS,T1)	F	Y	N	C	3	Inserts the element T1 after the indexed position POS in list L1. Returns the new list. Returns 'error' if POS is not a good index for list L1 (it should be in range 0 to length-1).
max_in_list(L)	F	Y	Y	C	3	Determines a maximum value of the numerical elements in the given list. Returns 'undef_number' if L is not a list, or if the maximum numeric item in the list was 'undef_number'.
min_in_list(L)	F	Y	Y	C	3	Determines a minimum value of the numerical elements in the given list. Returns 'undef_number' if L is not a list, or if the minimum numeric item in the list was 'undef_number'.
echo(Term)	P	Y	Y	C	3	Diagnostic feature. When executed, this predicate will evaluate Term and print the result to the standard error stream, cerr (which will usually print it to the screen).
cond(Condition, Term1,Term2)	F	Y	Y	D	3	Function evaluates the condition given and if true, returns the value of Term1 when evaluated, otherwise returns the value of Term2 when evaluated. Analogous to the cond function in LISP.

Prototype	P/F	Imp?	Used?	System	Group	Description
GROUP 4: PLANT, FLUID AND FAULT PATH DATA ACCESS						
max_port _diameter	F	Y	N	D	4	Determines the largest diameter of the ports associated with the current context unit.
get_attribute (AttName)	F	Y	Y	C	4	Returns the value of the named attribute for the current context unit in the plant model. Returns an Atom for 'is' slots, or a ListType for 'info' slots. If the attribute is not found or doesn't have a value, returns 'undefined'.
get_fluid (Port)	F	Y	Y	C	4	Access to the current fluid for the given port. Returns 'error' if the fluid cannot be retrieved.
get_nominal _fluid(Port)	F	Y	Y	C	4	Access to the nominal (plant description) fluid for the port given.
set_fluid (Port,F1)	P	Y	Y	C	4	Set the current fluid information for the given port to be the fluid F1.
get_pressure (Fluid)	F	Y	Y	C	4	Returns the numerical value of the pressure for the given fluid.
get _temperature (Fluid)	F	Y	Y	C	4	Returns the numerical value of the temperature for the given fluid.
get _composition (Fluid,Comp)	F	Y	N	C	4	Returns the mole fraction of the component in the fluid given.
set_pressure (Fluid,Value)	F	Y	N	C	4	Sets the pressure of the given fluid to be Value, returning the modified fluid.
set _temperature (Fluid,Value)	F	Y	Y	C	4	Sets the temperature of the given fluid to be Value, returning the modified fluid.
set _composition (Fluid,Comp, Val)	F	Y	N	C	4	Sets the composition of the component in the given fluid, returning the modified fluid. If the named component is not in the fluid, a warning is issued and the function returns the unchanged fluid.

Prototype	P/F	Imp?	Used?	System	Group	Description
this_unit	F	Y	N	C	4	Returns a string giving the name of the current context equipment item.
insulation	P	Y	Y	D	4	Is the current plant unit insulated ?
dead_heading _pressure	F	Y	Y	D	4	Retrieves the dead-heading pressure for the unit concerned (typically a pump), from the attribute "dead_head_pressure". Returns undef_number if not defined.
full_dh _pressure (Port)	F	Y	Y	D	4	Determines the maximum pressure a pump or compressor will see if its discharge (Port) is blocked off. This is the sum of the dead-heading pressure and the operating pressure of the pump inlet. Returns undef_number if either data are not available.
vessel_height	F	Y	N	D	4	Gets the height, in metres, of the current unit (typically a vessel), from the attribute "vessel_height". Returns undef_number if not defined.
vessel_volume	F	Y	N	D	4	Gets the volume, in cubic metres, of the current unit (typically a vessel), from the attribute "vessel_volume". Returns undef_number if not defined.
max_design _pressure	F	Y	Y	D	4	Finds the maximum design pressure for the equipment item being considered. Uses the attribute "max_allowable_pressure". Returns undef_number if no value is found.
min_design _pressure	F	Y	Y	D	4	Finds the minimum design pressure for the equipment item being considered. Uses the attribute "min_allowable_pressure". Returns undef_number if no value is found.
min_design _temperature	F	Y	Y	D	4	Finds the minimum allowable temperature for the equipment being examined.
max_design _temperature	F	Y	Y	D	4	Finds the maximum allowable temperature for the equipment being examined.

Prototype	P/F	Imp?	Used?	System	Group	Description
GROUP 5: LIMIT DATA ACCESS						
Note: Three types of operation are implemented in this part of the FMS: 1. The functions beginning with 'get_min_' and 'get_max_' return the values of the relevant limit, for the fluid given as the first argument of the function. 2. The functions beginning with 'set_min_' and 'set_max_' modify the limit data for the fluid in the first argument. They return the modified fluid, but do not change the data associated with any port in the current fluids list. 3. The predicates beginning with 'assign_' are used to change the current fluid data associated with the given port, so that it has the given limit value. They always return true.						
get_min_temperature(Fluid)	F	Y	Y	C	5	Finds the minimum temperature for the given fluid.
get_max_temperature(Fluid)	F	Y	Y	C	5	Finds the maximum temperature for the given fluid.
get_min_pressure(Fluid)	F	Y	Y	C	5	Finds the minimum pressure for the given fluid.
get_max_pressure(Fluid)	F	Y	Y	C	5	Finds the maximum pressure for the given fluid.
get_min_composition(Fluid, Comp)	F	Y	N	C	5	Gets the minimum composition of the component in the fluid given.
get_max_composition(Fluid, Comp)	F	Y	N	C	5	Gets the maximum composition of the component in the fluid given.
set_min_temperature(Fluid, Value)	F	Y	Y	C	5	Sets the minimum temperature of the given fluid to Value. Returns the modified fluid.
set_max_temperature(Fluid, Value)	F	Y	Y	C	5	Sets the maximum temperature of the given fluid to Value. Returns the modified fluid.
set_min_pressure(Fluid, Value)	F	Y	Y	C	5	Sets the minimum pressure of the given fluid to Value. Returns the modified fluid.

Prototype	P/F	Imp?	Used?	System	Group	Description
GROUP 6: COMBINING FLUIDS (INCLUDING COMPATIBILITY CHECKS)						
fluid_mixture (Flu1,Flu2)	F	Y	Y	C	6	Finds the fluid corresponding to mixing the two given fluids together, without doing any compatibility checks.
mix_fluids (F1,F2)	F	Y	Y	D	6	Mixes the fluids F1 and F2 together to produce a third fluid, which is returned. Calls on the compatibility table checks, which may generate side-effects. These side-effects may be used to annotate the current fluids in the fault path being considered.
compatibility _check(F1,F2)	F	Y	Y	C	6	Runs check on the compatibility of the components in the given fluids. This checks the components in the fluids via the reactivity group matrix of VTT. The result is a list of Structures, of the form [heat_generation(Comp1, Comp2, TempMax), ...]. The possible interactions are listed in Section 5.2.8. Implemented by VTT.
add_to_compat _report(Rep)	P	Y	Y	C	6	Adds the results (Rep) produced by the compatibility check to the overall compatibility report for the HAZOP.
GROUP 7: PROPERTIES OF SINGLE FLUIDS						
liquid(Port)	P	Y	Y	D	7	Could the fluid associated with the given port contain a liquid phase component ? Defaults to true if fluid state is not known.
solidsPresent (Port)	P	N	Y	C	7	Could solids be present in the fluid in Port ? Returns a default value at the moment.

Prototype	P/F	Imp?	Used?	System	Group	Description
freezing(Port)	P	Y	Y	C	7	Determines if any of the components of the fluid associated with the given port are below their freezing point at the current temperature. Does not use limit temperatures, just the current fluid data.
flammable (Port)	P	Y	Y	C	7	Determines if the fluid in the given port is flammable. Simply tests each of the components to see if any qualify.
toxic(Port)	P	Y	Y	D	7	Determines if the fluid in the given port is toxic. Uses the function toxicity(), which relies on fluid library info.
crystalliser (Port)	P	N	Y	C	7	Determines if the fluid in the given port is likely to crystallise. Uses a default return value at the moment, because no data are available to test the condition.
polymeriser (Port)	P	N	Y	C	7	Determines if the fluid in the given port is likely to polymerise. Uses a default return value at the moment, because no data are available to test the condition.
dissolvedGas (Port)	P	N	Y	C	7	Determines if the fluid in the given port contains dissolved gas components. Uses a default return value at the moment, because no data are available to test the condition.
brittle(Port)	P	N	Y	C	7	Determines if the materials of construction associated with the given port are likely to become brittle at a low temperature.
decomp(Port)	P	N	Y	C	7	Determines if the fluid in the given port is likely to undergo decomposition.

Prototype	P/F	Imp?	Used?	System	Group	Description
state(Fluid)	F	Y	N	C	7	Given a fluid, determine its state, as one of the following: [unknown, vapour, liquid, solid, vap_liq, solid_vap, solid_liq, solid_vap_liq]. Uses physical properties package requests or C++ functions as appropriate.
boiling_temp _range(Fluid)	F	Y	N	C	7	Finds the range of temperatures over which the given fluid will boil at its current pressure. Returned in the form of a list: [lowvalue, highvalue]. Uses property package requests or fluid library information as appropriate.
mol_weight (Fluid)	F	Y	N	C	7	Returns the average molecular weight of the given fluid. Returns the value undef_number if this cannot be calculated.
freezing_temp (Fluid)	F	Y	N	C	7	Returns the temperature at which the first component in the fluid begins to freeze, from liquid. Uses property package requests or fluid library information as appropriate. There may be problems running this request using ASPEN Properties Plus. C++ version of function not capable of dealing with mixtures of components. Returns undef_number if freezing point not available.
vapour _pressure (Fluid)	F	Y	Y	C	7	Returns the vapour pressure exerted by the fluid at its current temperature. Uses property package requests or the fluid library information, as appropriate.
viscosity (Fluid)	F	Y	N	C	7	Returns the viscosity of the given fluid at current conditions.
density(Fluid)	F	Y	N	C	7	Returns the density of the given fluid at current conditions. Uses property package requests or fluid library data as appropriate.

Prototype	P/F	Imp?	Used?	System	Group	Description
enthalpy (Fluid)	F	Y	N	C	7	Calculates the specific enthalpy of the given fluid.
specific_heat (Fluid)	F	Y	N	C	7	Calculates the specific heat capacity of the given fluid. Uses property package requests or fluid library information as appropriate.
latent_heat _fusion(Fluid)	F	Y	N	C	7	Calculates the latent heat of fusion for the given fluid.
latent_heat _evap(Fluid)	F	Y	N	C	7	Calculates the latent heat of evaporation for the given fluid. Uses property package requests or fluid library information as appropriate.
phase_temperat ures(Fluid)	F	Y	N	C	7	Calculates the temperature limits of phase change for the given fluid. Returns in the form of [freezing_point, boiling_point]. There may be problems running this request using ASPEN Properties Plus.
phase _pressures (Fluid)	F	Y	N	C	7	Calculates the pressure limits of phase change for the given fluid. Returns in the form of [press_vapour, press_solid]. There may be problems running this request using ASPEN Properties Plus.
flashpoint _temp(Fluid)	F	Y	N	C	7	Returns the closed cup flash point temperature of the given fluid. There may be problems running this request using ASPEN Properties Plus.
autoignition _temp(Fluid)	F	Y	N	C	7	Returns the AIT of the given fluid. There may be problems running this request using ASPEN Properties Plus.
lower_flamm _limit(Fluid)	F	Y	N	C	7	Return the lower flammable limit of the given fluid. There may be problems running this request using ASPEN Properties Plus.
upper_flamm _limit(Fluid)	F	Y	N	C	7	Return the upper flammable limit of the given fluid. There may be problems running this request using ASPEN Properties Plus.

Prototype	P/F	Imp?	Used?	System	Group	Description
cas_number (Comp)	F	Y	N	C	7	Returns the CAS number of the given fluid component.
vacuum(Port)	P	Y	Y	D	7	Is the port under vacuum ?
pressurised (Port)	P	Y	Y	D	7	Is the port under pressure ?
nearBoilingPoint(Port)	P	Y	Y	C	7	Is the fluid in Port near its boiling point ?
vapour(Port)	P	Y	Y	C	7	Does the fluid in Port contain vapour?
flashRelease (Port)	P	Y	Y	C	7	Would the fluid in Port flash if depressurised to 1 bara?
brittleFlash (Port)	P	Y	N	C	7	Check to see if any of the components in the fluid at the given port will cause the material of construction to be weakened if flashed to atmospheric pressure.
foamer(Port)	P	N	Y	C	7	Check to see if the fluid in the named port contains a component liable to cause foaming. Implemented to return a default value at the moment, because the information needed is not available yet.
solid(Port)	P	Y	N	V	7	VTT predicate. Does the fluid present for Port contain solid?
corrosion (Port)	P	N	Y	C	7	Are the materials associated with Port susceptible to corrosion ? Returns a default value at the moment, because data for deciding query are not available.
hydrocarbon (Port)	P	Y	Y	C	7	Succeeds if the fluid associated with the named port contains a hydrocarbon component. Returns a default value at the moment, because data for deciding query are not available.
exothermicReaction(Port)	P	Y	Y	C	7	Succeeds if an exothermic reaction is intended at the given port. Returns a default value so far, because no data are available to decide the condition.

Prototype	P/F	Imp?	Used?	System	Group	Description
endothermicReaction(Port)	P	Y	Y	C	7	Succeeds if an endothermic reaction is intended at the given port. Returns a default value so far, because no data are available to decide the condition.
hazardous (Port)	P	Y	Y	D	7	Returns true if the fluid at the given port is toxic or flammable.
non_hazardous (Port)	P	Y	Y	D	7	Returns true if the fluid at the given port is non-toxic and non-flammable.
toxicity (Fluid)	F	Y	N	C	7	Returns the toxicity of the given fluid, according to the data in the fluid library. This is the max. value for the components in the fluid, or -1 if some value or component is unknown to the fluid library.
vp_at_given_temp(Fluid,Temp)	F	Y	Y	D	7	Determines the vapour pressure of the given fluid at the given temperature. Used in vle_min_pressure_limit().and vle_max_pressure_limit().
fluid_can_freeze(Port)	P	Y	Y	D	7	Succeeds if the current fluid associated with the given port can attain a temperature below its freezing point. Makes use of lower limit temperature of fluid. Defaults to true if there is no minimum temperature defined or if the freezing point cannot be found.
GROUP 8: CONSEQUENCE EVALUATION						
get _consequence	F	Y	N	C	8	Gets the consequence belonging to the current fault path, or 'error' if the path is not a completed one.
is_consequence _type (Conseq,Code)	P	Y	N	C	8	Checks the consequence given to see if it has the given code value as a standard type of consequence.
get _consequence _rank(Conseq)	F	Y	N	C	8	Returns the rank number of the given consequence.

Prototype	P/F	Imp?	Used?	System	Group	Description
get _consequence _cat(Conseq)	F	Y	N	C	8	Returns the category of the given consequence (from none, haz, op, haz_op).
loc_eval (Fluid,Type)	F	N	N		8	Loss of containment evaluation. Given a fluid and the type either "toxic" or "flammable", the function determines a rank value for the generic loss of containment event for that fluid. Not fully implemented yet.
GROUP 9: CONTAMINATION						
add_air _contamination (Port)	P	Y	Y	D	9	Adds air as a contaminant to the current fluid at Port, changing the current fluid there.
add_contamination(Fluid, CmpList)	F	Y	Y	D	9	Add a number of compounds as contaminants to the fluid, returning the new fluid.
fluid_from _components (CompList)	F	Y	Y	C	9	Given a list of component names, makes a fluid containing those components. Used by add_contamination() to produce a fluid containing a list of named contaminants.
make_fluid _contaminant (Fluid)	F	Y	Y	C	9	Makes all the components of the fluid into contaminants, returning the modified fluid. Also used by add_contamination() to add named contaminants to another fluid.
becomes_toxic (Port)	P	Y	N	D	9	Detects if the fluid belonging to the named port has changed from a nominal fluid which is not toxic, to a current fluid which is toxic.
becomes _flammable (Port)	P	N	N	D	9	Detects if the fluid belonging to the named port has changed from a nominal fluid which is not flammable, to a current fluid which is flammable. Not yet implemented.

Prototype	P/F	Imp?	Used?	System	Group	Description
port_port_contamination (HP_Port, LP_Port)	P	Y	Y	D	9	Transfers the fluid present in the first (high pressure) port to the second (lower pressure) port, as a contaminant. Includes a call to the fluid compatibility checks. Sets the composition of LP_Port to the mixture of components, for use in (for example) contamination arcs attached to interface failure in heat exchangers.
GROUP 10: DESIGN PARAMETER CHECKS						
exceed_design_pressure (Port)	P	Y	Y	D	10	Determines if the maximum pressure at the port can exceed the design pressure of the unit. Defaults to true if any data are missing.
exceed_design_vacuum(Port)	P	Y	N	D	10	Determines if the minimum pressure at the port can go below the minimum design pressure of the unit. Defaults to true if any data are missing.
design_overTemp (Port)	P	Y	Y	D	10	Can the fluid at the given port exceed the upper design temperature of the equipment? Defaults to true if any data are missing.
design_underTemp (Port)	P	Y	N	D	10	Can the fluid at the given port be less than the lower design temperature limit of the equipment? Defaults to true if any data are missing.
GROUP 11: MISCELLANEOUS PHYSICAL CHECKS						
boiling (Port1,Port2)	P	Y	Y	D	11	Does the fluid boil between Port1 and Port2?
rollOver(Port)	P	Y	Y	C	11	Checks to see if the vessel containing the given port is large enough to experience the "rollover" phenomenon. This limit is arbitrarily set at 50 cubic metres.
hot(Port)	P	Y	Y	D	11	Arbitrary test to see if the given port is above ambient temperature (35 degrees C).

Prototype	P/F	Imp?	Used?	System	Group	Description
low_press (Port)	P	Y	Y	D	11	Test to see if the pressure of the given port is less than 2 bara. Used for classifying vessels.
hot_weather _temp	F	Y	Y	D	11	Returns the maximum ambient temperature for hot weather (currently set at 40 °C).
cold_weather _temp	F	Y	Y	D	11	Returns the minimum ambient temperature for cold weather (currently set at -30°C).
GROUP 12: LEAKAGE CHECKS AND LIMITATIONS						
pressureLeak (Port)	P	Y	Y	D	12	Predicate for setting the low pressure limit value for a scenario involving a leak out of a pressurised system. Tests that the port is pressurised and if it is, sets the minimum pressure limit for that port to be 1.0 bara, for the leak scenario only.
vacuumLeak (Port)	P	Y	Y	D	12	Predicate for setting the high pressure limit value for a scenario involving a leak into a vacuum process. Tests that the port is under vacuum and if it is, sets the maximum pressure for that port to be 1.0 bara, for the leak scenario only.
GROUP 13: CHECKS ON VLE PRESSURE LIMITATIONS						
vle_pressure _limits(L,V)	P	Y	Y	D	13	Sets the scenario pressure limits for a vapour port (V) based on the vapour liquid equilibrium between V and the liquid port (L). Uses the limit values of temperature for the liquid port and a calculation of vapour pressure for the liquid. Changes the limit values of the current fluid data for V.

Prototype	P/F	Imp?	Used?	System	Group	Description
vle_min_pressure_limit(L,V)	P	Y	Y	D	13	Sets the minimum pressure limit for the vapour port (V) based on the vapour pressure of the liquid in the liquid port (L) at the minimum temperature limit so far determined (in the current scenario) for the liquid. Changes the lower pressure limit of the current fluid data for V.
vle_max_pressure_limit(L,V)	P	Y	Y	D	13	Sets the maximum pressure limit for the vapour port (V) based on the vapour pressure of the liquid in the liquid port (L) at the maximum temperature limit so far determined (in the current scenario) for the liquid. Changes the upper pressure limit of the current fluid data for V.
GROUP 14: PRESSURE LIMITS IN FLOW PATHS WHEN RESISTANCE CHANGES						
res_dsp_limit (USPort, DSPort)	P	Y	Y	D	14	Sets the maximum attainable pressure of the downstream port, DSPort, to be the maximum pressure of the upstream port, USPort, or the nominal pressure, if there is no defined maximum for USPort. The nominal pressure of a port is the pressure specified for that port in the plant model. Used in the flowpath() template.
res_usp_limit (USPort, DSPort)	P	Y	Y	D	14	Sets the minimum attainable pressure of the upstream port, USPort, to be the minimum pressure of the downstream port, DSPort, or the nominal pressure, if there is no defined minimum for DSPort. The nominal pressure of a port is the pressure specified for that port in the plant model. Used in the flowpath() template.

Appendix F : Minutes of Meeting to Discuss Limits of Variable Deviations

This appendix presents, for reference, the minutes of a meeting held between myself and Prof. Lees, to discuss the idea of rules for the estimation of the limits on process plant deviations. Many of the ideas discussed have not so far been implemented in the AutoHAZID system, but could be developed further.

It should be noted that, in the following, completeness cannot be guaranteed. The method used was directed at finding limits for pressures and temperatures only and used a guide word approach for stimulating ideas. Also, the scenarios identified may not "cleanly" define a single fault propagation chain, but very often involve a whole family of constraints which may or may not be easily formalised for implementation in AutoHAZID.

The original minutes are presented below:

Introductory Notes

Prof. Lees and I met on 5th August 1996 to discuss in greater detail the problems behind the estimation of landmark values on deviations in plant process variables.

We decided to examine the limits on pressures and temperatures in plant in a "brain-storming" way, using a table from Bunn and Lees (1988) as a prompt for stimulating ideas about possible phenomena to consider.

We made the assumption that fault propagation does not attempt to consider more than one scenario (fault-consequence pair) at a time, and that the mechanical integrity of the plant can be assumed unless the fault or consequence dictates otherwise. Essentially, this boils down to the assumption that the only deviations which need to be considered are those belonging to the fault-consequence chain being examined.

In the notes that follow there may be many maximum and/or minimum figures for the pressures and temperatures considered. The actual envelope of the variable could be determined by taking the smallest of the maxima and the largest of the minima appropriate for that variable.

Implementation of the following ideas is left completely open for the moment. It is possible that the implementation could take the shape of generally applicable rules or characteristics of particular types of equipment (limits described in the unit model library, for example), or conditions expressed in individual arcs.

Consideration of Limits of Variable Deviations

In systems containing liquids, the lower limit of pressure is the vapour pressure of the liquid present. The vapour pressure is, of course, affected by the temperature of the system. An example of the vapour pressure dependence on temperature is the reduction of pressure in an ammonia storage sphere caused by a cooling shower of rain on the outside of the vessel.

The pressure drop caused by leakage from a pressurised vessel to atmosphere is limited to 1 bara. The pressure rise caused by a leak of air into a vacuum system is limited to 1 bara.

If a small hole in a vessel leads to depressurisation of the vessel and subsequently to flash vaporisation of some of the liquid contents, then cooling can take place, giving rise to brittle fracture of the vessel and a larger leak.

Pressurised fluid being released as a jet from a small hole in a vessel can impinge on other equipment, causing non-process escalation of the effects - this is known as the "domino effect".

Vacuum relief devices will limit the minimum pressure in a vacuum system. Pressure relief devices will limit the maximum pressure in a pressurised system. Such devices may include bursting disks as well as relief valves. Note that these are protection devices, which may fail - how should we deal with these?

Mechanical "burst pressure" for a pressurised system, if there is no relief device attached to it.

Nominal minimum/maximum inlet pressures and temperatures may be given. Care should be taken that these can be trusted to be the real limits of these variables, as they may correspond to the design condition envelope for the plant.

Maximum delivery pressure of a pressure raiser. Note that this maximum is also dependent on the pressure on the suction side of the pressure raiser. If the pressure raiser is a positive-displacement type, the pressure due to dead-heading it will be much higher - the possibility of isolating the pressure raiser discharge must be considered in determining the maximum here.

Minimum suction pressure of a vacuum pump. Note also the limit of vapour pressure in systems with liquid in them, as mentioned above.

Gas breakthrough at the base of a column, or in a vessel, could expose some usually liquid-filled components of the plant to the pressure of the gas or vapour-filled parts. In this case, the relevant pressure to consider is the nominal pressure of the vapour filled sections (*e.g.* the nominal discharge pressure of the compressor used in that system).

Heat exchanger interface failure will cause the low pressure side of the exchanger to be exposed to the full pressure of the high pressure side. The maximum here is the nominal pressure of the inlet to the high pressure side of the exchanger.

High pressures generated by non-intentional combustion of gases in process equipment are limited by the appropriate constant volume combustion calculation. The most pessimistic estimate of pressure-rise would use a stoichiometric basis for the combustion, but very often this is not realistic.

In the case of heating due to an external fire, where relief or fire valves are not present, the pressure limit may be that pressure generated by the system fluid at the temperature where the metal in the system fails. In this case, the other effect, of overpressure failure of the system, may also take place. The examination of the interplay of these two effects is potentially quite complicated.

Thermal expansion of liquid-filled systems is relevant when considering locked in fluids subject to a temperature rise caused by heat exchange with the environment. Some calculation involving the coefficient of thermal expansion, β, would be appropriate here, to calculate the highest expected pressure, dependent on an estimated maximum ambient temperature.

The problem of water in hot oil (the "chip-pan effect") is typical of those effects where the magnitude of the pressure increase is not easy to determine. In this case, some quantity of water makes its way into a hot oil system and there boils rapidly, causing an expansion. The amount of water and the volume of the system, temperature of the oil, *etc.*, are all needed for this calculation. Since the amount of the contaminant (water) in the system is highly uncertain, the possibility of making a reasonably confident "safe" calculation of the pressure rise is very slim.

In this problem, it is enough to detect that the water contamination would in fact boil when it gets into the hot oil.

A similar sort of quantification problem occurs when we consider the Bhopal disaster. It is thought that a quantity of water got into a storage tank containing methyl isocyanate, and there caused a runaway reaction, leading to an overpressure release from the vessel. Here it is also difficult to quantify the amount of the contaminant and, although the runaway phenomenon is quite different from the hot oil problem, the magnitude of the pressure change cannot be deduced for the same reasons. Here, a compatibility matrix should warn of the dangerous runaway reaction between the process fluid and contaminant.

Accumulation of inert/non-condensable gases at high points in a plant may cause blockages and other problems too.

For heat exchangers, where the process fluid is heated by some heat transfer fluid or steam, the maximum temperature for the process fluid is the maximum temperature expected from the heat transfer medium. The maximum process pressure is determined by considering the process fluid blocked in at such a temperature.

In furnaces and burners, which can be extremely hot, the best estimate of the maximum process side conditions is the failure of the tube metal due to heat or overpressure. This establishes limits on the maximum temperature and pressure in the process fluid side of the furnace tubes.

In the event of loss of cooling medium in a cooler, the maximum process fluid temperature at the outlet of the exchanger will be the nominal process fluid inlet temperature.

Loss of cooling in a condenser will lead to vapour accumulation in the process side and possible breakthrough of vapour into the condensate outlet. In the case of a distillation column, the pressure of the column will increase until the process temperature in the reboiler is the same as the steam temperature, or the relief pressure is reached, or the burst pressure of the column is reached, whichever is the lowest.

The coolant in a cooler must remain flowing in order to cool the process fluid. Therefore, the minimum temperature that the process fluid can get to is either its own freezing point or the freezing point of the coolant, whichever is higher.

The weather will have certain characteristic temperature limits, depending on the part of the world in which the plant is situated. These will define the envelope for environmental temperature.

The brittle fracture temperature of the materials of construction is an important temperature minimum.

Freezing expansion of water in pipes, as a result of cold weather, gives rise to blockage and a pressure effect on the pipes, possibly damaging them. Some calculation might be devised to determine if the pipe will be endangered by freezing in this way. Do any other fluids expand on freezing, as water does?

For systems containing liquids, when a leak to environment occurs the liquid will depressurise. If the fluid would normally be vapour at ambient conditions, it will flash. The evaporation of the process fluid can chill the equipment to a minimum of the boiling temperature of the fluid at 1 bara. A similar principle applies where the evaporative cooling happens within a system: the minimum temperature is the saturation temperature at the lower pressure.

For gases/vapours, typically, cooling occurs on expansion and heating on compression, due to the Joule-Thompson effect. It is likely that calculations could be found to estimate the size of these effects, for application in processes where expanders or compressors are found.

Mixing with another cold fluid can cause some process materials to freeze, *e.g.* benzene plus cold slugs of ethylene in a flare stack, freezing the benzene.

If fluid is erroneously introduced (in a batch process, for example) to a cold vessel, it could freeze, causing problems, such as freezing the impeller in a reaction vessel, plugging inlets or outlets in the vessel, or measurement points, inconvenience generally...

In runaway reactions, one temperature limit is the "adiabatic reaction temperature" (typically for batch or semi-batch reactors). Another is the temperature at which the venting on the reactor operates.

Pumps and compressors are a source of high temperature when dead-heading or overheating, or when recycling fluid (under spill-back, for example). In all these cases, the magnitude of the effect is not easy to quantify without some arbitrary judgements about the process.

For compressors, if the coolers which should remove the heat of compression from the process fluid are lost, then it may be possible to calculate the maximum to which the discharge temperature would go. This is not straightforward, however.

Loss of tracing (steam or electric) on traced pipework could drop the temperature to ambient.

If steam tracing goes wrong and more heat than intended is given to the process, then the trace steam temperature could be a useful guide to the maximum process temperature reached.

Some materials have a very high heat of solution, and this could be a factor in some cases. Calculations of temperatures here have the same problem as the water in hot oil example above - that too many data are needed for the calculation which cannot usually be pinned down exactly. Detection of the problem using compatibility matrices, plus the judgement that the temperature cannot go above the boiling point of the solvent, may help in this case.

Shock compression of gas by slugs of fast-moving liquid may give rise to large compressive heat effects, which sometimes are big enough to cause problems.

Appendix G : Future work changes to HAZID

A number of important but quite trivial changes should be made to the HAZID system in the future. These are in addition to the more difficult changes noted in Chapter 6:

- Consequences without a defined importance rank in the model library are always screened out of the results set, because of the way the consequence thresholding operation has been implemented. There are no such consequences in the library at the moment, but they could be added in future. Consequences without rank information should instead be reported wherever they are found (or a warning should be issued when a consequence is found without a rank number). This is a trivial coding change to the thresholding function.
- A user option (flag) could be added, to switch the fluid compatibility checking functionality in AutoHAZID on or off.
- Consider making the "stopping points" feature an option on the flags menu.
- Consider making all flag options configurable from the `hazpaths.dos` configuration file.
- The numerical value –999.0 is used for undefined values in the fluid model system and elsewhere. In the future, this value may be required as a legitimate defined value. The functions and predicates of the FMS should use some type of "not a number" symbol (*e.g.* the Atom, `'undefined'`), instead of a valid numerical value, when they are not capable of giving a value for a calculation. This is part of the larger problem of developing a consistent approach to missing information in the FMS.
- The definitions of fluid model system predicates and functions should be separated from the unit model library and put in a library file of their own.
- Recursive calls between fluid model functions or predicates should be detected and prevented, or warnings should be issued. Until there is some reliable way of eliminating infinite recursion in the FMS, recursion and iteration should be avoided.