OPTIMIZATION OF PROCESSES FOR SUSTAINABILITY

By

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OPTIMIZATION OF PROCESSES FOR

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DEDICATIONS

This thesis is dedicated to my parents Mr.S.Govindarajan and Mrs.Jayashree, my brother Ashwin, cousins Badri, Meera, Sachin, Sriram, Naveen, Anusha, Varsha, Shyam and Varun. To our Guru Sri.Sadasiva Bhramendrar for his blessings. To my grandparents Mr.R.Sathianathan and Mrs.Jembagalakshmi for their blessings and good wishes.

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CHAPTER I

INTRODUCTION

Against the backdrop of the Deepwater Horizon oil spill in April 2010, society has been very vocal in demanding that by meeting the economic and developmental needs of the present, the social and environmental needs, which invariably affect the future, cannot be compromised. Back in 1987, the World Commission on Environment and Development, Our Common Future, defined sustainability as “development that meets the needs of the present without compromising the ability of future generations to meet their own needs” (Brundtland, 1987).This turned out to be the first clear and concise definition for sustainability. Further, it has been agreed that sustainability has three dimensions-social, economic and environmental. Figure 1.1 shows a Venn diagram illustrating this concept. A process (or any other activity for that matter) is considered viable if it is economic and environmentally friendly, equitable if it is economic and socially beneficial, bearable if it is environmentally friendly and socially beneficial. However, when a process is viable, bearable and equitable, it is considered sustainable.

Traditionally, sustainability has been measured using various indices such as material, water and energy intensities (Tanzil et al., 2003). However, measuring the viability

of a process (product) versus designing one that is going to be inherently sustainable are different things. The former situation gives the option of evaluating the impact ofan existing industry. The latter presents a more complex situation because the process has to be designed for sustainability.

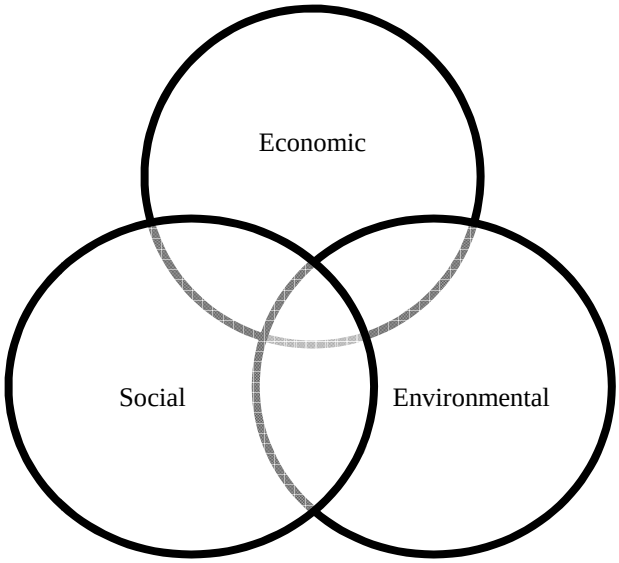

Figure 1.1 Dimensions of Sustainability (Adams, 2006)

This essentially means social parameters are needed in addition to the numerous process, environmental and economic parameters. While parameterizing social factors is a challenge, what is more complex is the incorporation of social parameters into design. For instance processing more raw materials affects the economics of operation, and possibly also increases waste products; but how does a process design engineer account for what happens to the society? How does it affect the people in the neighborhood? At this juncture it is pertinent to mention that there are well developed indices for the measurement of health and safety which fall under the social impact. There are several other aspects of social impact which have to be surveyed for specific data (specificity is all encompassing, meaning each situation has a different geo-political scenario, different

sensibilities, different standards, etc.). Process design can no longer be accomplished by just a chemical engineer with knowledge of economics. A process designer is now expected to have exemplary knowledge on other aspects of sustainability aside from process design and economics. Therefore, process designers need one tool/software to design their processes and then another tool/software to evaluate their process for sustainability.

Designing processes has become easier these days with the advent of the computer and process simulators such as Aspen Plus, CHEMCAD, HYSYS, PROSIM. Process simulators may be categorized into sequential modular simulators and equation oriented simulators. A sequential modular simulator simulates the process by solving the equations for the process equipment sequentially (Aspen Tech Inc., 2003). These are simple, graphic and user friendly. Aspen Plus and CHEMCAD are examples of sequential modular simulators. Many of the commercial process simulators have inbuilt optimization routines, sensitivity analysis tools and options to specify design specifications to design for environmentally compliant processes. In equation oriented simulators, all the non linear and differential/algebraic equations representing the process are solved simultaneously using matrix methods. Although the results obtained from the equation oriented simulators are more accurate, these are typically used by advanced users and for complex optimization problems. This research uses the sequential modular simulator Aspen Plus to optimize processes for sustainability as it is readily available at Oklahoma State University (OSU).

Optimization routines in Aspen Plus can only solve for single objectives with multiple constraints. However, multiple objectives can be specified, and can be solved

sequentially, which means, they have to be independent of each other, or non-conflicting. More often than not sustainability objectives are conflicting. This research seeks to convert multiobjective problems to single objective problems by using two methods. The first is a constraints method, wherein one objective is retained and the rest are converted to constraints. The second method used in this research is to weigh the multiple objectives and then optimize the process using Aspen Plus. The above optimization methods have previously been used by other researchers. However, optimizing a process for sustainability by involving economic, environmental and social objectives using inbuilt routines in Aspen Plus is new. In reality when a multiobjective optimization needs to be performed, a complex interface is required between sequential modular simulators and programming platforms such as C, C++ or Visual Basic. This involves considerable effort and expertise, which might not be warranted at a design stage of the process. Therefore this research is significant in that an existing simulation software (Aspen Plus) is used to solve a multiobjective problem by converting it into a single objective problem.

Sustainability metrics are simple measures of performance of a product/process/industry across different aspects of sustainability (Tanzil et al., 2003). For instance, safety indices, material intensity, reaction efficiency, etc. are examples of sustainable metrics concerning processes. One way of incorporating sustainability criteria into process simulators is to use metrics that can be directly related to material and energy balances. Over the past two decades several researchers have contributed to development of sustainability metrics. Prominent amongst them are the Inherent Process Safety Index (Heikkila, 1999), AICHE Center for Waste Reduction Sustainability Metrics (AIChE Center for Waste Reduction Technology- Institute for Sustainability, 2000), Dow Jones

Sustainability Index (Knoepfel, 2001), IChemE Sustainability Metrics (Institution of Chemical Engineers, 2002), Bridges Sustainability Index (Tanzil et al., 2006), AIChE Sustainability Index (Cobb et al., 2009). The pros and cons of metrics that have been developed have been listed in Shadiya (2010). The problem with the metrics listed above is that they are tools that evaluate sustainability of a process. Shadiya (2010) developed a framework to design processes for sustainability during early stages of design. In addition, an easy to use tool the SUSTAINABILITY EVALUATOR (SE) was created for use by process designers to evaluate processes for sustainability. The tool has been described in brief detail in subsequent chapters. The metrics associated with the SE have to be incorporated within the simulator, to optimize for sustainability using Aspen Plus. This research uses metrics from the SE and relates them with material and energy balances enabling their usage in Aspen Plus.

Thus the objectives of this research are three fold:

a. To develop a methodology to optimize processes for sustainability using Aspen Plus and information from the SE developed at OSU.
b. To convert the multiobjective optimization problem of sustainability into a single objective problem by using the constraints and the weighted methods.
c. To demonstrate this methodology on the allyl chloride process using Aspen Plus.

CHAPTER II

LITERATURE REVIEW

This chapter reviews existing literature concerning the development of sustainability metrics, optimization of processes in general and for sustainability. Since the Brundtland report's definition of sustainability (Brundtland, 1987), there have been several others who have defined sustainability in other ways (Serageldin, 1993; Hart, 1997; de Beer et al., 2000). For process engineers, a definition of sustainability was of no help. Without quantitative features in the definition, they were of no practical significance to the process designer/engineer. This was the first stumbling block that process designers faced. During the 1990's, sustainability was understood as being profitable and environmentally friendly (better understood as compliant with the EPA norms for emissions). Much of the improvements in processes in this phase (1990's) were centered on improving profit, while at the same time being compliant with all the regulatory standards. Other factors such as safety, stakeholder demands, health, etc. were not factored into the design and operation of chemical processes.

Around the late 1990's the concept of sustainability was transformed to the concept of the triple bottom line approach. The triple bottom line stood for people, profits and planet

(Elkington, 1994; Elkington, 1998). However, for a manufacturing process this would effectively translate into resource, waste, hazard and cost (Lange, 2009).Researchers have often mentioned that measuring sustainability is akin to measuring the immeasurable (Böhringer et al., 2007). So, the first challenge is to develop metrics/indices for measuring sustainability of processes. The next step is to modify processes to improve the sustainability indices, by using process intensification, process modification, controls and optimization. Most of the work concerning sustainability and the process industries has been an afterthought. Seldom have processes been designed for sustainability. Measuring how sustainable a processes is (and carrying out improvements on them) and designing a process to be inherently sustainable are altogether different things. Process designers need a well defined methodology to design for sustainability. Therefore, subsequent sections in this chapter are aimed at addressing the development of sustainability metrics (2.1), optimization of processes (2.2) and sustainability and optimization of processes (2.3) summary (2.4).

2.1 Development of Sustainability Metrics

Metrics are required to transfer the concepts of sustainability into action. Working groups like AIChE and ICheme have developed indices for measuring process sustainability (AIChE Center for Waste Reduction Technology- Institute for Sustainability, 2000). Sustainability metrics go beyond traditional economic analysis, and includes resource usage efficiency, energy efficiency, safety indices, etc. (Goodstein, 1999; AIChE Center for Waste Reduction Technology- Institute for Sustainability, 2000; Sagoff, 2000). The complexity of the industries and stakeholders involved directly translates to a sea of work contributing to the literature on metrics. Until now, there has been no effort in

consolidation and standardization of metrics. Shadiya (2010) did a thorough review of existing literature concerning sustainability metrics and indicator systems. Table 2.1 shows a list of proposed sustainability metrics and indicator systems as also the concerns they address.

Table 2.1: Proposed Sustainability Metric and Indicator Systems (Shadiya, 2010)

System	Applications	Limitations
Sustainable Process Index (Krotscheck et al., 1996)	Detailed process design	No social concerns are addressed
Inherent Process Safety Index (Heikkila, 1999)	Assessing safety of process	No economic and environmental concerns
Sustainability Indicators(Afgan et al., 2000)	Sustainability of process during early design stages	Better suited for energy systems
AICHE/ CWRT Sustainability Metrics(Center for Waste Reduction Technologies (CWRT) AIChE, 2000)	Environmental impact of process	No Economic and Social Concerns
Dow Jones Sustainability Index (Knoepfel, 2001)	Evaluate Corporate performance	Not applicable to chemical processes
BASF Socio-Eco-efficiency Metrics (Saling et al., 2002)	Evaluate impact of products/process during detail design	Requires extensive data, social metrics do not directly correlate with process design parameters
Green Metrics (Constable et al., 2002)	Evaluate efficiency of chemical reactions	No economic, environmental and social concerns
IChemE Sustainability Metrics (Institution of Chemical Engineers, 2002)	Evaluate the sustainability of production processes	Difficult to correlate social metrics with process design parameters.
Indicators of sustainable production (Krajnc et al., 2003)	Evaluating the sustainability of an operating unit	Only limited application to early stages of design

Global Environmental Risk Assessment (GERA) Index (Achour et al., 2005)	Evaluate health and safety risks of operating units	No economic and environmental concerns
BRIDGES to Sustainability Metrics (Tanzil et al., 2003)	Evaluate environmental impact of chemical processes	No economic and social concerns
Three Dimensional Sustainability Metrics (Martins et al., 2007)	Evaluate environmental impact, health and safety risks of an industrial process	No direct correlation between process design parameters and risk or environmental impact
Sustainability Indices (Tugnoli et al., 2008)	Evaluate sustainability of chemical process alternatives	Limited applicability to early stages of design
AIChE Sustainability Index(Calvin Cobb et al., 2009)	Evaluate Corporate Performance	Not applicable to chemical processes

It is evident from Table 2.1 that while there is a wealth of information concerning sustainability metrics, there is lack of information concerning social indicators. The boundaries for social indicators need to be clearly defined. Also, social indicators, unlike economic and environmental indicators, change from region to region, so the problems are compounded. One approach is to included health and safety under social metrics (Shadiya, 2010). The SE includes health and safety under social metrics to quantify the impact of the process on the society. The next subsection describes the SE in brief detail.

2.1.1 SUSTAINABILITY EVALUATOR (SE)

The SE is a Microsoft Excel-based impact assessment tool developed at Oklahoma State University by Shadiya (2010) for evaluating sustainability of processes. This tool uses a set of 41 indicators for evaluating economic, environmental, health and safety concerns. This tool requires inputs of material and energy flows, capital and operating costs (from a process simulator such as Aspen Plus), cost of raw materials, waste processing and

selling price of products. Figure 2.1 summarizes how the SE functions and Figure 2.2 shows the outputs of the SE.

Figure 2.1 Functioning of the SE

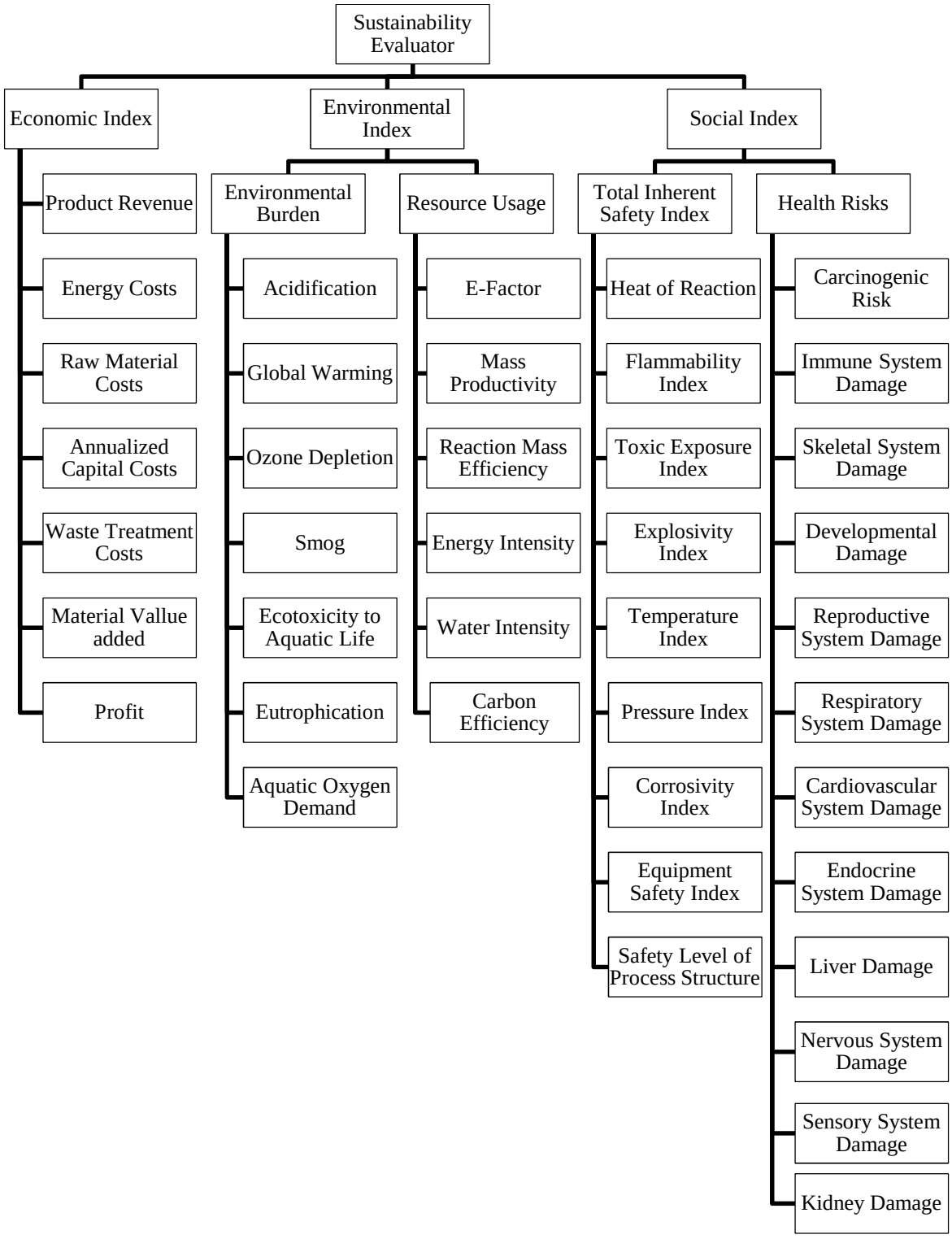

Figure 2.2 SE Outputs (Shadiya., 2010)

2.2 Optimization of Processes

Optimization is a technique of finding the best values of an objective function, where best may be the maximum or the minimum. Essentially optimization is a mathematical technique and a multitude of them have already been developed. For simple functions which are continuous and differentiable, Newton or Secant methods might be used (Rhinehart, 2010). More often than not in the process industries, the objective may not be a function, and an explicit function might be difficult to obtain. Commonly, an algebraic expression derived using regression of the input-output variables (dependent and independent variables) is also used.

The main focus of optimization in chemical engineering has been on optimizing for a single objective (SOO) such as profit/operating conditions/equipment design parameters (Rangaiah, 2008). In reality, there is more than one objective that needs to be satisfied in a chemical process, for instance meeting a certain product demand and at the same time meeting a emission regulation. These two objectives are conflicting: with increasing production, there is increasing emission. In this case, a tradeoff between the two objectives might be required. Process designers might be better off generating a set of solutions involving the two objectives and presenting it to the decision makers and managers who can then make decisions based on other external considerations best known to them. This technique is called multi objective optimization (MOO). Unlike SOO, which gives an unique solution, MOO gives rise to a number of solutions, unless the objectives are non conflicting, where the MOO scenario will also yield an unique solution.

Several methods are available for solving the MOO problem. Many of them involve converting the MOO into a SOO and subsequently solving the problem. Figure 2.3 shows the classification of the methods used to solve MOO problems. The primary classification of MOO methods fall into generating and preference based methods. Preference based methods require prior knowledge and also input from a decision maker, while generating methods provide an exact or approximate Pareto set (Rangaiah, 2008).

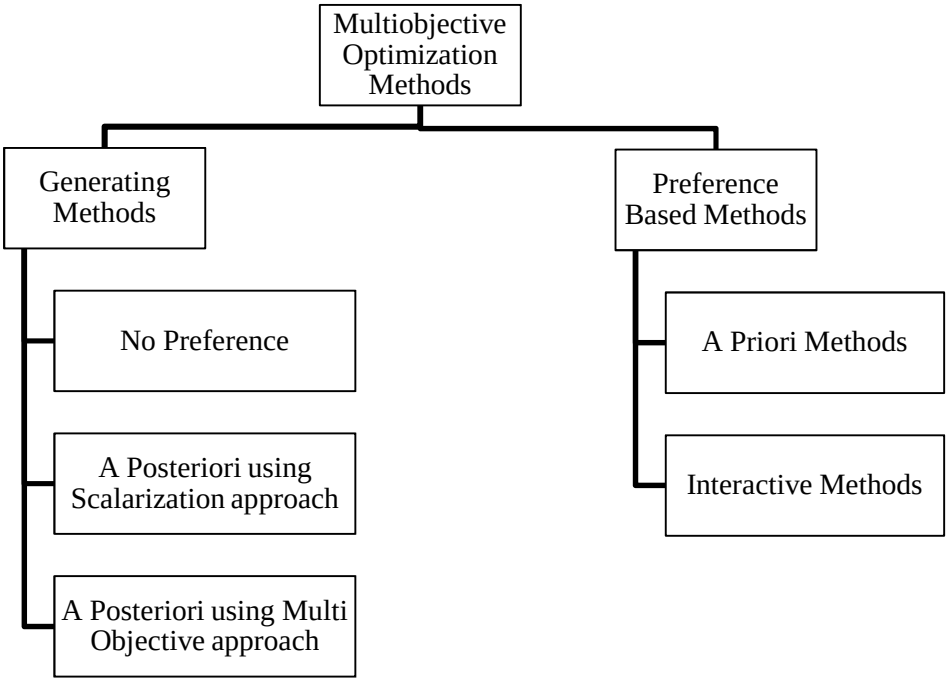

Figure 2.3 Classification of Multiobjective Methods (Rangaiah, 2008)

Preference based methods use the decision maker's preferences to generate solutions. They reduce mathematical and computational complexity, but require a thorough understanding and knowledge of the factors governing the process. Generating methods on the other hand "generate" results, and do not require preferences. However the scalarization approach requires the MOO to be converted to a SOO problem, which requires human intervention. A summary of the advantages and disadvantages of each method is provided in Table 2.2

Table 2.2 Merits and Demerits of MOO Methods (Rangaiah, 2008)

Method	Merits	Demerits
No Preference Methods	No inputs required from a decision maker at any stage	Computationally intensive for complicated problems, Not universally applicable
A Posteriori using Scalarization approach	Computational simplicity Very effective for low number of objectives	Difficulty in selecting weights and constraint bounds. Some solutions may not be found.
A Posteriori using MOO approach	Provides more Pareto sets than scalarization.	Computationally intensive, more results than necessary can lead to wastage of computational resources
A Priori Methods	Provides one optimal solution consistent with preferences	Requires prior knowledge of process to estimate preferences
Interactive Methods	Active role of decision maker, provides ideal tradeoff between computational resource and complexity	Requires decision maker's constant presence, full range of Pareto Optimal solutions may not be available

Conversion of MOO to SOO can be achieved in a number of ways. Most commonly used approaches to convert MOO to SOO are shown in Figure 2.4. Weighted objective method involves assigning weights to each of the objectives and combining them as a weighted sum.

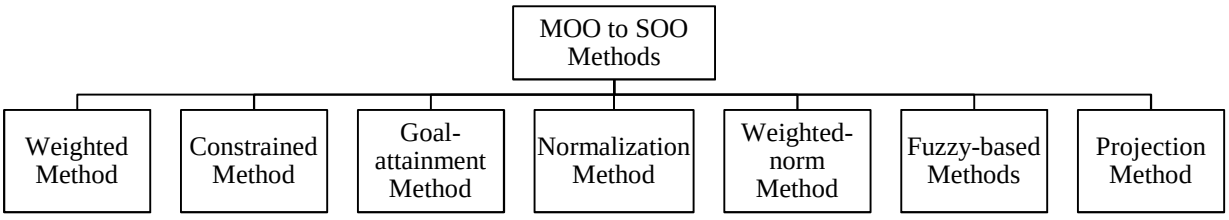

Figure 2.4 Approaches Used to Convert MOO to SOO Methods (Li et al., 2008)

Constrained method involves converting all but one objective into inequality constraints and then solving the subsequent SOO problem. In the goal attainment method, the desired goal for each objective is specified as an ideal point by the decision maker and the objective is formulated to attain this goal. Table 2.3 summarizes some of the MOO-SOO conversion options. For details of the other methods, one may refer to the work by (Li et al., 2008).

Table 2.3 MOO-SOO Conversion Methods (Li et al., 2008; Rangaiah, 2008)

Method	Objective Function Formulation
Weighted Method	$\max J = w_i(J_i)$
Constrained Method	$\max J = f_k(x)$; where f_k is the selected objective s.t. $f_i(x) \leq \varepsilon_i$; where f_i is the constraint for the i^{th} objective
Goal-attainment Method	$\min J_i = (f_i - f_{ideal})$; where f_{ideal} is the ideal or the goal that decision maker wishes to achieve for the i^{th} objective. Subsequently multiple objectives can be combined using the Weighted or Constrained Method
Normalization Method	$\min J_i = \frac{f_i - f_{i,min}}{f_{i,max} - f_{i,min}}$; where fi,min and fi,max are the upper and lower boundaries of the i^{th} objective. Subsequently multiple objectives can be combined using the Weighted or Constrained Method

A new approach to multi-objective optimization was introduced by (Fu et al., 2004). This method converts the MOO to SOO using the constrained approach. Figure 2.5 details the steps involved in this method. This method avoids the generation of a Monte-Carlo simulation by using a Hammersley Sequence Sampling (HSS) technique. By reducing the computational burden but retaining the efficiency of the solutions, this method provides for an ideal tradeoff between effort and results.

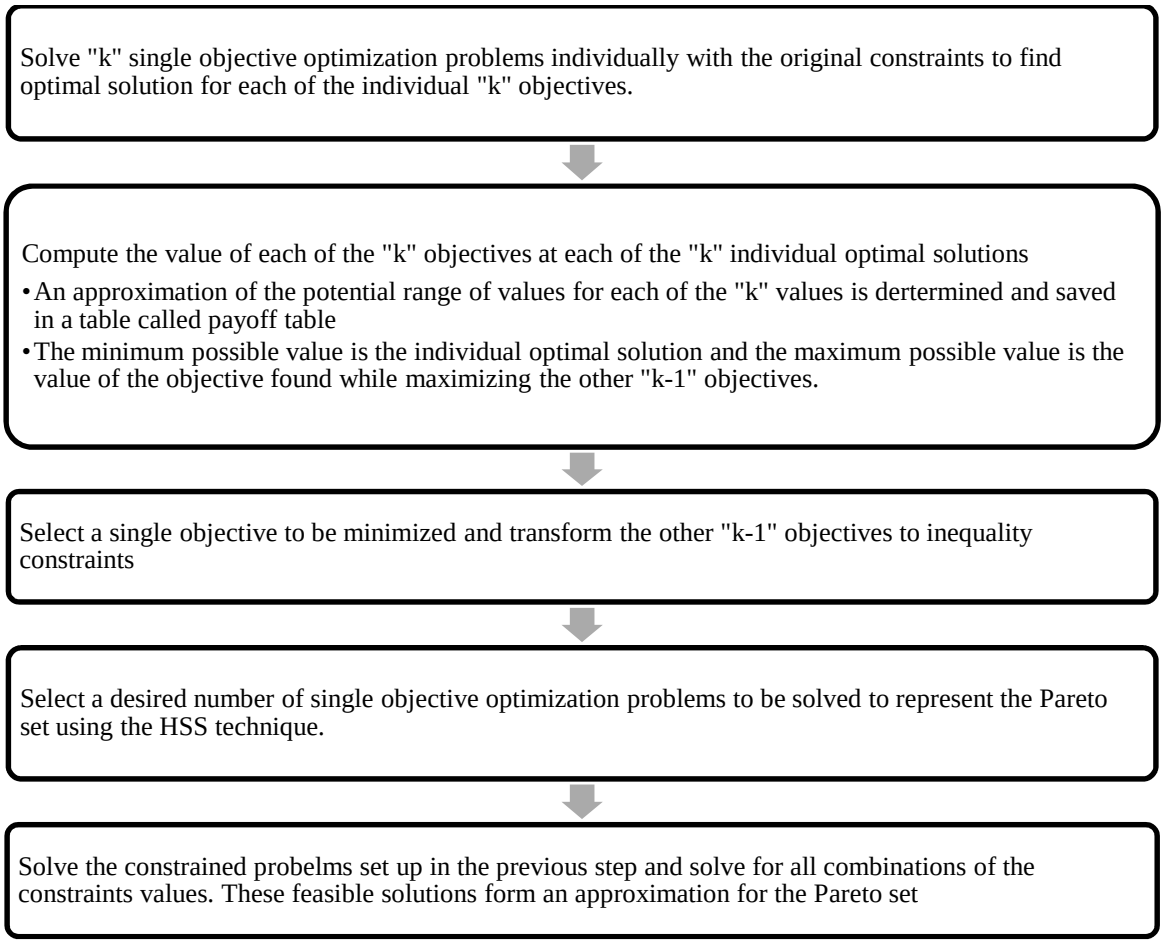

Figure 2.5 MINSOOP Algorithm to Solve “k” Multiobjective Problems (Fu et al., 2004)

2.3 Optimization and Sustainability

Previous researchers at OSU and elsewhere have addressed sustainability using several approaches. Jin (2005) incorporated multicriteria decision analysis (MCDA) into engineering design. A four-step metric classification system was developed to identify environmental metrics that assist decision makers in selecting an environment friendly process. Dantus (1999) focused on retrofit applications by classifying waste streams, assessing environmental impacts, developing process models and implementing pollution prevention techniques. The source reduction variables (SRV) are identified and the

alternatives used to construct a superstructure that is solved using a Mixed Integer Non-Linear Programming (MINLP). The superstructure was optimized using an economic model based on the net present value method. Further MCDA was implemented to address conflicting economic and environmental concerns via goal programming (Dantus et al., 1996; Gollapalli et al., 2000).

van der Helm's (1997) work focused on minimizing waste while considering economic tradeoffs. Process modification was used to reduce process waste. The approach involved three steps; process modeling, selection of source reduction variables and optimization of an economic objective function (van der Helm et al., 1998). Venkataraman (1996) used multiobjective optimization techniques to simultaneously optimize revenue while minimizing waste through source reduction. Process modeling and analysis, identification and selection of process alternatives and incorporation of multiobjective optimization were used (Venkataraman, 1996). All the above work focus on waste minimization and (or) economic-environmental objectives. None of them address social concerns of sustainability.

Outside of OSU (Gutowski et al., 2009), viewed sustainability from the perspective of ecosphere interactions between the various spheres in the earth and used a thermodynamic framework for the analysis. (Sengupta et al., 2008) developed a chemical complex analysis system using multicriteria optimization to determine the optimal configuration of plants in a chemical complex based on economy, energy, environment and sustainable costs. (Singh et al., 2006) developed a novel hierarchical Pareto optimization methodology used to achieve the most sustainable solution for industrial ecosystems. (Othman et al., 2010) addressed sustainability concerns using a multi-criteria

analytical process hierarchy. (Piluso et al., 2009) devised a framework for industrial sustainability using forecasting and profitable pollution prevention. (Sun et al., 2008) developed a strategy for multiobjective optimization for chemical processes.

2.4 Summary

In this chapter the following areas were explored

a) Development of metrics to evaluate sustainability and tools available for process designers to evaluate sustainability
b) SOO and MOO methods for optimizing processes and converting MOO to SOO problems
c) Optimization and its use in sustainable process development

Despite the wealth of information that was available in literature to optimize process,

a) There is no methodology that incorporates sustainability metrics into process optimization using a process simulator.
b) Most of the MOO methods require intensive computation and programming, and at the design stage, this kind of time and effort is not always required.
c) Though MOO-SOO conversion methods exist, they have not been implemented using sequential process simulators such as Aspen Plus to optimize processes for sustainability

CHAPTER III

METHODS

Process optimization for sustainability follows a sequence of steps. Figure 3.1 shows the proposed steps involved in this sequence. Subsequent sections in this chapter describe each of these steps in detail.

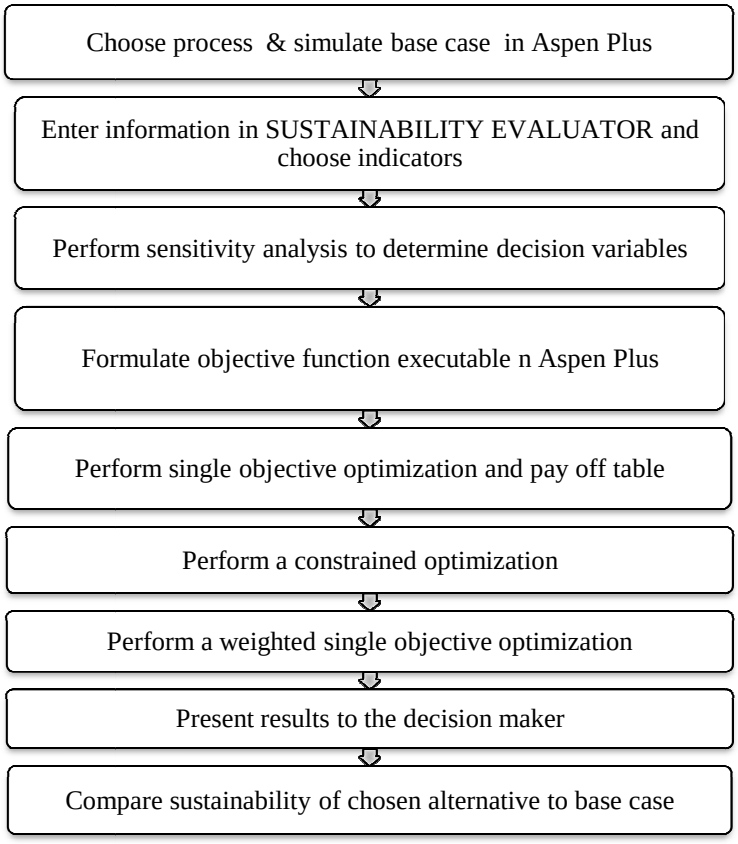

Figure 3.1 Proposed Methodology for Optimizing Processes for Sustainability

3.1 Choose Process and Simulate Base Case in Aspen Plus

The allyl chloride manufacturing process is selected because allyl chloride and the byproducts arising out of side reactions of its manufacturing process are regulated (van der Helm, 1997) under the Clean Air Act and the Clean Water Act. Further the global production of allyl chloride exceeds 1 million tons per annum, so an improvement in this process is bound to have a high impact. Commercial scale allyl chloride manufacture involves the high temperature chlorination of propylene in a plug flow reactor, typically adiabatic (Fairbairn et al., 1947). Equation 3.1a is the main reaction of the process giving allyl chloride and HCl. Equations 3.1b and 3.1c are the side reactions of the process. Equation 3.1b occurs at low temperatures (<400°F) by addition to give rise to 1,2 DCP, which is why the reactor is operated at high temperatures (Fairbairn et al., 1947 ; Krahling et al., 2000). Equation 3.1c occurs by an substitution reaction where the allyl chloride formed reacts further with chlorine to give 1,3, DCP.

$$\underset{\text{Propylene}}{C_3H_6} + \underset{\text{Chlorine}}{Cl_2} \rightarrow \underset{\text{Allyl Chloride}}{C_3H_5Cl} + \underset{\text{Hydrochloric acid}}{HCl} \quad (3.1a)$$

$$\underset{\text{Propylene}}{C_3H_6} + Cl_2 \rightarrow \underset{\text{1,2-dichloropropane}}{C_3H_6Cl_2} \quad (3.1b)$$

$$\underset{\text{Allyl Chloride}}{C_3H_5Cl} + Cl_2 \rightarrow \underset{\text{1,3-dichloropropene}}{C_3H_4Cl_2} + HCl \quad (3.1c)$$

The products coming out of the reactor are purified using a series of distillation columns to separate the unreacted excess propylene, purify allyl chloride and separate the wastes. Figure 3.2 is a schematic of the allyl chloride process simulated in this work. Both the adiabatic and isothermal reactor schemes are simulated for this work. Heated propylene and chlorine are fed to a plug flow reactor in adiabatic operation, and the reaction products containing a mixture of allyl chloride, 1,2 DCP, 1,3 DCP and HCl are fed to a

prefractionator column, where the excess propylene and HCl are separated from the chlorides. The allyl chloride is purified by another distillation tower. The HCl and propylene coming out of the top of the prefractionator pass through an absorber where HCl is absorbed in water and sold, while the propylene is compressed and recycled back to the feed heater.

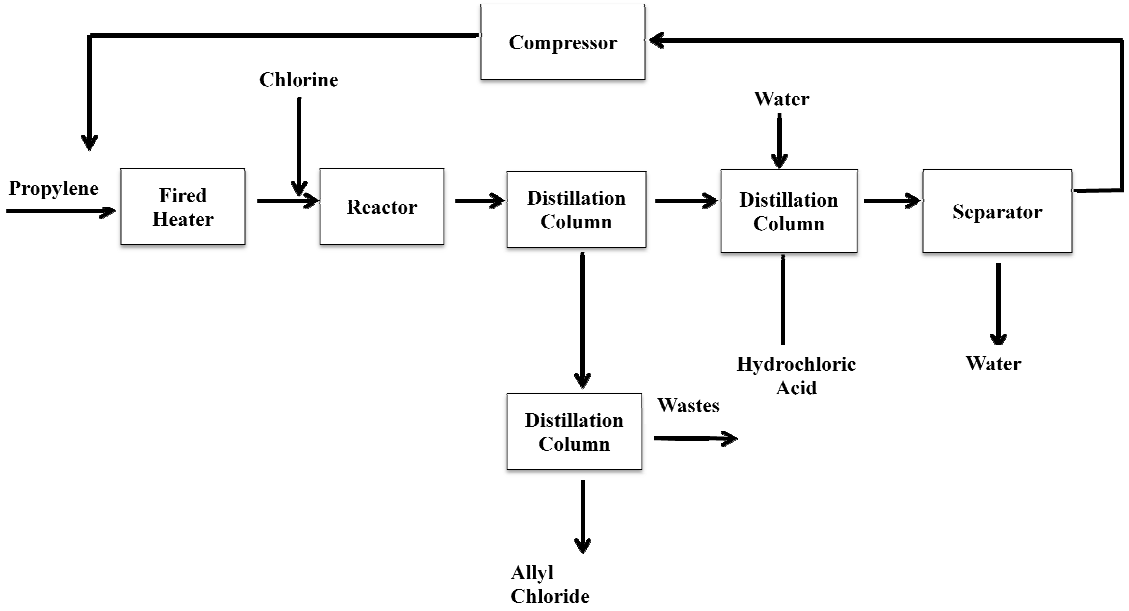

Figure 3.2 Schematic of the Allyl Chloride Manufacturing Process

Using kinetic and operating conditions from literature (Fairbairn et al., 1947 ; van der Helm, 1997; Krahling et al., 2000) this process is simulated in Aspen Plus. Aspen Plus is a sequential modular simulator where each unit operation block is solved in a certain sequence. For simulating a process, Aspen Plus requires input of component flows, temperature, pressures and reactions for absorbers and reactors. Input summaries of all simulations are provided in the appendix. Several options are provided for each type of equipment, for instance distillation columns can be simulated using shortcut distillation calculations with the DSTW block and using rigorous simulation with the RADFRAC block. Details and step-by-step procedures on how a flow sheet is set up and process

operating conditions are entered into Aspen Plus can be found in (Aspen Tech Inc., 2008). The allyl chloride process was earlier simulated by van der Helm (1997). This work uses Aspen Plus input summary files from that work along with information from literature to build the process model. Table 3.1 shows the details of the blocks used to simulate the allyl chloride process.

Table 3.1 Details of Aspen Plus Models Used to Simulate the Allyl Chloride Process

Equipment	Aspen Plus Model
Propylene Feed Heater	HEATER
Plug Flow Reactor	RPLUG
Continuous Stirred Tank Reactor	RCSTR
Reactor Effluent Cooler	HEATER
Prefractionator	RADFRAC
HCl Absorber	RADFRAC
Separator	SEP
Allyl Chloride Purification Column	RADFRAC
Compressor	COMP

Once the base case process has been simulated, the economic evaluation is completed using Aspen's economic evaluation tool. This requires a series of steps starting from initializing the costing tool, loading simulation data, mapping the equipments in the flow sheet, sizing and then evaluating the cost. Capital and operating cost information is obtained at the end of these steps. The equipment summary tab also tells the user about any errors and issues if any in sizing and costing. The material and energy balance results and costing results obtained from this simulation are used to enter information into the SUSTAINABILITY EVALUATOR.

3.2 Enter Information in the SUSTAINABILITY EVALUATOR and Choose Indicators

The SUSTAINABILITY EVALUATOR (SE) is an impact assessment tool developed by Shadiya (2010). The SE requires inputs of material flows, energy flows, capital and operating costs from Aspen Plus for economic evaluation, environmental evaluation and social evaluation. Table 3.2 shows the inputs given to the SE for the economic evaluation.

Table 3.2 Inputs to the SE for Economic Evaluation

Item	Value ($/lb)
Allyl Chloride Price (Hexion Speciality Chemicals)	0.82
HCl Price (ICIS)	0.063
Chlorine Cost (ICIS)	0.16
Propylene Cost (ICIS)	0.45
Waste Treatment Cost (Ulrich et al., 2007)	0.0011

The environmental and social evaluation sections of the evaluator have a list of chemicals in their drop down menus for the different aspects of environmental and social impact such as safety, carcinogenic risk, neurological damage, etc. There are 41 indicators that the SE provides as output to evaluate the impact of a process. In order to compare different processes it is necessary to have a smaller number of indicators or lump some of the indicators. Some of the indices such as profit, health impact, safety index are composite indicators. The composite indicators have sub indices, for instance profit accounts for revenue, waste costs, raw material costs etc. So, using profit as an indicator of comparison actually accounts for revenue, waste costs, raw material costs etc. Thus the number of indicators used (after lumping the sub indices) to represent the output of the SE is 16. Table 3.3 shows the list of the indicators chosen, their units and the sustainability dimension.

Table 3.3 List of indicators chosen for sustainability evaluation

Indicator	Units	Sustainability Dimension
Global warming	lb equivalent per year	Environmental
Health impact	lb equivalent per year	Social
Safety Index	No units	Social
Material intensity	Lb/lb	Resource Usage
Energy intensity	kW per lb	Resource Usage
Water intensity	lb/lb	Resource Usage
E-factor	lb/lb	Resource Usage
Reaction Mass Efficiency	%	Resource Usage
Effective Mass Yield	%	Resource Usage
Atom Economy	%	Resource Usage
Mass Intensity	lb/lb	Resource Usage
Mass Productivity	lb/lb	Resource Usage
Profit	$ per year	Economic
Annualized Capital Cost	$ per year	Economic
Waste cost	$ per year	Economic
Material Value Added	$ per year	Economic

All of the health impacts were summed up to represent the health impact in pounds equivalent (Equation 3.5). Global warming (due to 1,2 DCP and 1,3 DCP) is the only environmental impact arising out of this process, and is included in our analysis.

3.3 Sensitivity Analysis to Determine Decision Variables

To determine the variables that are to be used for optimization, a sensitivity analysis is carried out with the base case. The effect of the variables on process performance in terms of moles of the main product produced, profit, health impact and mass productivity (MP) is studied. MP is used as an objective rather than material intensity because, it

accounts for both efficiency and resource usage. MP is defined in Equation 3.2, profit by Equation 3.3 and Health Impact by Equation 3.5.

$$\text{Mass productivity (MP)} = \frac{\text{Mass of reactants used}}{\text{Mass of reactants fed}} \quad (3.2)$$

$$\text{Profit} = \text{Revenue from Products-Raw Material Cost-Utility Cost-Waste Cost} \quad (3.3)$$

There are several sources available in literature (Fairbairn et al., 1947 ; Krahling et al., 2000) that state the effect of changing different process variables on the molar yields of the process. However there is no information that states how changes in process variables affect profit, health impact and MP. A sensitivity analysis that looks at these presents a much better idea when it comes to optimization, because profit, health impact and MP are going to be the objective functions. Table 3.4 lists the variables used along with the ranges used to ascertain their effects on the process and the different objectives.

Table 3.4 Variables Used for Sensitivity Analysis and their Ranges

Variable	Range
Temperature of propylene feed heater	400-1000°F
Reactor Pressure	15-150 psia
Molar Feed Ratio (C_3H_6/Cl_2)	1-8
Temperature of reactor (if isothermal)	400-1000°F

Aspen Plus has a built-in feature to carry out sensitivity analysis within the model analysis tools tab. This requires a definition of the variables that are going to be manipulated and the variables that are going to be calculated and tabulated. Aspen Plus cannot calculate health, MP or profit unless they are defined using FORTRAN Statements. FORTRAN statements were used to define and specify the calculation sequence of such variables. The FORTRAN statements used in this study can be found in

Appendix. Step by step instructions on performing sensitivity analysis using Aspen can be found in (Aspen Tech Inc., 2008). From the results of the sensitivity analysis the decision variables to be used in optimization along with their ranges are identified.

3.4 Formulating an Objective Function Executable in Aspen Plus

An objective function is a function that is to be maximized or minimized using an optimization algorithm. A general formulation of a single objective optimization problem would look like Equation 3.4.

$$\max_{\{a,b\}} J=f(x,y) \tag{3.4}$$

There can be constraints on the values of the objective function J and (or) on the values that a and b, the decision variables can take. Conventionally a process is optimized for profit, without considerations for health and (or) the environment. In this work it is proposed to optimize the process to make it more sustainable as opposed to making it more profitable. Hence we have three objectives, one in each dimension of sustainability- profit, MP and health. From Equation 3.5 and 3.6 it is clear that health impact and environment go together and it would suffice to have just one of them as an objective. Health and environmental impact are in lb equivalent and component flows in lb.

$$\text{Health Impact}=\sum_{i=1}^{N} \text{Potency factors from } SE_i * \text{Component flow rate}_i \tag{3.5}$$

$$\text{Environmental Impact}_i=\text{Potency factors from } SE_i * \text{Component flow rate}_i \tag{3.6}$$

Aspen Plus has inbuilt optimization routines within the model analysis tools tab for optimizing processes. This requires a definition of all the variables that would be used in the optimization, both the manipulated variables (decision variables) and the variables used to calculate the objective function. As in the sensitivity analysis, Aspen Plus requires inline FORTRAN statements to compute profit, health impact and MP. The

FORTRAN statements used are very similar to the ones in sensitivity analysis and can be found in the Appendix. The default optimization algorithm in Aspen Plus is Successive Quadratic Programming (SQP). Other essential information used in optimizing this process with Aspen Plus is listed in Table 3.5.

Table 3.5 Aspen Plus Optimization Parameters

Algorithm	Sequential Quadratic Programming
Tolerance	0.001
Maximum number of flow sheet iterations	100

3.5 Single Objective Optimization and Payoff Table

The next step in the methodology is to carry out a single objective optimization of all the objective functions and generate a payoff table. This procedure is partly along the lines prescribed by (Fu et al., 2004). Figure 3.3 shows the steps involved in the MINSOOP method. For this research the first three steps are implemented in accordance with this method. The fourth and fifth steps are slightly modified. Instead of selecting a number of problems to solve, only one objective of profit is selected. The objectives of MP and health were converted to constraints and the right hand sides of the constraints are obtained by dividing the region between the maximum and the minimum into five equally spaced intervals (five is demonstrative of this methodology and more number of intervals can be chosen). Constraints can be added to the optimization statement in Aspen Plus. Using this feature, a representative set of the constrained optimization results was obtained and the points plotted on a two dimensional graph. Subsequently the dominant sets are eliminated and only the non-dominant sets of Pareto optimal solutions are presented to the decision maker.

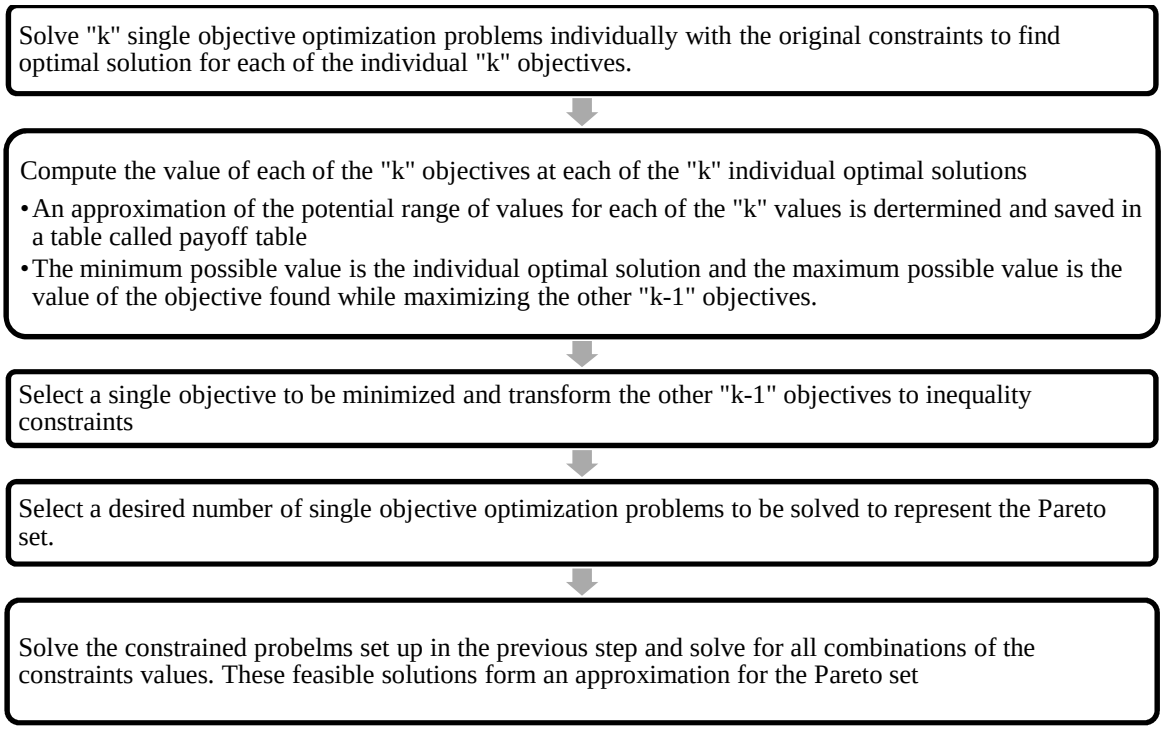

Figure 3.3 MINSOOP Algorithm to Solve “k” Multiobjective problems (Fu et al., 2004)

3.6 Weighted Single Objective Optimization

The second method adopted to convert the multi objective optimization problem to single objective under the generating methods was the method of weights. By using the method of weights the multi optimization statement was reduced to a single objective statement and each of the objectives was weighed. When combining multiple objectives it was necessary to normalize the objectives to have consistent units for the function. Each objective was normalized by dividing it by the maximum value obtained from the payoff table. The following example illustrates the conversion of a multiobjective problem into a weighted single objective problem. Equations 3.7 to 3.9 represent a multiobjective scenario.

$$\max_{\{a,b\}} J_1 = f(x,y) \tag{3.7}$$

$$\min_{\{a,b\}} J_2 = g(x,y) \tag{3.8}$$

$$\max_{\{a,b\}} J_3 = h(x,y) \quad (3.9)$$

Equations 3.10 to 3.11 represent the weighted, normalized, single objective function.

$$\max_{\{a,b\}} J = w_1\left(\frac{J_1}{\bar{J}_1}\right) - w_2\left(\frac{J_2}{\bar{J}_2}\right) + w_3\left(\frac{J_3}{\bar{J}_3}\right) \quad (3.10)$$

$$\sum w_i = 1 \quad (3.11)$$

Here J_1, J_2, J_3 are profit, health impact and MP respectively. $\bar{J_1}$, $\bar{J_2}$ and $\bar{J_3}$ are the bounds of these objectives determined from the payoff table that is used to normalize the objectives. The implementation of the weighted normalized objective function is similar to the single objective optimization method, with only the objective function statement being different. Since the primary objectives do not have any constraints the weighted normalized optimization is not constrained. The weights of the objectives viz. profit, MP and health impact are varied from 0 to 1. The sum of all the weights is always one (though it need not be so). The results obtained for different weights were plotted on a two dimensional graph and dominant sets were eliminated before presenting to a decision maker.

For a decision maker choosing a constrained optimization versus the weighted optimization is a decision by itself. The computational burden of the constrained method is higher than the weighted method, because of the constraints (Fu et al., 2004). Constrained methods offer better control over the exploration of the optimizer. For instance, the decision maker decides that the value of his profit has to be at a particular value, and there cannot be a compromise on it. Now, the optimizer has to search along the line/surface that has different combinations for the other two objectives-health impact and mass productivity. The weighted method is more intuitive and requires sound

knowledge of the process and its intricacies from a decision maker. Most often than not, the choice of weights is subject to debate.

3.7 Comparing Sustainability of Chosen Optimized Case with the Base Case

When the decision maker is presented with results from the weighted or the constrained optimization, he/she has to preferentially choose one optimum solution over another. At any given point, there cannot be an improvement in one objective without compromising on others. This is the reason that the decision maker is presented with a number of alternatives to choose from based on his current priorities.

Amoeba charts (Rutgers et al., 2008) have been used in literature to compare multiple values on a same graphic. This research uses the amoeba chart approach to compare the chosen optimized case with the base case. The results of the various indicators for the optimized case are normalized with respect to the base case which is considered unity. The resulting amoeba chart provides with an instant visual comparison of whether an indicator has improved or worsened. Figure 3.4 is an illustrative example of an amoeba chart. The dark lines are the ones of the base case (where all the indicators are valued as unity) while the light lines represent the optimized case.

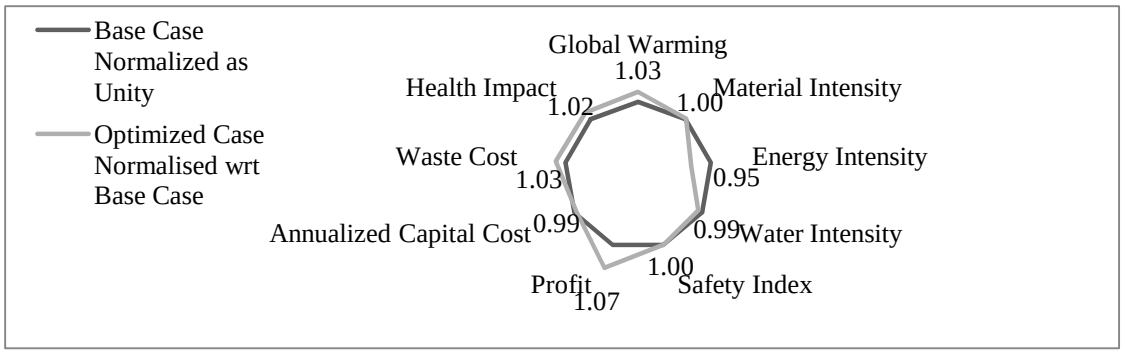

Figure 3.4 Illustrative Example of an Amoeba Chart

CHAPTER IV

RESULTS AND DISCUSSION

4.1 Base Case Modeling of Process Using Aspen Plus and Sustainability Evaluation

Based on environmental and social concerns (regulated under the Clean Air Act and Clean Water Act) the allyl chloride process is selected to be examined. The process is simulated using information from literature (Fairbairn et al., 1947 ; van der Helm, 1997; Krahling et al., 2000). Two process schemes-one with an isothermal plug flow reactor (PFR) and one with an adiabatic PFR reactor are simulated. The pre-exponential factors used for the reactions have already been mentioned in the Appendix. The Aspen Plus economic evaluation program is used to estimate the capital and operating costs of the process. The information from the base case presented in Table 4.1 is used to carry out the sustainability impact assessment using the SE. The results obtained from the SE using the information in Table 4.1 are presented in Tables 4.2, 4.3, 4.4, 4.5 and 4.6.

Table 4.1 Base Case Simulation Results for Adiabatic and Isothermal Case

	Adiabatic	Isothermal	Units
Allyl Chloride production	49.0	44.0	10^6 lb/year
By product HCl production (32 wt.%)	137.0	149.0	10^6 lb/year
Chlorine usage	103.0	103.0	10^6 lb/year
Propylene usage	48.0	45.0	10^6 lb/year
Water usage (coolers, condensers, absorber)	4813.0	4712.0	10^6 lb/year
Energy usage (compressor, reboilers, heaters)	54.0	52.0	10^6 kWh/year
Total waste generated (1,2 DCP & 1,3 DCP)	56.0	53.0	10^6 lb/year
Capital Cost (from Aspen in 2008$)	5.4	5.6	10^6 $
Operating Cost (from Aspen in 2008$)	2.8	3.3	10^6 $/year
Allyl Chloride Price (Hexion Speciality Chemicals; Rangaiah, 2008)	0.88	0.88	$/lb
HCl Price (ICIS)	0.063	0.063	$/lb
Chlorine Cost (ICIS)	0.16	0.16	$/lb
Propylene Cost (ICIS)	0.45	0.45	$/lb
Waste treatment cost (Ulrich et al., 2007)	0.0011	0.0011	$/lb

Table 4.2 Economic Assessment Results from SE

OUTPUTS for Economic Evaluation		
	Adiabatic ($10^6$$/year)	Isothermal ($10^6$$/year)
Revenue	52.4	48.7
Utility Costs (2008$)	2.8	3.3
Waste Treatment Costs	0.6	0.6
Raw Material Costs	38.2	35.5
Capital Costs (2008$)	5.4	5.6
Annualized Capital Cost	0.6	0.7
Material Value Added	14.1	12.2
Profit	10.7	8.2

The outputs of the economic evaluation indicate that the adiabatic process with a profit of $10.72 million is more profitable than the isothermal process with a profit of $8.21 million. This is in concurrence with industrial operation of the allyl chloride process

where the reactor is operated adiabatically than isothermally (Fairbairn et al., 1947 ; van der Helm, 1997; Krahling et al., 2000). Further it is clear that the utility and capital costs for the adiabatic case are lower than the isothermal case. So at the outset it is clear that operating adiabatically is a better option than operating isothermally. However, in order to compare the sustainability of both the processes using the methodology proposed in this work, both are subsequently optimized.

Table 4.3 shows the results from the health impact assessment of the process. Again it is observed that in most cases, the health impact of the adiabatic process is much lower than the isothermal process. The health impact was calculated by the SE using potency factors and component flow rates according to Equation 3.5. The health impact is modified as Equation 3.5 so that it can be used in Aspen Plus using inline FORTRAN statements for sensitivity analysis and optimization. The damage caused to health is regarded as social impact. 1,2 DCP and 1,3 DCP, the primary wastes of this process are responsible for the different health impacts.

Table 4.3 Health Impact Assessment Results from SE (adiabatic reactor)

Health Impact	Equivalent impact ($x10^{-3}$ lb/year)		Causative Chemical
	Adiabatic	Isothermal	
Carcinogenic Risk	29000.0	30000.0	1,2 DCP & 1,3 DCP
Immune System Damage	20000.0	26000.0	1,3 DCP
Skeletal System Damage	0.0	0.0	N/A
Developmental Damage	0.0	0.0	N/A
Reproductive System Damage	33000.0	32000.0	1,2 DCP & 1,3 DCP
Kidney System Damage	20000.0	26000.0	1,3 DCP
Respiratory System Damage	33000.0	32000.0	1,2 DCP & 1,3 DCP
Cardiovascular System Damage	13000.0	5200.0	1,2 DCP
Endocrine System Damage	13000.0	5200.0	1,2 DCP
Liver Damage	33000.0	32000.0	1,2 DCP & 1,3 DCP
Nervous System Damage	33000.0	32000.0	1,2 DCP & 1,3 DCP
Sensory System Damage	33000.0	32000.0	1,2 DCP & 1,3 DCP

Results of the environmental impact assessment are presented in Table 4.4. For the allyl chloride process the only environmental impact is the global warming impact measured in thousands of pounds CO_2 equivalent.

Table 4.4 Environmental Impact Assessment Results from SE

	Adiabatic	Isothermal	Units
Atmospheric Acidification	0.0	0.0	1000s lb/year SO_2 Equivalent
Global Warming	611115.0	578015.0	1000s lb/year CO_2 Equivalent
Stratospheric Ozone Depletion	0.0	0.0	1000s lb/year TCFM Equivalent
Photochemical Smog Formation	0.0	0.0	1000s lb/year C_2H_4 Equivalent
Aquatic Acidification	0.0	0.0	1000s lb/year H^+ ions Equivalent
Aquatic Oxygen Demand	0.0	0.0	1000s lb/year O_2 Equivalent
Ecotoxicity to Aquatic life	0.0	0.0	1000s lb/year Copper Equivalent
Eutrophication	0.0	0.0	1000s lb/year Phosphate Equivalent

Resource usage evaluation results are presented in Table 4.5. These results indicate the resource consumed to produce one pound of allyl chloride product. Resource evaluation ensures that energy, water and raw material usage are accounted for.

Table 4.5 Results of Resource Usage Evaluation from SE

	Adiabatic	Isothermal	Units
Mass productivity	64.0	63.0	%
E-Factor	0.6	0.6	lb/lb
Atom Economy	100.0	100.0	%
Mass Intensity	1.5	1.6	lb/lb
Mass Productivity	64.0	63.0	%
Reaction Mass Efficiency	20.0	20.0	%
Material Intensity	4.0	3.9	lb/lb
Energy Intensity/ Fossil Fuel Usage	0.5	0.6	kW/lb
Water Intensity	49.0	50.0	lb/lb

Table 4.6 shows the results of the safety evaluation from the SE. The maximum possible safety index for any process is 100. The adiabatic base case has a lower safety index than the isothermal case. However as stated earlier, improving the safety of the process is outside the scope of this work, so no effort is devoted towards that end.

Table 4.6 Results of Safety Evaluation from SE

	Adiabatic	Isothermal	Maximum Value
Heat of main reaction index	0	4	8
Heat of side reaction index	0	0	8
Flammability index	8	8	8
Explosiveness index	2	2	8
Toxic Exposure Index	24	24	30
Corrosiveness index	2	2	4
Temperature index	6	6	8
Pressure index	0	0	8
Equipment safety index	6	6	8
Safety Level of Process Structure index	4	4	10
Total Inherent Safety index	52	56	100

At this stage, a representative indicators are selected, to represent the three dimensions of sustainability i.e. economic, social and environmental. The indicators shown in Table 4.7 are selected for use in the amoeba charts.

Table 4.7 Selected Indicators for use in Amoeba Charts

Indicator	Sustainability Dimension
Global warming	Environmental
Health impact	Social
Safety Index	Social
Material intensity	Resource Usage (Environmental)
Energy intensity	Resource Usage (Environmental)
Water intensity	Resource Usage (Environmental)
E-factor	Resource Usage
Reaction Mass Efficiency	Resource Usage
Effective Mass Yield	Resource Usage
Atom Economy	Resource Usage
Mass Intensity	Resource Usage
Mass Productivity	Resource Usage
Profit	Economic
Annualized Capital Cost	Economic
Waste cost	Economic
Material Value Added	Economic

4.2 Sensitivity Analysis

A sensitivity analysis is carried out to determine the operating parameters that affect the extent of the main reaction and also profit, health impact and mass productivity. The equations used in the sensitivity analysis and optimization are profit (Equation 3.2), health impact (Equation 3.5) and MP (Equation 3.2). These equations are defined in the FORTRAN block of the sensitivity analysis tab in Aspen Plus. The FORTRAN statements and the variables used are shown in the Appendix. The list of operating parameters used to carry out a sensitivity analysis and their ranges are presented in Table 4.8(a).

Table 4.8(a) Sensitivity Analysis Parameters

Variable	Range	
	Adiabatic	Isothermal
Feed Ratio (C_3H_6/Cl_2)	1-8	1-8
Temperature of C3H6 feed heater	400-1000°F	400-1000°F
Temperature of reactor	N/A	400-1000°F
Pressure of reactor	15-150 psia	15-150 psia

4.2.1 Adiabatic Reactor Case Sensitivity Analysis

Results of the sensitivity analysis for increasing feed ratio for an adiabatic reactor are presented in Figure 4.1 (a) and (b). Figure 4.1 (b) has two vertical axes, one for profit and one for mass productivity. With increasing feed ratio, the molar yield of allyl chloride increases and the yield of 1,2 DCP and 1,3 DCP decrease. The yield of 1,3 DCP decreases much more rapidly than the yield of 1,2 DCP. Allyl chloride formation peaks between a feed ratio of 4 and 6. However from Figure 4.1 (b) it is evident that profit peaks at a feed ratio just over 4. The health impact decreases with increasing feed ratio and MP increases with increasing feed ratio. This analysis indicates that the range for feed ratio should be between 1 and 6. Beyond 6, there is no improvement in product formation, profit decreases rapidly and health impact does not decrease significantly.

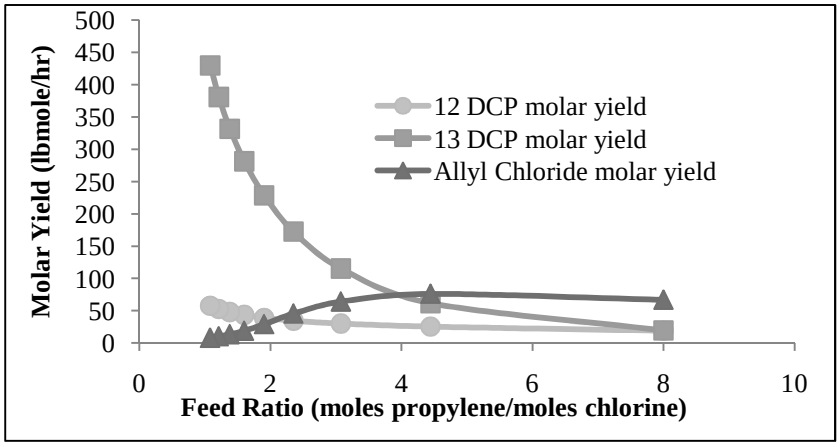

Figure 4.1 (a) Effect of Feed Ratio on Molar Yield (Adiabatic)

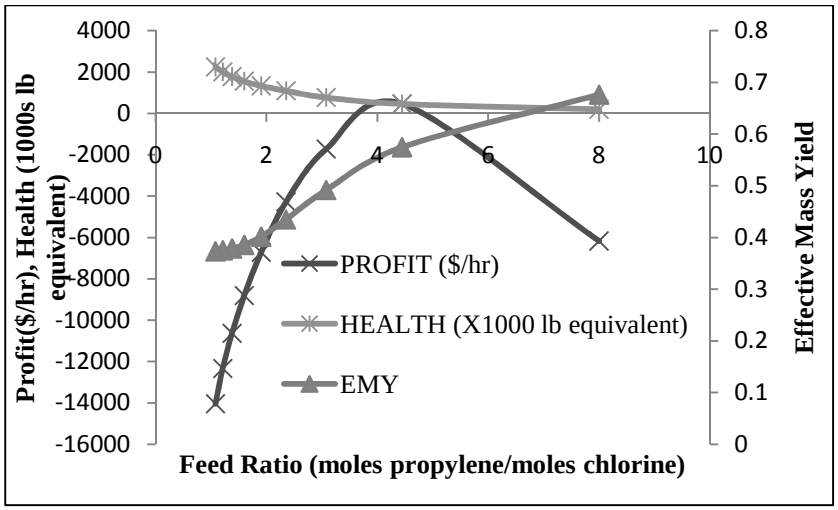

Figure 4.1(b) Effect of Feed Ratio on Profit, Health and MP (adiabatic)

Next, the sensitivity to the temperature of the feed heater is studied. This is done because increasing temperature of the feed increases the temperature of the reactor effluent stream. A change in reactor outlet temperature essentially means a change in the molar yields and consequently all our objectives. Figure 4.2 (a) and (b) show the effect of varying the feed heater temperature. With increasing temperature of the feed heater, allyl chloride formation increases slightly before decreasing at temperatures above 550°F. With increasing temperature 1,2 DCP formation decreases and 1,3 DCP formation increases both of which are in accordance with literature. The profit increases until 600°F and then decreases. MP increases upto 700°F and then decreases indicating that there is a conflict between when profit attains the maximum and when the MP attains the maximum. The gradient in health impact is very gradual, it decreases till about 600°F and increases thereafter. So, the three objectives competing against each other. It is therefore advisable to vary temperature of the feed heater from 400-700°F.

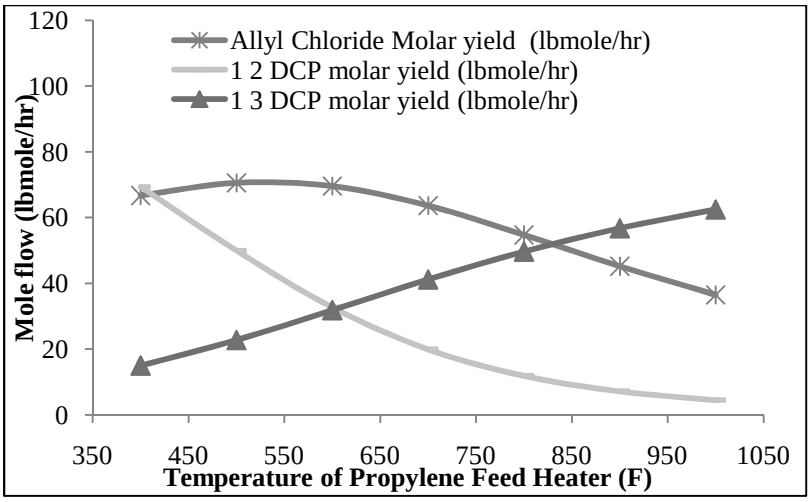

Figure 4.2 (a) Effect of Propylene Feed Heater Temperature on Molar Yield (Adiabatic)

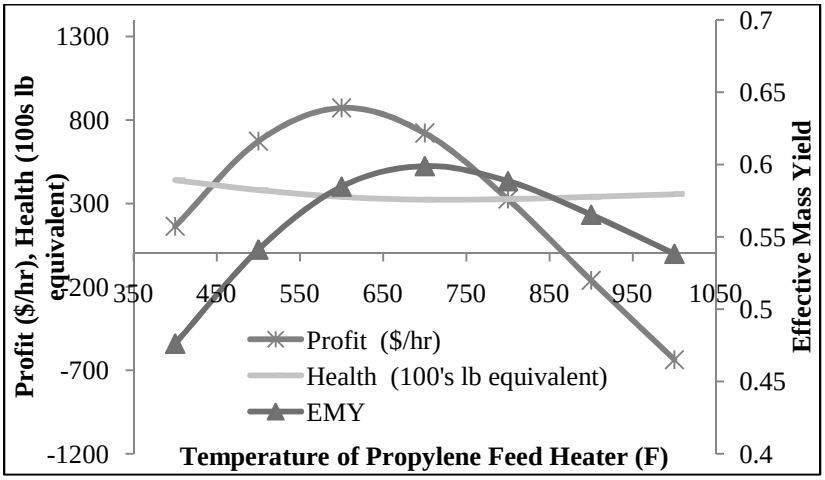

Figure 4.2 (b) Effect of Propylene Feed Heater Temperature on Profit, Health and MP (Adiabatic)

The next step is to vary reactor pressure for the adiabatic case. From Figure 4.3(a) and 4.3 (b) it is clear that changing reactor pressure does not have any impact on the molar yields or any of the objectives.

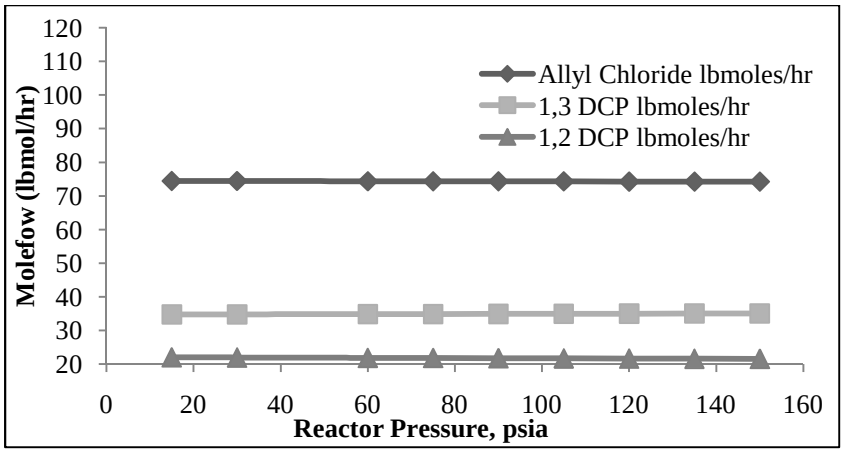

Figure 4.3 (a) Effect of Reactor Pressure on Molar Yield (Adiabatic)

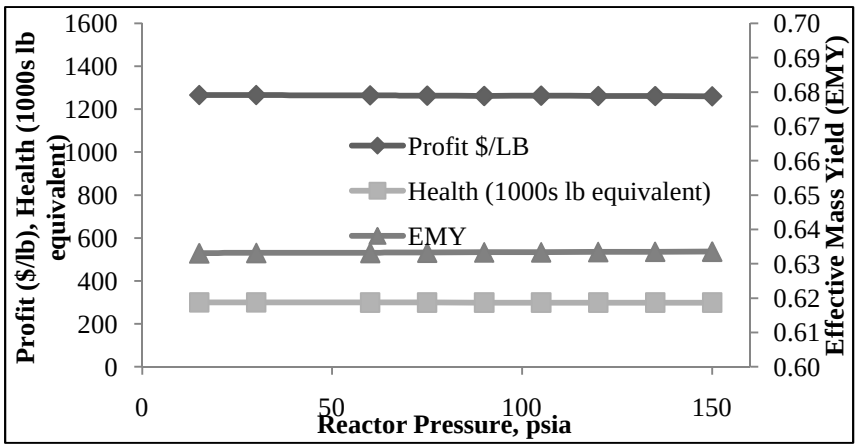

Figure 4.3 (b) Effect of Reactor Pressure on Profit, Health and MP (Adiabatic)

4.2.2 Isothermal Reactor Case Sensitivity Analysis

The sensitivity analysis is repeated for the isothermal case, with the only difference being, that instead of reactor pressure, reactor temperature is used. Results of the sensitivity analysis for increasing feed ratio for an isothermal reactor are presented in Figure 4.4 (a) and (b). With increasing feed ratio, the molar yield of allyl chloride, 1,2 DCP and 1,3 DCP decreases. The yield of 1,2 DCP decreases much more rapidly than the yield of 1,3 DCP. Allyl chloride formation is highest for a feed ratio of 1. However from Figure 4.1 (b) it is evident that the highest value of profit is not at a feed ratio of 1, rather it is at a feed ratio of about 4. The health impact decreases with increasing feed

ratio and MP increases with increasing feed ratio. This analysis indicates that the range for feed ratio should be between 1 and 6. Beyond a feed ratio of 6, 13 DCP formation does not decrease anymore, profit decreases rapidly and health impact does not decrease significantly.

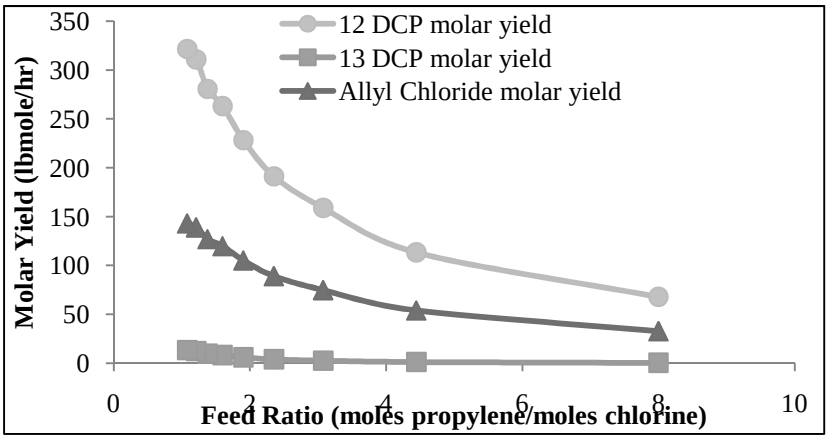

Figure 4.4 (a) Effect of Feed Ratio on Molar Yield (Isothermal)

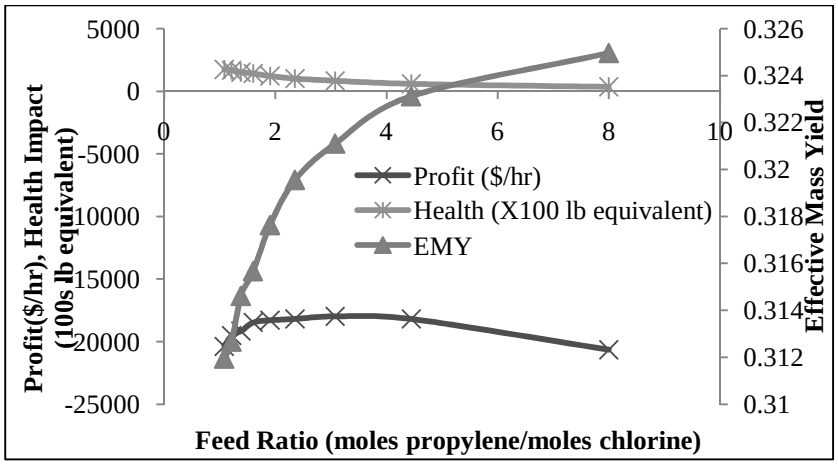

Figure 4.4 (b) Effect of Feed Ratio on Profit, Health and MP (Isothermal)

Next, the sensitivity to the temperature of the reactor is studied. A change in reactor temperature essentially means a change in the molar yields and consequently all our objectives. Figure 4.5 (a) and (b) show the effect of varying the reactor temperature. With increasing temperature allyl chloride formation increases before decreasing at temperatures above 700°F. With increasing temperature 1,2 DCP formation decreases

and 1,3 DCP formation increases both of which are in accordance with literature. Profit increases till about 700°F and then decreases. MP increases till about 800°F and decreases indicating that there is a conflict between when profit attains the maximum and when the MP attains the maximum. The gradient in health impact is very gradual, it increases till 550 °F and then decreases till about 800°F and increases gradually thereafter. Again, all the three objectives are competing against each other. Therefore it is advisable to vary temperature of the reactor from 500-1000°F to allow the decision variables to search for optimum values to maximize profit, health impact and MP.

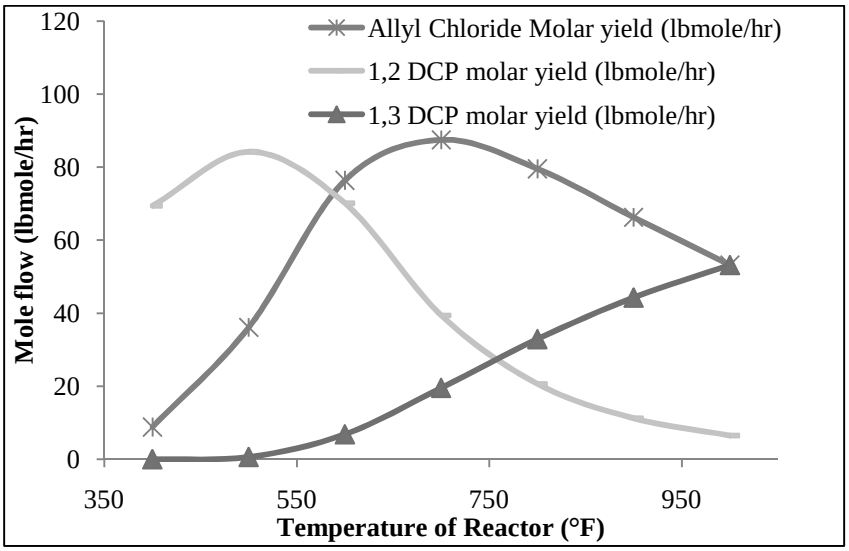

Figure 4.5 (a) Effect of Reactor Temperature on Molar Yield (Isothermal)

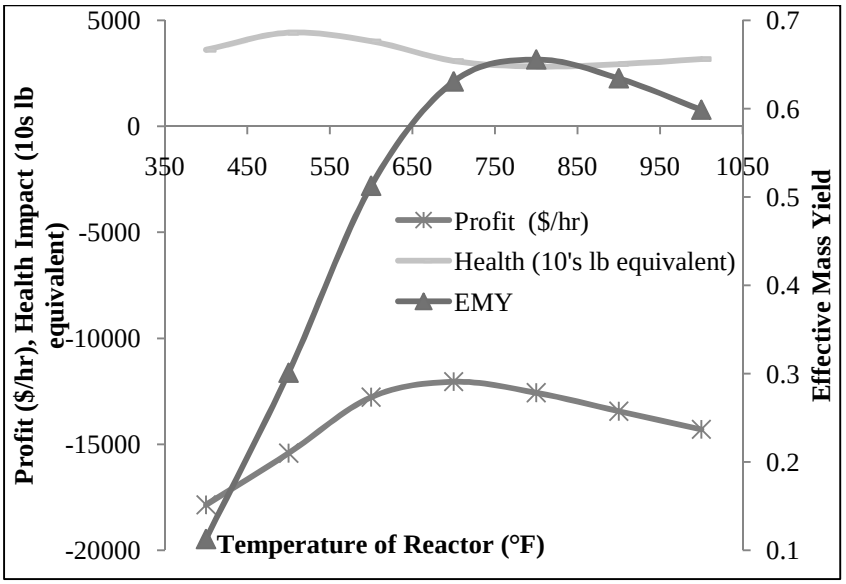

Figure 4.5 (b) Effect of Reactor Temperature on Profit, Health and MP (Isothermal)

The next step is to vary the feed heater temperature for the isothermal case. From Figure 4.6 (a) it is clear that changing feed heater temperature does not have any impact on the molar yields. But from Figure 4.6 (b) it is observed that with increasing feed heater temperature there is a decrease in the profit. This is because of the increase in operating costs due to the increase in feed heater duty. In the isothermal operation, change in feed heater temperature affects only the heat duty requirement of the reactor, and nothing downstream. For the reason that it affects profit, because of increasing operating costs this decision variable is retained.

After the sensitivity analysis is carried out and the decision variables and their ranges identified, the single objective optimization is carried out using Aspen Plus for the objectives of profit, health and MP.

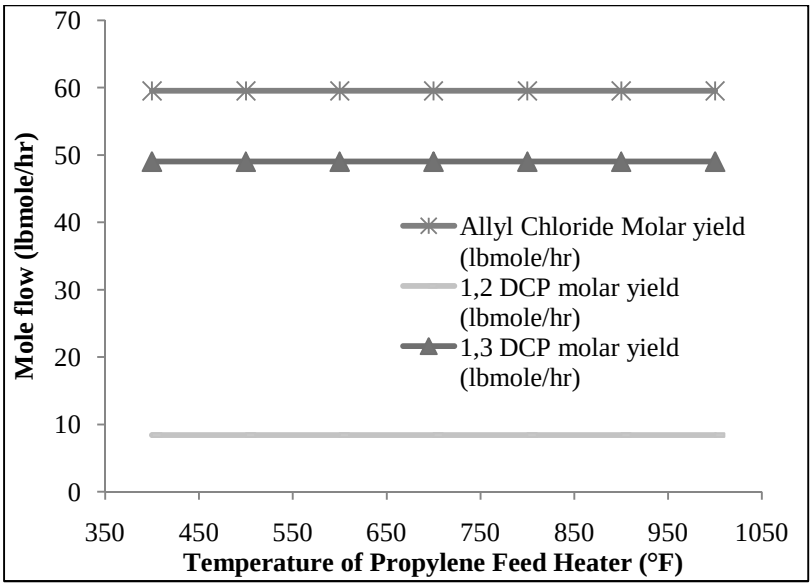

Figure 4.6 (a) Effect of Propylene Feed Heater Temperature on Molar Yield (Isothermal)

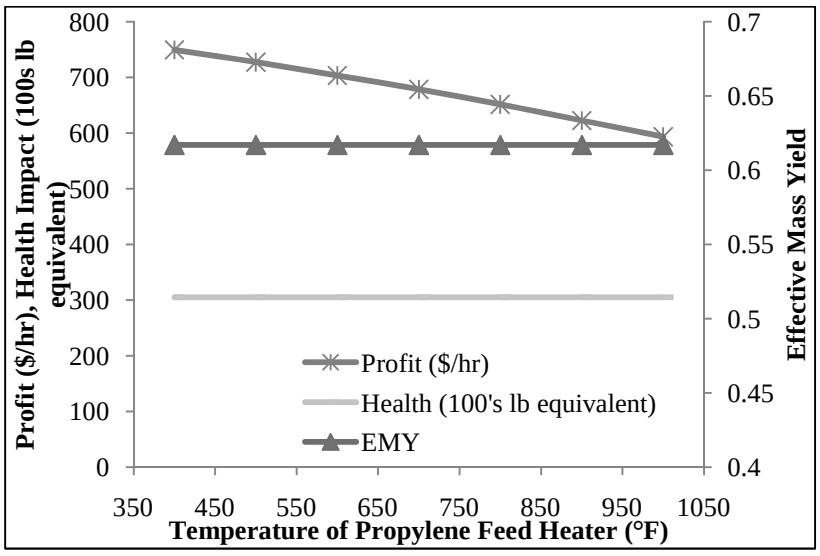

Figure 4.6 (b) Effect of Propylene Feed Heater Temperature on Profit, Health and MP (Isothermal)

4.3 Single Objective Optimization and Generation of Payoff Table

As discussed in the methods section, Aspen Plus is used to carry out a single objective optimization. The objective functions are formulated according to Equations 3.2, 3.3 and 3.5. The decision variables are chosen according to the inferences made during sensitivity analysis and are listed in Table 4.8 (b).

Table 4.8 (b) Decision Variable Ranges

Variable	Range	
	Adiabatic	Isothermal
Feed Ratio (C_3H_6/Cl_2)	1-6	1-6
Temperature of C_3H_6 feed heater	400-700°F	400-700°F
Temperature of reactor	N/A	500-1000°F
Pressure of reactor	15-150 psia	15-150 psia

4.3.1 Adiabatic Case

Table 4.9 presents the results of the single objective optimization. At each of the optimums, the values of the other objective functions are also calculated. From the results it is again established that when one objective is at its optimum, the other objective degenerates. For instance from a maximization of profit to a minimization of health impact, the value of the profit decreases, but the health impact is reduced and MP improves. Moving to the maximization of MP, it is observed that while profit improves, the value of health impact increases (thereby degenerating). A payoff table is generated from the data in Table 4.9. This is presented in Table 4.10. This payoff table is the step 2 of the MINSOOP algorithm (Fu et al., 2004). The upper and lower bounds are indicated in the payoff table as UB and LB respectively. This is essential to decide on the value of the constraints in the subsequent steps.

Table 4.9 Results of Single Objective Optimization of Each Objective (Adiabatic)

Objective	Profit ($/hr)	Health Impact (lb equivalent)	MP	Temperature of Propylene Feed Heater (°F)	Feed Ratio	Reactor Pressure (psia)
Max Profit	1360.2	31029.5	0.6234	638.0	6.0	41.3
Min Health Impact	1065.7	29740.4	0.6325	729.2	6.0	39.9
Max MP	1210.5	29754.9	0.6344	721.3	6.0	40.1

Table 4.10 Payoff Table (Adiabatic)

Objective	Profit ($/hr)	Health Impact (lb equivalent)	MP
Max Profit	1360.2 (UB)	31029.5 (UB)	0.6234 (LB)
Min Health Impact	1065.7 (LB)	29740.4 (LB)	0.6325
Max MP	1210.5	29754.9	0.6344 (UB)

4.3.2 Isothermal Case

Table 4.11 presents results of the single objective optimization for the isothermal case. As in the adiabatic case, the values of the other objective functions are also calculated and a payoff table generated, that is shown as Table 4.12. A pattern of results similar to the adiabatic case is observed in the isothermal case with each objective in conflict with the other.

Table 4.11 Results of Single Objective Optimization of Each Objective (Isothermal)

Objective	Profit ($/hr)	Health Impact (lb equivalent)	MP	Temperature of Propylene Feed Heater (°F)	Feed Ratio	Reactor Temperature (°F)
Max Profit	2237.7	41613.9	0.6321	500.0	4.4	726.3
Min Health Impact	1869.6	26587.9	0.6772	700.8	6.0	815.6
Max MP	1905.8	26595.5	0.6776	700.3	6.0	807.4

Table 4.12 Payoff Table (Isothermal)

Objective	Profit ($/hr)	Health Impact (lb equivalent)	MP
Max Profit	2237.7 (UB)	41613.9 (UB)	0.6321 (LB)
Min Health Impact	1869.6 (LB)	26587.9 (LB)	0.6772
Max MP	1905.8	26595.5	0.6776 (UB)

4.4 Constrained Optimization

According to the MINSOOP algorithm once the payoff table is generated, one of the objectives is retained as an objective and the rest are converted to inequality constraints. Accordingly, profit is retained as the objective function and health and MP are converted to inequality constraints. Based on the information available in the payoff table, the lower and upper bounds of the constraints-health and MP are now known. This interval is split into 5 to generate a reasonable number of results to present to the decision maker. The constraints are changed in the corresponding forms in Aspen Plus after each optimization run is complete.

4.4.1 Adiabatic Case

Table 4.13 shows the results of the constrained optimization for the adiabatic case. Figure 4.7 represents the information contained in Table 4.13.The results are in increasing order of profit. There is no clear trend in the results. As profit increases to $1233.7/hr, the MP also increases. At this point, as profit increases MP decreases. Health impact increases until profit reaches $1319.6/hr and then decrease with increasing profit until $1330.2/hr. After this point, the variation in health impact with profit is random, increasing and

decreasing with increasing profit. The points in the graph are numbered, to identify the corresponding point from the table. However, these results do not represent the Pareto optimal solution set. Figure 4.8 represents the Pareto optimal solutions for the adiabatic case. At each of the points in the graph, another point better than the current one cannot be obtained without sacrificing on one of the objectives. These sets of points are called the non-dominated solutions. This set of results is presented to the decision maker who takes the final decision.

Table 4.13 Results of the Constrained Optimization (Adiabatic)

Point No.	Profit ($/hr)	Health Impact (lb equivalent)	MP
1	1065.7	29740.4	0.633
2	1198.7	29740.5	0.635
3	1210.5	29755.0	0.635
4	1233.7	29792.2	0.634
5	1297.9	29984.6	0.633
6	1300.3	29997.0	0.633
7	1313.0	30108.5	0.632
8	1319.6	30768.1	0.629
9	1329.0	30254.1	0.631
10	1330.2	30253.5	0.631
11	1336.9	31028.9	0.626
12	1337.3	31029.0	0.626
13	1343.2	30365.9	0.630
14	1346.9	30768.0	0.627
15	1347.0	30511.0	0.629
16	1352.0	30587.3	0.628
17	1357.8	30767.9	0.626
18	1360.2	31029.6	0.623
19	1360.4	31029.2	0.623
20	1362.3	30817.9	0.626

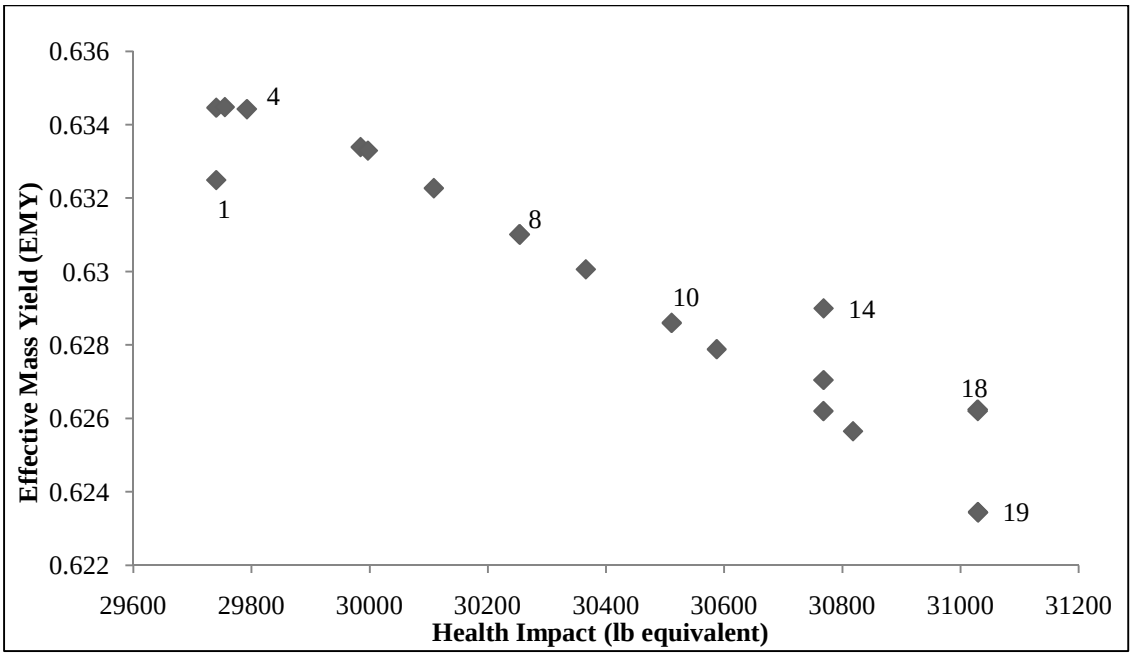

Figure 4.7 Constrained Optimization Results (Adiabatic)

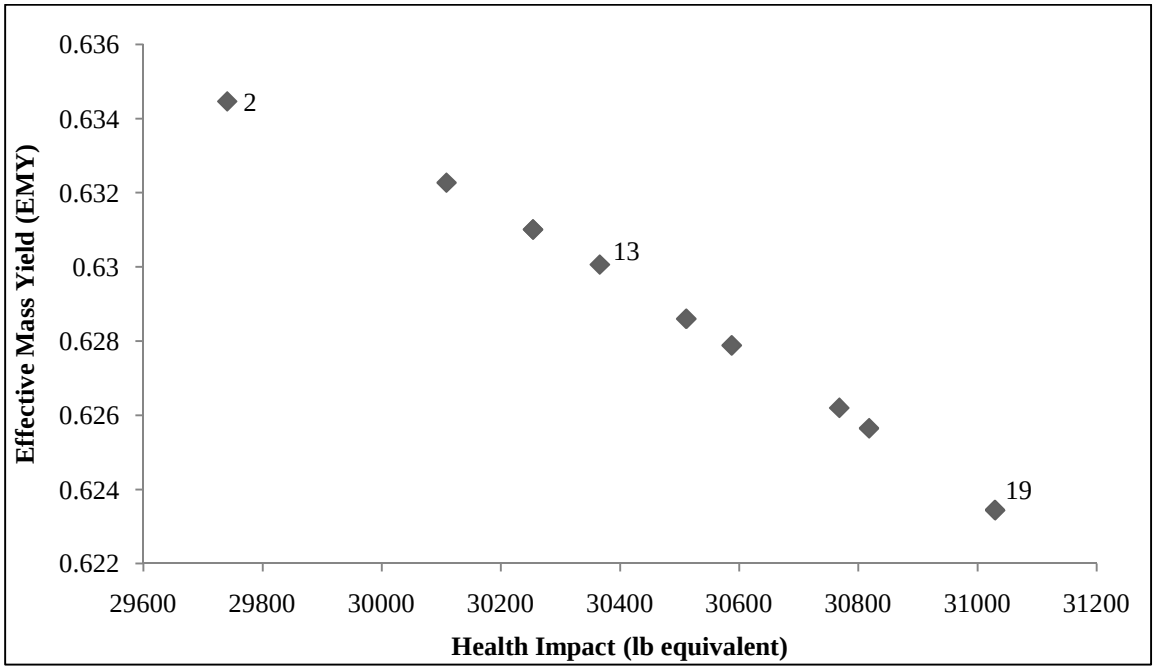

Figure 4.8 Non-dominant Solutions of the Constrained Optimization Results (Adiabatic)

4.4.2 Isothermal Case

Table 4.14 shows the results of the constrained optimization for the isothermal case.

Figure 4.9 represents the information contained in Table 4.14. These results do not

represent the Pareto optimal solution set. Figure 4.10 represents the Pareto optimal solutions for the isothermal case. This set of results is presented to the decision maker who takes the final decision.

Table 4.14 Results of the Constrained Optimization (Isothermal)

Point No.	Profit ($/hr)	Health Impact (lb equivalent)	MP
1	1667.6	41646.2	0.632
2	1859.5	29592.5	0.667
3	1938.9	41613.2	0.637
4	1957.5	26591.7	0.678
5	2002.9	30111.5	0.642
6	2022.1	26671.8	0.678
7	2049.2	28076.5	0.673
8	2060.0	31104.4	0.664
9	2063.9	35604.0	0.652
10	2077.8	31096.8	0.664
11	2101.8	35839.2	0.651
12	2119.7	28091.7	0.670
13	2124.3	35026.1	0.653
14	2157.0	34101.0	0.655
15	2166.2	31949.1	0.659
16	2177.8	35713.3	0.650
17	2180.4	37107.0	0.647
18	2181.0	37591.0	0.646
19	2187.0	38609.0	0.643
20	2191.1	40112.0	0.640
21	2193.4	39341.6	0.641
22	2214.1	41614.0	0.635

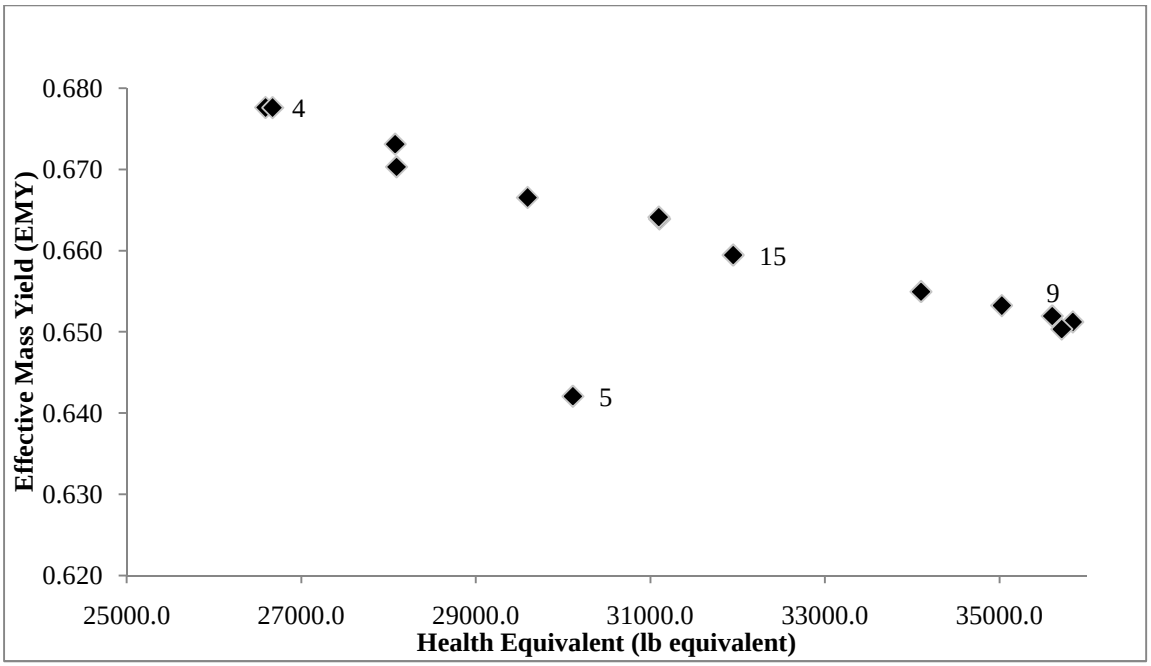

Figure 4.9 Constrained Optimization Results (Isothermal)

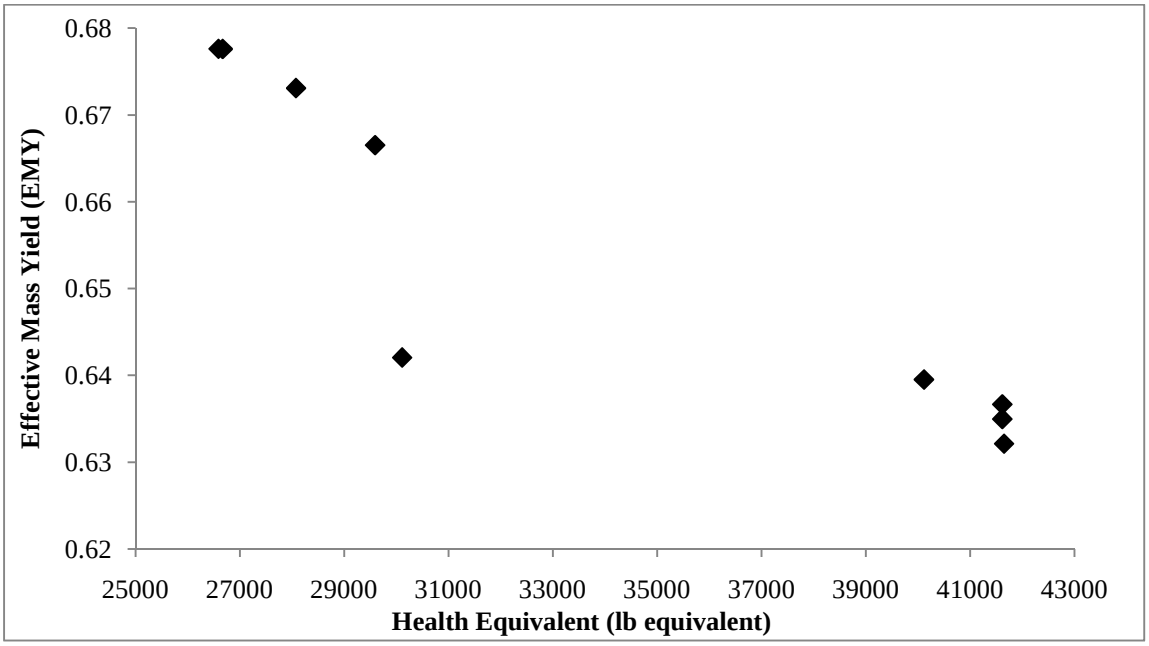

Figure 4.10 Non-dominant Solutions of the Constrained Optimization Results (Isothermal)

4.5 Weighted Optimization

Next, an approach of weighing the three objectives of profit, health and MP is carried out. The weights of the objective functions are varied from 0 to 1. The objective function is

modified and formulated according to Equation 3.10. This is then inserted in the constraints form of the optimization tool in Aspen Plus.

$$\max_{\{a,b\}} J = w_1\left(\frac{J_1}{\bar{J}_1}\right) - w_2\left(\frac{J_2}{\bar{J}_2}\right) + w_3\left(\frac{J_3}{\bar{J}_3}\right) \tag{3.10}$$

4.5.1 Adiabatic Case

Table 4.15 presents the results of the weighted optimization. Figure 4.11 presents the results of the weighted optimization. Again, these results are not Pareto optimal and Figure 4.12 represents the Pareto optimal solutions for the adiabatic case.

Table 4.15 Results of the Weighted Optimization (Adiabatic)

Point No.	Profit ($/hr)	w1	Health Impact (lb equivalent)	w2	MP	w3
1	1114.6	0.0	29712.7	0.2	0.634	0.8
2	1136.5	0.0	29709.2	0.4	0.634	0.6
3	1158.2	0.0	29712.9	0.6	0.634	0.4
4	1180.5	0.0	29724.1	0.8	0.634	0.2
5	1252.8	0.1	29839.2	0.1	0.634	0.8
6	1262.8	0.1	29869.0	0.3	0.634	0.6
7	1272.0	0.1	29902.6	0.5	0.634	0.4
8	1289.0	0.1	29971.8	0.7	0.633	0.2
9	1296.9	0.1	30012.3	0.8	0.633	0.1
10	1315.8	0.2	30136.2	0.0	0.632	0.8
11	1328.0	0.2	30244.7	0.2	0.631	0.6
12	1329.4	0.3	30259.3	0.1	0.631	0.6
13	1333.2	0.3	30309.7	0.3	0.631	0.4
14	1338.2	0.2	30366.1	0.4	0.630	0.4
15	1339.9	0.4	30395.8	0.0	0.630	0.6
16	1345.9	0.3	30493.7	0.3	0.629	0.3
17	1346.7	0.2	30501.4	0.6	0.629	0.2
18	1350.7	0.3	30593.9	0.4	0.628	0.4
19	1352.1	0.4	30628.7	0.2	0.628	0.4
20	1352.5	0.4	30632.4	0.6	0.627	0.0
21	1352.8	0.3	30645.9	0.6	0.627	0.1
22	1353.1	0.4	30652.6	0.3	0.627	0.3
23	1353.1	0.2	30650.7	0.8	0.627	0.0
24	1353.9	0.4	30676.4	0.4	0.627	0.2
25	1354.0	0.5	30679.5	0.1	0.627	0.4

26	1354.6	0.5	30693.7	0.4	0.627	0.1
27	1355.4	0.6	30725.2	0.0	0.627	0.4
28	1356.7	0.6	30769.8	0.2	0.626	0.2
29	1357.5	0.7	30807.4	0.1	0.626	0.2
30	1357.7	0.6	30817.5	0.4	0.626	0.0
31	1358.2	0.7	30844.7	0.2	0.625	0.1
32	1358.4	0.8	30865.8	0.0	0.625	0.2
33	1114.6	0.0	29712.7	0.2	0.634	0.8
34	1136.5	0.0	29709.2	0.4	0.634	0.6

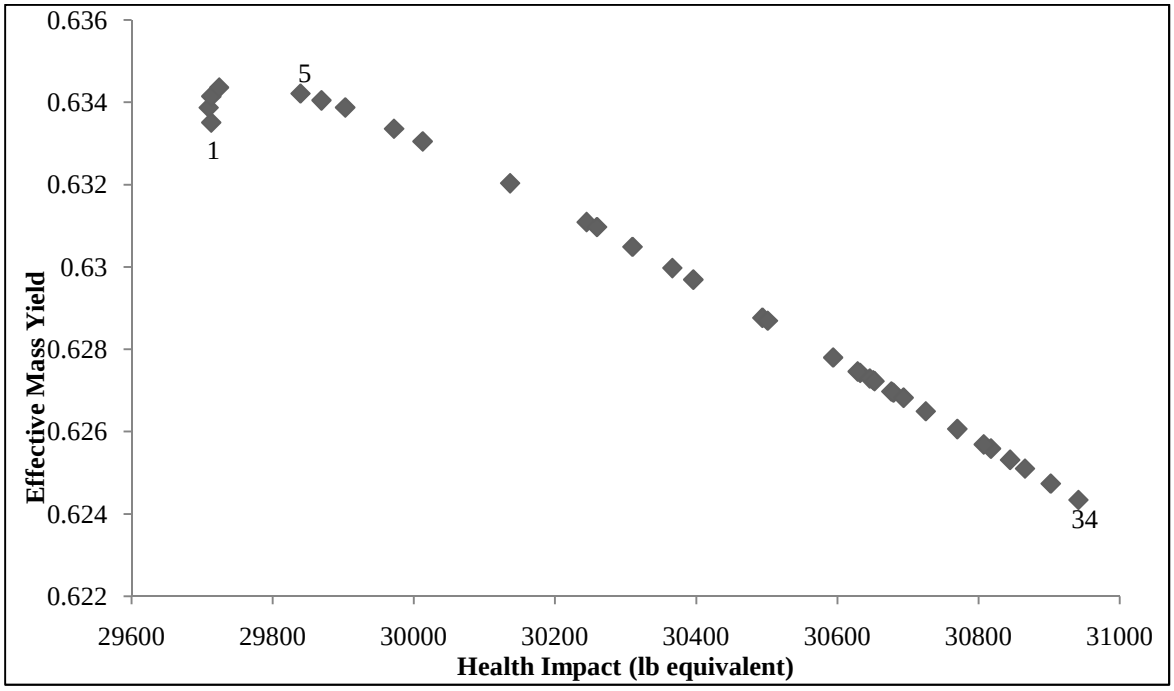

Figure 4.11 Weighted Optimization Results (Adiabatic)

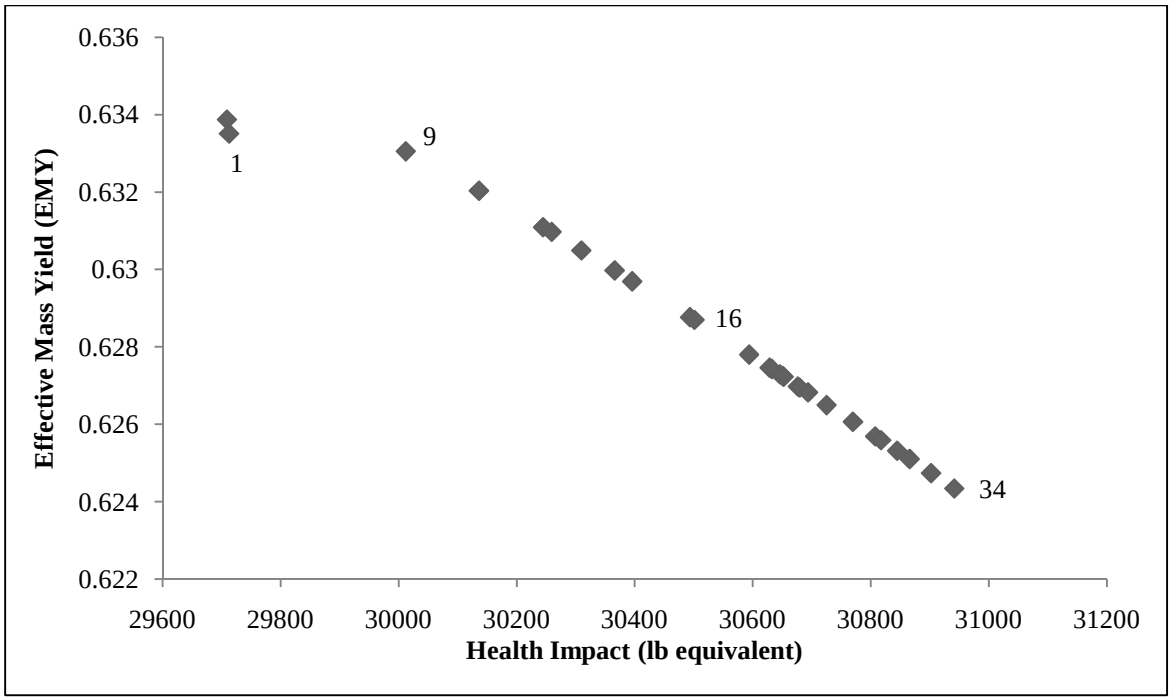

Figure 4.12 Non-dominant Solutions of the Weighted Optimization Results (Adiabatic)

4.5.2 Isothermal Case

Table 4.16 presents the results of the weighted optimization for the isothermal case. Figure 4.13 presents the results of the weighted optimization. Again, these results are not the Pareto optimal and Figure 4.14 represents the Pareto optimal solutions for the isothermal case. The results from the weighted optimization are presented to the decision maker who then makes the choice, with the explicit understanding that improvement in one of the objectives is not possible without a loss in another.

Table 4.16 Results of the Weighted Optimization (Isothermal)

Point No.	Profit ($/hr)	w1	Health Impact (lb equivalent)	w2	MP	w3
1	1863.5	0.0	26588.4	0.8	0.6772	0.2
2	1869.6	0.0	26587.6	1.0	0.6773	0.0
3	1886.2	0.0	26589.5	0.6	0.6775	0.4
4	1895.2	0.0	26590.7	0.2	0.6776	0.8
5	1905.8	0.0	26595.5	0.0	0.6777	1.0

6	1945.6	0.1	26629.3	0.8	0.6778	0.1
7	1959.7	0.1	26653.5	0.4	0.6777	0.5
8	1966.4	0.1	26667.7	0.2	0.6776	0.7
9	1968.9	0.2	26662.5	0.8	0.6776	0.0
10	1971.0	0.1	26678.7	0.1	0.6776	0.8
11	1974.8	0.2	26676.1	0.6	0.6776	0.2
12	1985.5	0.2	26704.9	0.4	0.6774	0.4
13	2011.2	0.0	26860.8	0.4	0.6762	0.6
14	2023.1	0.2	26747.7	0.0	0.6771	0.8
15	2030.1	0.1	26692.0	0.6	0.6775	0.3
16	2038.5	0.3	27457.1	0.1	0.6743	0.6
17	2070.2	0.3	27024.3	0.6	0.6748	0.1
18	2084.2	0.2	27110.2	0.2	0.6740	0.6
19	2089.0	0.5	31272.0	0.4	0.6636	0.5
20	2091.2	0.4	27128.9	0.2	0.6738	0.4
21	2094.1	0.4	27159.2	0.0	0.6735	0.4
22	2097.4	0.33	27091.1	0.33	0.6742	0.33
23	2100.3	0.3	27130.3	0.4	0.6738	0.3
24	2101.2	0.6	27143.9	0.4	0.6737	0.0
25	2102.2	0.3	27158.2	0.3	0.6735	0.4
26	2102.7	0.6	27167.1	0.0	0.6735	0.4
27	2104.3	0.5	27193.7	0.4	0.6732	0.1
28	2104.6	0.4	27198.4	0.3	0.6732	0.3
29	2104.9	0.4	27204.6	0.4	0.6731	0.2
30	2104.9	0.6	27219.4	0.2	0.6731	0.2
31	2131.6	0.6	29234.4	0.0	0.6674	0.4
32	2139.4	0.7	29196.7	0.2	0.6629	0.1
33	2153.2	0.8	30305.2	0.0	0.6588	0.2
34	2166.8	0.8	31002.9	0.2	0.6581	0.0
35	2175.7	0.7	31839.4	0.1	0.6551	0.2
36	2195.5	0.8	33641.1	0.1	0.6501	0.1
37	2237.7	1.0	41614.0	0.0	0.6321	0.0

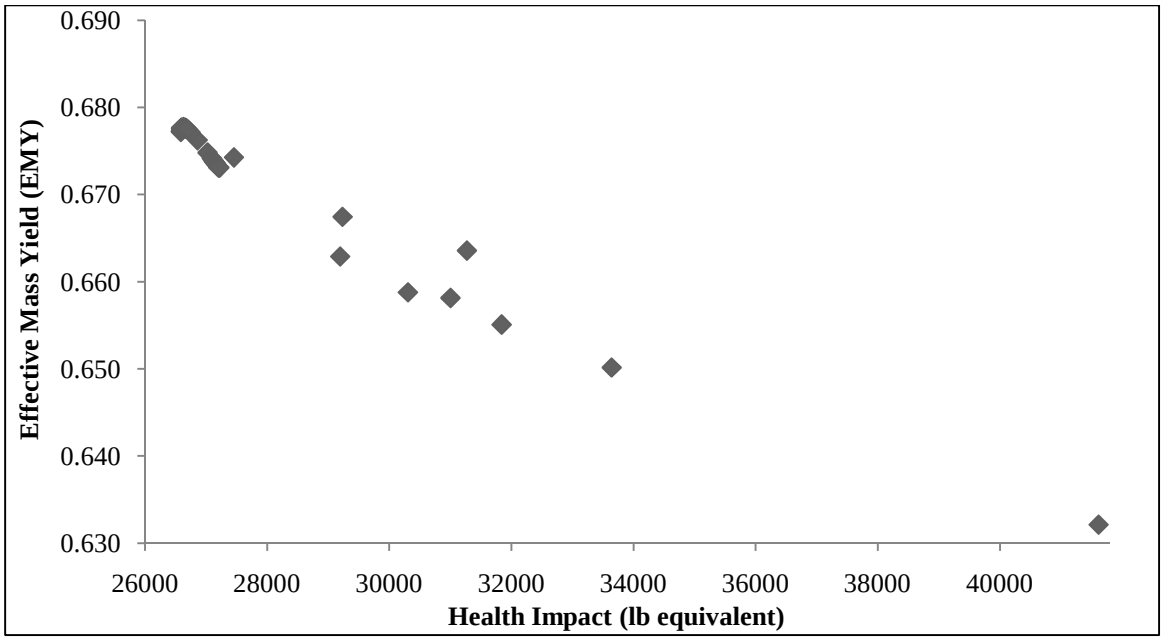

Figure 4.13 Weighted Optimization Results (Isothermal)

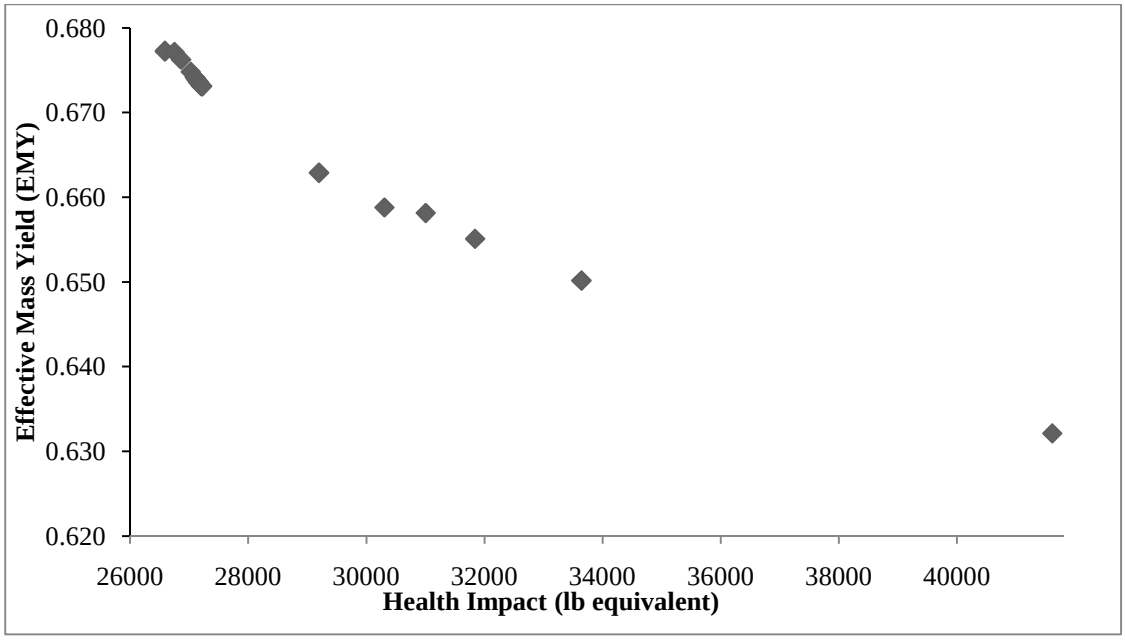

Figure 4.14 Non-dominant Solutions of the Weighted Optimization Results (Isothermal)

4.6 Comparison of Base and Optimized Case Results

As a final step the results from the base and optimized case are compared using the amoeba charts. The results from the base case for the 9 indicators selected according to Table 4.2 are used to compare the base and optimized case. For the decision maker to compare the results of one of the optimized cases, constrained or weighted, the values of the indicators mentioned are plotted against the base case, by normalizing the base case values to unity.

If the decision maker chooses to compare a weighted optimized case of the isothermal reactor described by point 1 in Table 4.16 then Figure 4.15 shows the amoeba chart with the values of the optimized case plotted against the base case. Table 4.17 shows the value of the indicators, for the base and selected optimized case. The amoeba chart gives a visual graphic for the decision maker. It shows how each of the indicators has improved or worsened. In the instant case it is seen that profit improves by almost 86% while health impact is reduced by 7%. Overall the process has improved from an environmental, economic and social point of view. Barring safety, where no improvements are made and a slight increase in the annualized capital cost the selected optimized case is better than base case in all other aspects. This is reflected in Figure 4.15, where the value of the optimized case is indicated along with the axis label, for quick viewing. If the decision maker feels there must be further improvement, or wants to explore other options presented to him, the optimized cases are compared in a similar manner and finally a decision is made by the decision maker.

Table 4.17 Comparison of Base Case and Selected Optimized Case

Indicator	Base Case	Selected Optimized Case Normalized wrt Base Case	% Improvement
Global Warming	1	0.938	(6.2)
Material Intensity	1	0.899	(10.1)
Energy Intensity	1	0.964	(3.6)
Water Intensity	1	0.828	(17.2)
Safety Index	1	1.000	0
Profit	1	1.857	85.7
Annualized Capital Cost	1	1.032	3.2
Waste Cost	1	0.939	(6.1)
Health Impact	1	0.929	(7.1)
Material Value Added	1	1.599	59.9
E-factor	1	0.833	(16.7)
Reaction Mass Efficiency	1	1.100	10
Effective Mass Yield	1	1.063	6.3
Atom Economy	1	1.000	0.0
Mass Intensity	1	0.955	(4.5)
Mass Productivity	1	1.063	6.3

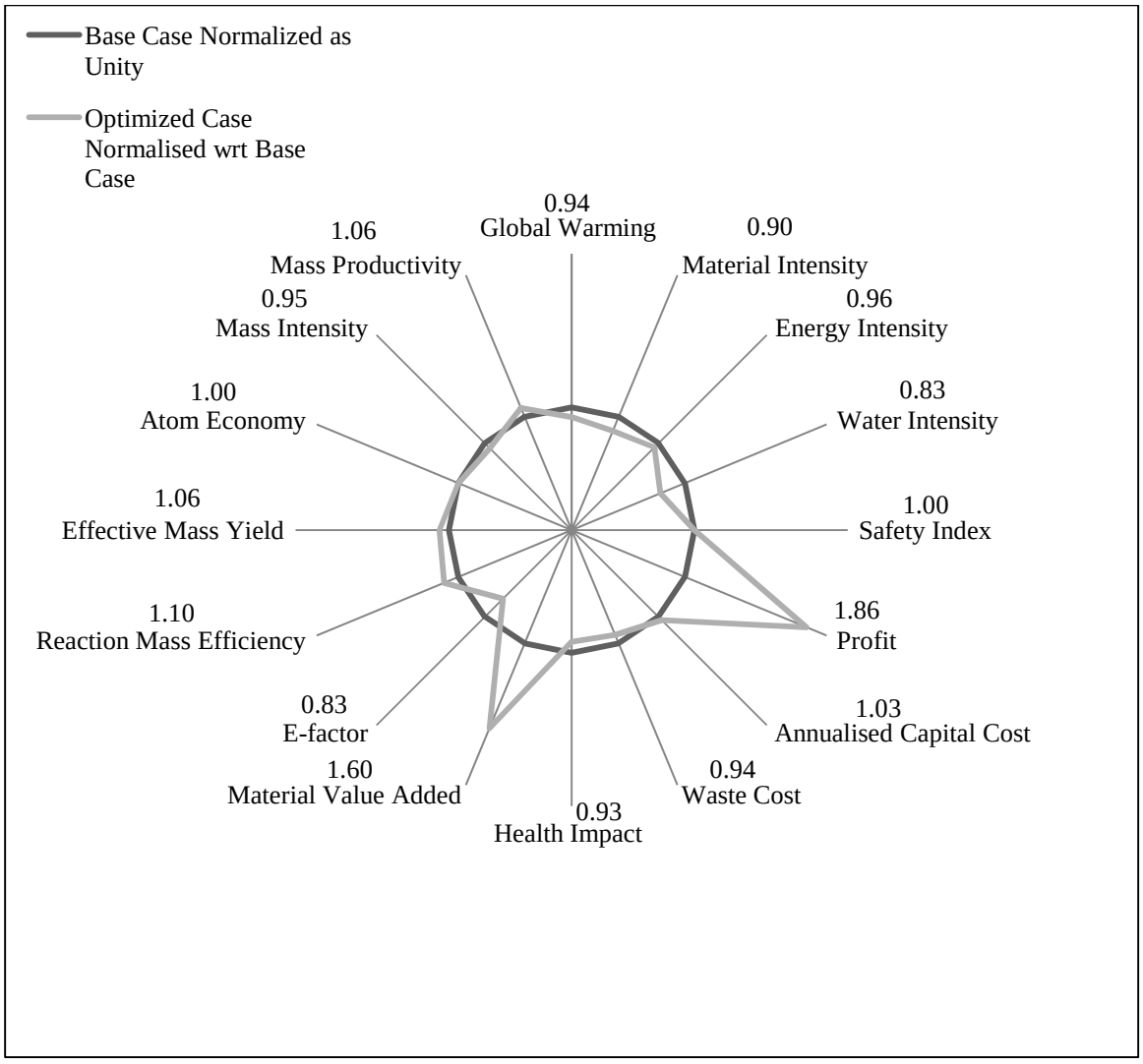

Figure 4.15 Amoeba Chart Comparing a Base Case and an Optimized Case Selected by the Decision Maker*

*Comparison of base case with point 1 of Table 4.16, where health impact is 26588.4 lb equivalent, MP is 0.6772 and profit is 1863.5 $/hr.

CHAPTER V

CONCLUSIONS AND RECOMMENDATIONS

Conclusions

There is an increasing need to fill the gap between a high-level complicated MOO for sustainability concerns and a simple SOO for profit. At the design stage there is not enough time and effort with proposal and design managers to use a MOO framework. Most of the MOO methods are not user friendly and require training of the designer in complicated programming logic. This work is a tradeoff between effort and result.

In the context of research at OSU this work fits in by taking forward the current state of research in sustainability. At present a methodology for addressing sustainability concerns during early stages of design has been developed (Shadiya, 2010). Taking this forward, as a next step a MOO problem was formulated and solved by converting it into a SOO problem using the constrained and weighted optimization methods. As a next step, the MOO problem of sustainability can be solved by using the MOO methods.

A methodology was developed for optimization of chemical processes that can be implemented on a commercially available process simulator such as Aspen Plus.

This methodology involves the simulation of the base case of the process in Aspen Plus followed by the identification of the decision variables using a sensitivity analysis. Information from the base case was entered in the SE and then a set of metrics is selected for comparison with the optimized case. Next, an objective function that can be implemented using Aspen Plus was formulated. A payoff table was generated by optimizing each of the objectives according to the MINSOOP method (Fu et al., 2004). As a final step, a set of Pareto optimal solutions is generated using the constrained and weighted method. These sets of results are presented to the decision maker who decides which result is implemented.

The proposed methodology was implemented using the allyl chloride manufacturing process case study. The allyl chloride process was selected because it is a highly regulated chemical and its production exceeds 1 million tonnes every year in the United States alone (van der Helm, 1998). Allyl chloride is manufactured by the high temperature chlorination of propylene in an adiabatic reactor. 1,2 DCP and 1,3 DCP are both by-products of this reaction and extremely hazardous. For the purpose of this research they were considered wastes (despite a small dwindling market existing for 1,2 DCP and 1,3 DCP). A base case process using an isothermal reactor and an adiabatic reactor was simulated. Information from the base case was entered in the SE, and a sustainability evaluation was carried out.

As a next step, an objective function was formulated and a FORTRAN code was written to define all the objectives in Aspen Plus. Three objectives: Profit, Health Impact and Mass productivity (MP) were formulated. Each of the objectives was optimized and a payoff table was generated. Profit was retained as an objective and health impact and MP

were converted to constraints. Using information from the payoff table the limits of the constraints are entered in Aspen Plus and a representative set of Pareto optimal results is obtained. Similarly for the weighted optimization method, the objectives were normalized and combined into a single objective using weights. Optimum points are generated for different weights. Some of the solutions generated were inferior solutions, and they are eliminated and only the non-dominant results are presented to the decision maker. From the results it was clear that the isothermal process offers a higher profit than the adiabatic process, but with a higher impact on the health and environment.

In summary this research proposes a methodology to optimize processes during the design stage, by combining the SE and Aspen Plus. The proposed methodology is an ideal tradeoff between effort invested and results generated. This research is novel because it develops a methodology to optimize processes for sustainability using information from the SE and using Aspen Plus. The SE developed at OSU is a simple but effective tool to gauge the impact of processes on sustainability; Aspen Plus is one of the most commonly used process simulation software tools in the industry. Using these two tools in tandem without complicated programming for optimization, to explore a multiobjective problem in single objective sense and generate options for a decision maker is a step forward in designing processes for sustainability.

Recommendations

Exploring the multiobjective problem of sustainability in a single objective sense, has certain limitations, such as loss of few Pareto optimal solutions. This can be avoided, by using a multiobjective algorithm such as Genetic Algorithm, Simulated Annealing, etc.

Multiobjective algorithms require complicated programming and optimization expertise, which may not be warranted for small process plants, but may be worth the effort for huge plants, such as power stations, refineries, etc. Exploring the problem (opportunity) of optimizing processes for sustainability using multiobjective techniques will involve developing multiobjective optimization under uncertainties to satisfy social, economic and environmental objectives. In this work, it is left to the decision maker to implement a solution out of the non-dominated solutions. However future work must also focus on a decision making procedure to select the most suitable alternative.

This work does not have a seamless connection between the SE tool and Aspen Plus. The process designer is the interface between the two tools. To improve the reliability of this methodology and to increase the speed at which this methodology is completed, a platform has to be created to interface both tools together. Further, during optimization stages, changing the constraints and weights each time manually in Aspen Plus is cumbersome. A platform that connects both will avoid this problem and possibly errors associated with continuous human interference.

There is no contribution to improving the safety of the process in the current research. Improving the safety of the process needs to be addressed especially after incidents such as Japan's Nuclear Disaster in 2011, Chernobyl and Bhopal. The industry continues to compromise on safety despite tremendous advancements in process and control engineering. Safety can be incorporated into this methodology by using a step-by-step decision making methodology that goes hand-in-hand with the decision making of the optimization algorithm. Some researchers in the past have contributed to developing a methodology for safety as a standalone procedure and not one integrated with

optimization (Srinivasan et al., 2008). Future work should, therefore, address safety and optimization simultaneously.

As far as sustainability and sustainability metrics is concerned, there is tremendous scope for improvements. It is a fact that there are no metrics that calculate or indicate the impact of a process or energy plant on the surrounding geography. More often than not geo-political considerations decide locations of process and energy plants with scant regard for ecosystems, water availability, land quality, etc. (Govindarajan et al., 2011). Additional metrics from a regulatory and process design standpoint that reflect on the impact of water usage, process plant footprint, economic and job forecasting, etc. need to be developed. Although economic and job forecasting may be out of the scope of a process engineer, the best person to address these issues remains a process engineer.

Right now sustainability is no longer an option and a bare minimum necessity. It is only a matter of time before safety, water use impact, land quality, etc. get factored into sustainable process design. In the end, it is essential to understand and acknowledge that there can be no process which is absolutely benign to nature, rather it is only relative.

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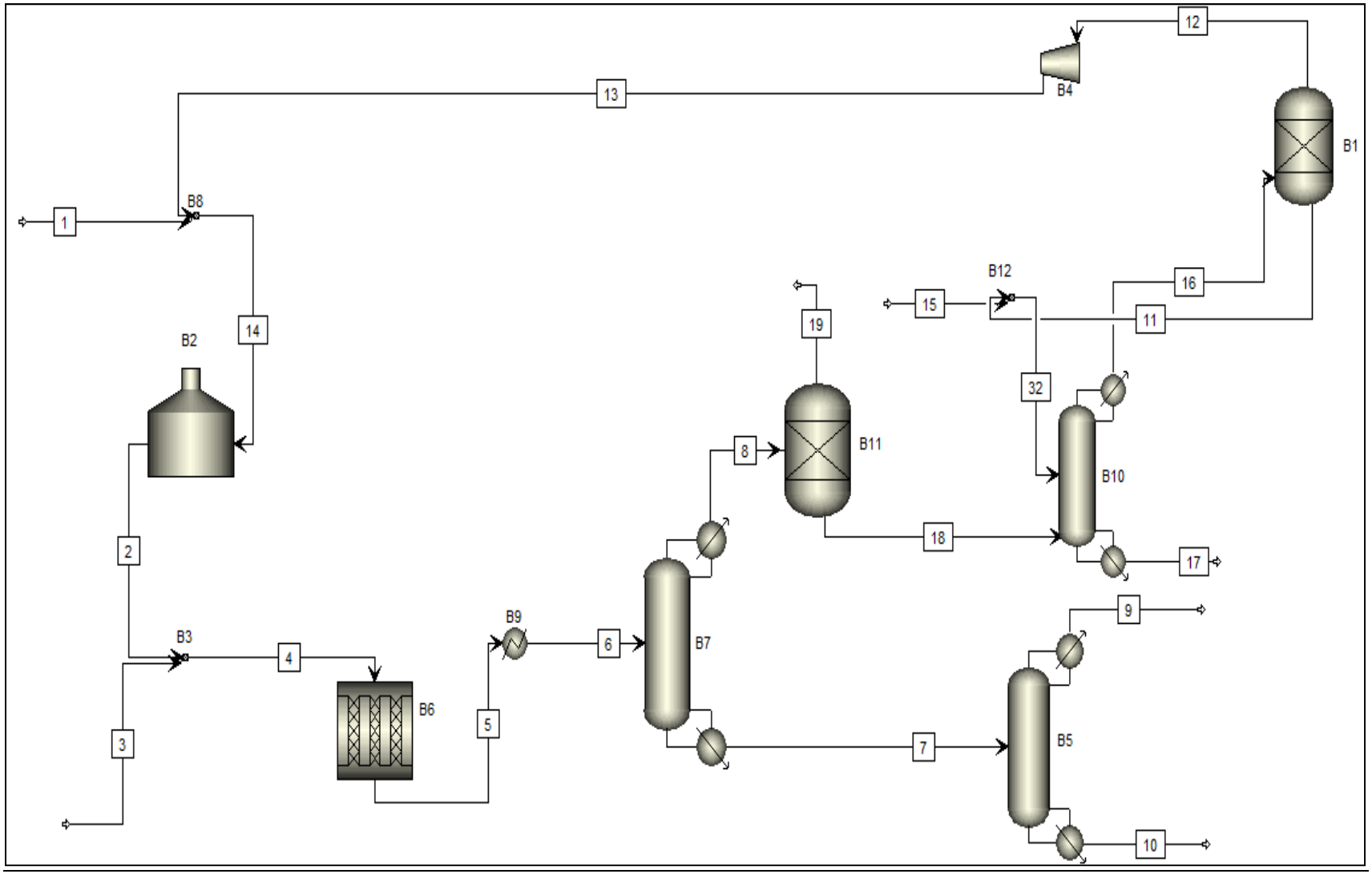
APPENDIX;PROCESS FLOW DIAGRAM USED FOR SIMULATION AND OPTIMIZATION



APPPENDICES

INPUT SUMMARY FOR BASE CASE-ADIABATIC REACTOR

```
IN-UNITS ENG
DEF-STREAMS CONVEN ALL
SIM-OPTIONS OLD-DATABANK=YES
RUN-CONTROL MAX-TIME=100000. MAX-ERRORS=500
DESCRIPTION "
   General Simulation with English Units :
   F, psi, lb/hr, lbmol/hr, Btu/hr, cuft/hr.
   Property Method: None
   Flow basis for input: Mole
  Stream report composition: Mole flow
DATABANKS ASPENPCD  / AQUEOUS  / SOLIDS  / INORGANIC  /  &
      PURE22  / PURE10
PROP-SOURCES ASPENPCD  / AQUEOUS  / SOLIDS  / INORGANIC  /  &
      PURE22  / PURE10
COMPONENTS
   H2O H2O /
   HCL HCL /
   PROPENE C3H6-2 /
   CHLORINE CL2 /
   AC C3H5CL /
   12DCP C3H6CL2 /
   13DCP-C C3H4CL2-D1 /
   13DCP-T C3H4CL2-D2 /
   H+ H+ /
   CL- CL-
HENRY-COMPS HENRY CHLORINE HCL PROPENE
SOLVE
   RUN-MODE MODE=OPT
CHEMISTRY HCL
   STOIC 1 HCL -1 / H+ 1 / CL- 1
```

```
FLOWSHEET
   BLOCK B2 IN=14 OUT=2
   BLOCK B8 IN=1 13 OUT=14
   BLOCK B3 IN=2 3 OUT=4
   BLOCK B6 IN=4 OUT=5
   BLOCK B9 IN=5 OUT=6
   BLOCK B7 IN=6 OUT=8 7
   BLOCK B5 IN=7 OUT=9 10
   BLOCK B10 IN=18 32 OUT=16 17
   BLOCK B1 IN=16 OUT=12 11
   BLOCK B11 IN=8 OUT=18 19
   BLOCK B4 IN=12 OUT=13
   BLOCK B18 IN=15 11 OUT=32

PROPERTIES SYSOP0
   PROPERTIES ELECNRTL / UNIQ-RK / UNIQUAC

STRUCTURES
   STRUCTURES 13DCP-C CL1 C2 S / C2 C3 D / C3 C4 S /  &
      C4 CL5 S

ESTIMATE ALL

PROP-DATA PCES-1
   IN-UNITS ENG
   PROP-LIST DGAQHG / DHAQHG / S25HG / OMEGHG / DHVLB /  &
      VB / RGYR / VLSTD
   PVAL CHLORINE 2983.662941 / -10060.18917 / 28.90035349 /  &
      -17580.05159 / 8784.000000 / .7262124822 /  &
      3.2391732E-10 / .8579136616
   PROP-LIST DHVLB / VB / RGYR
   PVAL 13DCP-C 14431.51333 / 1.612466586 / 1.11089239E-9

PROP-DATA HENRY-1
   IN-UNITS ENG
   PROP-LIST HENRY
   BPVAL HCL H2O -49.78140336 2186.999983 8.370700000  &
      -5.3294445E-3 -3.999995968 68.00000346 0.0
   BPVAL CHLORINE H2O -116.9781387 4371.515965 19.18540000  &
      -4.9558834E-3 49.73000360 103.7300032 0.0
```

```
   BPVAL HCL 12DCP 10.00798341 -2648.879936 0.0 0.0  &
      -4.269995966 67.73000346 0.0
   BPVAL PROPENE H2O 326.3806995 -28021.26578 -41.73762000 0.0  &
      69.53000344 220.7300022 0.0
   BPVAL PROPENE 12DCP 12.93988341 -3932.459880 0.0 0.0  &
      -4.269995966 67.73000346 0.0

PROP-DATA UNIQ-1
   IN-UNITS ENG
   PROP-LIST UNIQ
   BPVAL H2O AC -4.247000000 2292.652782 0.0 0.0 109.9400031  &
      212.0000023 0.0
   BPVAL AC H2O 15.46800000 -10062.08074 0.0 0.0 109.9400031  &
      212.0000023 0.0
   BPVAL H2O 12DCP 0.0 -539.9468957 0.0 0.0 77.00000338  &
      77.00000338 0.0
   BPVAL 12DCP H2O 0.0 -2498.536780 0.0 0.0 77.00000338  &
      77.00000338 0.0

PROP-DATA VLCLK-1
   IN-UNITS ENG
   PROP-LIST VLCLK
   BPVAL H+ CL- .5534556926 .2140997389

PROP-DATA GMELCC-1
   IN-UNITS ENG
   PROP-LIST GMELCC
   PPVAL H2O ( H+ CL- ) 41.67400000
   PPVAL ( H+ CL- ) H2O -22.15400000
   PPVAL HCL ( H+ CL- ) 1.00000000E-3
   PPVAL ( H+ CL- ) HCL -1.0000000E-3

PROP-DATA GMELCD-1
   IN-UNITS ENG
   PROP-LIST GMELCD
   PPVAL H2O ( H+ CL- ) 9581.579923
   PPVAL ( H+ CL- ) H2O -3967.379968

PROP-DATA GMELCE-1
   IN-UNITS ENG
```

```
   PROP-LIST GMELCE
   PPVAL H2O ( H+ CL- ) -5.404000000
   PPVAL ( H+ CL- ) H2O 5.188000000

PROP-DATA GMELCN-1
   IN-UNITS ENG
   PROP-LIST GMELCN
   PPVAL H2O ( H+ CL- ) .0283500000

PCES-PROP-DATA
   IN-UNITS ENG
   GAMINF H2O 12DCP * * 68 2340 / * * 86 2310 / * *  &
      104 2090

PCES-PROP-DATA
   IN-UNITS ENG
   GAMINF H2O 13DCP-C * * 68 1360 / * * 86 1430 / * *  &
      104 1460

PROP-SET IPE-1 TEMP PRES MASSFLMX VOLFLMX MWMX MASSSFRA  &
      MASSVFRA MASSFLOW SUBSTREAM=ALL PHASE=T

PROP-SET IPE-2 CPMX MWMX MASSFLMX KMX SIGMAMX MUMX VOLFLMX
&
      UNITS='J/kg-K' SUBSTREAM=MIXED PHASE=L

PROP-SET IPE-3 VOLFLMX CPMX MUMX KMX MWMX MASSFLMX UNITS= &
      'J/kg-K' SUBSTREAM=MIXED PHASE=V

STREAM 1
   SUBSTREAM MIXED TEMP=80. PRES=74.7
   MOLE-FLOW PROPENE 1000.

STREAM 3
   SUBSTREAM MIXED TEMP=80. PRES=74.7
   MOLE-FLOW CHLORINE 166.

STREAM 15
   SUBSTREAM MIXED TEMP=70. PRES=14.7
   MOLE-FLOW H2O 325.
```

```
BLOCK B3 MIXER
   PROPERTIES UNIQ-RK FREE-WATER=STEAM-TA SOLU-WATER=3  &
      TRUE-COMPS=YES

BLOCK B8 MIXER
   PROPERTIES UNIQ-RK FREE-WATER=STEAM-TA SOLU-WATER=3  &
      TRUE-COMPS=YES

BLOCK B18 MIXER

BLOCK B1 SEP
   PARAM
   FRAC STREAM=12 SUBSTREAM=MIXED COMPS=PROPENE FRACS=1.
   PROPERTIES UNIQ-RK FREE-WATER=STEAM-TA SOLU-WATER=3  &
      TRUE-COMPS=YES

BLOCK B11 SEP
   PARAM
   FRAC STREAM=18 SUBSTREAM=MIXED COMPS=H2O HCL PROPENE  &
      CHLORINE AC 12DCP 13DCP-C 13DCP-T H+ CL- FRACS=1. 1.  &
      1. 1. 0. 0. 0. 0. 1. 1.
   PROPERTIES UNIQ-RK FREE-WATER=STEAM-TA SOLU-WATER=3  &
      TRUE-COMPS=YES

BLOCK B2 HEATER
   PARAM TEMP=700. PRES=74.7
   PROPERTIES UNIQ-RK FREE-WATER=STEAM-TA SOLU-WATER=3  &
      TRUE-COMPS=YES

BLOCK B9 HEATER
   PARAM TEMP=70. PRES=74.7
   PROPERTIES UNIQ-RK FREE-WATER=STEAM-TA SOLU-WATER=3  &
      TRUE-COMPS=YES

BLOCK B5 RADFRAC
   PARAM NSTAGE=15
   COL-CONFIG CONDENSER=PARTIAL-V
   FEEDS 7 6
   PRODUCTS 9 1 V / 10 15 L
   P-SPEC 1 16. / 15 25.
```

```
   COL-SPECS D:F=0.539038 MOLE-RR=4.02554
   SPEC 1 MOLE-RECOV 0.999 COMPS=AC STREAMS=9 BASE-STREAMS=7
   VARY 1 D:F 0.01 0.99
   PROPERTIES UNIQ-RK FREE-WATER=STEAM-TA SOLU-WATER=3  &
      TRUE-COMPS=YES

BLOCK B7 RADFRAC
   PARAM NSTAGE=15 ALGORITHM=STANDARD INIT-OPTION=STANDARD
&
      MAXOL=150 DAMPING=NONE
   COL-CONFIG CONDENSER=PARTIAL-V
   FEEDS 6 7
   PRODUCTS 8 1 V / 7 15 L
   P-SPEC 1 20. / 15 27.
   COL-SPECS D:F=0.8 MOLE-RR=0.4084
   SPEC 1 MOLE-RECOV 0.99 COMPS=AC STREAMS=7
   VARY 1 D:F 0.01 0.99
   PROPERTIES UNIQ-RK FREE-WATER=STEAM-TA SOLU-WATER=3  &
      TRUE-COMPS=YES

BLOCK B10 RADFRAC
   PARAM NSTAGE=10 ALGORITHM=NONIDEAL INIT-OPTION=STANDARD  &
      MAXOL=100 MAXIL=50
   COL-CONFIG CONDENSER=NONE REBOILER=NONE
   FEEDS 18 10 ON-STAGE / 32 1
   PRODUCTS 17 10 L / 16 1 V
   P-SPEC 1 14.7
   COL-SPECS
   T-EST 1 110. / 10 68.
   PROPERTIES ELECNRTL HENRY-COMPS=HENRY CHEMISTRY=HCL  &
      FREE-WATER=STEAM-TA SOLU-WATER=3 TRUE-COMPS=NO

BLOCK B6 RPLUG
   PARAM TYPE=ADIABATIC LENGTH=20. DIAM=6. PRES=40.  &
      INT-TOL=1E-005
   COOLANT MAXIT=50
   PROPERTIES UNIQ-RK FREE-WATER=STEAM-TA SOLU-WATER=3  &
      TRUE-COMPS=YES / SYSOP0
   REACTIONS RXN-IDS=R-1
```

```
BLOCK B4 COMPR
   PARAM TYPE=ASME-POLYTROP PRES=90.
   PROPERTIES UNIQ-RK FREE-WATER=STEAM-TA SOLU-WATER=3  &
      TRUE-COMPS=YES

DESIGN-SPEC FEED
   DEFINE S14 MOLE-FLOW STREAM=14 SUBSTREAM=MIXED  &
      COMPONENT=PROPENE
   SPEC "S14" TO "1000"
   TOL-SPEC "0.01"
   VARY MOLE-FLOW STREAM=1 SUBSTREAM=MIXED
COMPONENT=PROPENE
   LIMITS "5" "1000"

DESIGN-SPEC H20
   DEFINE HCL18 MASS-FLOW STREAM=18 SUBSTREAM=MIXED  &
      COMPONENT=HCL
   DEFINE H2032 MASS-FLOW STREAM=32 SUBSTREAM=MIXED  &
      COMPONENT=H2O
   SPEC "H2032" TO "2.1*HCL18"
   TOL-SPEC ".001"
   VARY STREAM-VAR STREAM=15 SUBSTREAM=MIXED VARIABLE=MASS-
FLOW
   LIMITS "10" "60000"

DESIGN-SPEC RESTM
   DEFINE RESTM BLOCK-VAR BLOCK=B6 VARIABLE=RES-TIME  &
      SENTENCE=PARAM
   SPEC "RESTM" TO "1.11E-3"
   TOL-SPEC ".0001"
   VARY BLOCK-VAR BLOCK=B6 VARIABLE=LENGTH SENTENCE=PARAM
   LIMITS "1" "200"


REACTIONS R-1 POWERLAW
   REAC-DATA 1 PHASE=V
   REAC-DATA 2 PHASE=V
   REAC-DATA 3 PHASE=V
   RATE-CON 1 PRE-EXP=40400000. ACT-ENERGY=74300000. <J/kmol>
   RATE-CON 2 PRE-EXP=2300. ACT-ENERGY=27300000. <J/kmol>
```

```
RATE-CON 3 PRE-EXP=90300000000. ACT-ENERGY=110000000. <J/kmol>
STOIC 1 MIXED PROPENE -1. / CHLORINE -1. / AC 1. /  &
   HCL 1.
STOIC 2 MIXED PROPENE -1. / CHLORINE -1. / 12DCP 1.
STOIC 3 MIXED AC -1. / CHLORINE -1. / 13DCP-C 1. /  &
   HCL 1.
POWLAW-EXP 1 MIXED PROPENE 1. / MIXED CHLORINE 1.
POWLAW-EXP 2 MIXED PROPENE 1. / MIXED CHLORINE 1.
POWLAW-EXP 3 MIXED AC 1. / MIXED CHLORINE 1.
```

OUTPUT STREAM SUMMARY-BASE CASE ADIABATIC REACTOR

STREAM	1	2	3	4	5	6	7	8	9
Temperature F	80	700	80	668.1	959.7	70	178.6	-43.5	117.9
Pressure psia	74.7	74.7	74.7	74.7	40	74.7	27	20	16
Vapor Frac	1	1	1	1	1	0.821	0	1	1
Mole Flow lbmol/hr	131.33	1000.00	166.00	1166.00	1144.02	1144.02	130.58	1013.44	73.83
Mass Flow lb/hr	5526.42	42080.64	11770.30	53850.94	53851.85	53851.85	11989.46	41862.39	5649.89
Mass Flow VAPOR lb/hr	5526.42	42080.64	11770.30	53850.94	53851.85	39703.85		41862.39	5649.89
Mass Flow LIQUID lb/hr						14148.00	11989.46		
Volume Flow cuft/hr	9469.78	165601.50	12095.54	187657.25	434972.28	66867.62	196.99	218819.11	27750.78
Volume Flow VAPOR cuft/hr	9469.78	165601.50	12095.54	187657.25	434972.28	66599.96		218819.11	27750.78
Volume Flow LIQUID cuft/hr						267.66	196.99		
Enthalpy MMBtu/hr	1.13	22.11	-0.03	22.09	22.09	-2.61	-3.45	0.25	0.03
Mole Flow lbmol/hr									
H2O	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
HCL	0.00	0.00	0.00	0.00	144.02	144.02	0.00	144.02	0.00
PROPENE	131.33	1000.00	0.00	1000.00	868.67	868.67	0.00	868.67	0.00
CHLORINE	0.00	0.00	166.00	166.00	0.00	0.00	0.00	0.00	0.00
AC	0.00	0.00	0.00	0.00	74.65	74.65	73.90	0.75	73.83
12DCP	0.00	0.00	0.00	0.00	21.99	21.99	21.99	0.00	0.00
13DCP-C	0.00	0.00	0.00	0.00	34.68	34.68	34.68	0.00	0.00
13DCP-T	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
H+	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
CL-	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

STREAM	10	11	12	13	14	15	16	17	18
Temperature F	248	85.7	85.7	269.8	245.7	70	85	104.7	-43.5
Pressure psia	25	14.7	14.7	90	74.7	14.7	14.7	14.7	20
Vapor Frac	0	0	1	1	1	0	1	0	1
Mole Flow lbmol/hr	56.75	37.45	868.67	868.67	1000.00	574.65	906.12	718.67	1012.69
Mass Flow lb/hr	6339.57	674.62	36554.22	36554.22	42080.64	10352.49	37228.85	15603.53	41805.26
Mass Flow VAPOR lb/hr			36554.22	36554.22	42080.64		37228.85		41805.26
Mass Flow LIQUID lb/hr	6339.57	674.62				10352.49		15603.53	
Volume Flow cuft/hr	96.32	10.93	341427.76	72961.37	98153.40	166.37	355715.52	271.72	218665.17
Volume Flow VAPOR cuft/hr			341427.76	72961.37	98153.40		355715.52		218665.17
Volume Flow LIQUID cuft/hr	96.32	10.93				166.37		271.72	
Enthalpy MMBtu/hr	-2.61	-4.60	7.71	10.41	11.54	-70.69	3.81	-78.84	0.26
Mole Flow lbmol/hr									
H2O	0.00	37.45	0.00	0.00	0.00	574.65	37.45	574.65	0.00
HCL	0.00	0.00	0.00	0.00	0.00	0.00	0.00	144.02	144.02
PROPENE	0.00	0.00	868.67	868.67	1000.00	0.00	868.67	0.00	868.67
CHLORINE	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
AC	0.07	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
12DCP	21.99	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
13DCP-C	34.68	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
13DCP-T	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
H+	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
CL-	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

STREAM	19	32
Temperature F	-43.5	71
Pressure psia	20	14.7
Vapor Frac	0	0
Mole Flow lbmol/hr	0.75	612.10
Mass Flow lb/hr	57.13	11027.12
Mass Flow VAPOR lb/hr		
Mass Flow LIQUID lb/hr	57.13	11027.12
Volume Flow cuft/hr	0.90	177.30
Volume Flow VAPOR cuft/hr		
Volume Flow LIQUID cuft/hr	0.90	177.30
Enthalpy MMBtu/hr	-0.01	-75.29
Mole Flow lbmol/hr		
H2O	0.00	612.10
HCL	0.00	0.00
PROPENE	0.00	0.00
CHLORINE	0.00	0.00
AC	0.75	0.00
12DCP	0.00	0.00
13DCP-C	0.00	0.00
13DCP-T	0.00	0.00
H+	0.00	0.00
CL-	0.00	0.00

INPUT SUMMARY OF WEIGHTED OPTIMIZATION-ADIABATIC PFR

```
IN-UNITS ENG
DEF-STREAMS CONVEN ALL
SIM-OPTIONS OLD-DATABANK=YES
RUN-CONTROL MAX-TIME=100000. MAX-ERRORS=500
DESCRIPTION "
   General Simulation with English Units :
   F, psi, lb/hr, lbmol/hr, Btu/hr, cuft/hr.
   Property Method: None
   Flow basis for input: Mole
   Stream report composition: Mole flow

DATABANKS ASPENPCD  / AQUEOUS  / SOLIDS  / INORGANIC  /  &
      PURE22  / PURE10

PROP-SOURCES ASPENPCD  / AQUEOUS  / SOLIDS  / INORGANIC  /  &
      PURE22  / PURE10

COMPONENTS
   H2O H2O /
   HCL HCL /
   PROPENE C3H6-2 /
   CHLORINE CL2 /
   AC C3H5CL /
   12DCP C3H6CL2 /
   13DCP-C C3H4CL2-D1 /
   13DCP-T C3H4CL2-D2 /
   H+ H+ /
   CL- CL-

HENRY-COMPS HENRY CHLORINE HCL PROPENE

SOLVE
   RUN-MODE MODE=OPT

CHEMISTRY HCL
   STOIC 1 HCL -1 / H+ 1 / CL- 1

FLOWSHEET
```

```
   BLOCK B2 IN=14 OUT=2
   BLOCK B8 IN=1 13 OUT=14
   BLOCK B3 IN=2 3 OUT=4
   BLOCK B6 IN=4 OUT=5
   BLOCK B9 IN=5 OUT=6
   BLOCK B7 IN=6 OUT=8 7
   BLOCK B5 IN=7 OUT=9 10
   BLOCK B10 IN=18 32 OUT=16 17
   BLOCK B1 IN=16 OUT=12 11
   BLOCK B11 IN=8 OUT=18 19
   BLOCK B4 IN=12 OUT=13
   BLOCK B18 IN=15 11 OUT=32

PROPERTIES SYSOP0
   PROPERTIES ELECNRTL / UNIQ-RK / UNIQUAC

STRUCTURES
   STRUCTURES 13DCP-C CL1 C2 S / C2 C3 D / C3 C4 S /  &
      C4 CL5 S

ESTIMATE ALL

PROP-DATA PCES-1
   IN-UNITS ENG
   PROP-LIST DGAQHG / DHAQHG / S25HG / OMEGHG / DHVLB /  &
      VB / RGYR / VLSTD
   PVAL CHLORINE 2983.662941 / -10060.18917 / 28.90035349 /  &
      -17580.05159 / 8784.000000 / .7262124822 /  &
      3.2391732E-10 / .8579136616
   PROP-LIST DHVLB / VB / RGYR
   PVAL 13DCP-C 14431.51333 / 1.612466586 / 1.11089239E-9

PROP-DATA HENRY-1
   IN-UNITS ENG
   PROP-LIST HENRY
   BPVAL HCL H2O -49.78140336 2186.999983 8.370700000  &
      -5.3294445E-3 -3.999995968 68.00000346 0.0
   BPVAL CHLORINE H2O -116.9781387 4371.515965 19.18540000  &
      -4.9558834E-3 49.73000360 103.7300032 0.0
   BPVAL HCL 12DCP 10.00798341 -2648.879936 0.0 0.0  &
```

```
      -4.269995966 67.73000346 0.0
   BPVAL PROPENE H2O 326.3806995 -28021.26578 -41.73762000 0.0  &
      69.53000344 220.7300022 0.0
   BPVAL PROPENE 12DCP 12.93988341 -3932.459880 0.0 0.0  &
      -4.269995966 67.73000346 0.0

PROP-DATA UNIQ-1
   IN-UNITS ENG
   PROP-LIST UNIQ
   BPVAL H2O AC -4.247000000 2292.652782 0.0 0.0 109.9400031  &
      212.0000023 0.0
   BPVAL AC H2O 15.46800000 -10062.08074 0.0 0.0 109.9400031  &
      212.0000023 0.0
   BPVAL H2O 12DCP 0.0 -539.9468957 0.0 0.0 77.00000338  &
      77.00000338 0.0
   BPVAL 12DCP H2O 0.0 -2498.536780 0.0 0.0 77.00000338  &
      77.00000338 0.0

PROP-DATA VLCLK-1
   IN-UNITS ENG
   PROP-LIST VLCLK
   BPVAL H+ CL- .5534556926 .2140997389

PROP-DATA GMELCC-1
   IN-UNITS ENG
   PROP-LIST GMELCC
   PPVAL H2O ( H+ CL- ) 41.67400000
   PPVAL ( H+ CL- ) H2O -22.15400000
   PPVAL HCL ( H+ CL- ) 1.00000000E-3
   PPVAL ( H+ CL- ) HCL -1.0000000E-3

PROP-DATA GMELCD-1
   IN-UNITS ENG
   PROP-LIST GMELCD
   PPVAL H2O ( H+ CL- ) 9581.579923
   PPVAL ( H+ CL- ) H2O -3967.379968

PROP-DATA GMELCE-1
   IN-UNITS ENG
   PROP-LIST GMELCE
```

```
   PPVAL H2O ( H+ CL- ) -5.404000000
   PPVAL ( H+ CL- ) H2O 5.188000000

PROP-DATA GMELCN-1
   IN-UNITS ENG
   PROP-LIST GMELCN
   PPVAL H2O ( H+ CL- ) .0283500000

PCES-PROP-DATA
   IN-UNITS ENG
   GAMINF H2O 12DCP * * 68 2340 / * * 86 2310 / * *  &
      104 2090

PCES-PROP-DATA
   IN-UNITS ENG
   GAMINF H2O 13DCP-C * * 68 1360 / * * 86 1430 / * *  &
      104 1460

PROP-SET IPE-1 TEMP PRES MASSFLMX VOLFLMX MWMX MASSSFRA  &
      MASSVFRA MASSFLOW SUBSTREAM=ALL PHASE=T

PROP-SET IPE-2 CPMX MWMX MASSFLMX KMX SIGMAMX MUMX VOLFLMX
&
      UNITS='J/kg-K' SUBSTREAM=MIXED PHASE=L

PROP-SET IPE-3 VOLFLMX CPMX MUMX KMX MWMX MASSFLMX UNITS= &
      'J/kg-K' SUBSTREAM=MIXED PHASE=V

STREAM 1
   SUBSTREAM MIXED TEMP=80. PRES=74.7
   MOLE-FLOW PROPENE 1000.

STREAM 3
   SUBSTREAM MIXED TEMP=80. PRES=74.7
   MOLE-FLOW CHLORINE 166.

STREAM 15
   SUBSTREAM MIXED TEMP=70. PRES=14.7
   MOLE-FLOW H2O 325.
```

```
BLOCK B3 MIXER
   PROPERTIES UNIQ-RK FREE-WATER=STEAM-TA SOLU-WATER=3  &
      TRUE-COMPS=YES

BLOCK B8 MIXER
   PROPERTIES UNIQ-RK FREE-WATER=STEAM-TA SOLU-WATER=3  &
      TRUE-COMPS=YES

BLOCK B18 MIXER

BLOCK B1 SEP
   PARAM
   FRAC STREAM=12 SUBSTREAM=MIXED COMPS=PROPENE FRACS=1.
   PROPERTIES UNIQ-RK FREE-WATER=STEAM-TA SOLU-WATER=3  &
      TRUE-COMPS=YES

BLOCK B11 SEP
   PARAM
   FRAC STREAM=18 SUBSTREAM=MIXED COMPS=H2O HCL PROPENE  &
      CHLORINE AC 12DCP 13DCP-C 13DCP-T H+ CL- FRACS=1. 1.  &
      1. 1. 0. 0. 0. 0. 1. 1.
   PROPERTIES UNIQ-RK FREE-WATER=STEAM-TA SOLU-WATER=3  &
      TRUE-COMPS=YES

BLOCK B2 HEATER
   PARAM TEMP=700. PRES=74.7
   PROPERTIES UNIQ-RK FREE-WATER=STEAM-TA SOLU-WATER=3  &
      TRUE-COMPS=YES

BLOCK B9 HEATER
   PARAM TEMP=70. PRES=74.7
   PROPERTIES UNIQ-RK FREE-WATER=STEAM-TA SOLU-WATER=3  &
      TRUE-COMPS=YES

BLOCK B5 RADFRAC
   PARAM NSTAGE=15
   COL-CONFIG CONDENSER=PARTIAL-V
   FEEDS 7 6
   PRODUCTS 9 1 V / 10 15 L
   P-SPEC 1 16. / 15 25.
```

```
   COL-SPECS D:F=0.539038 MOLE-RR=4.02554
   SPEC 1 MOLE-RECOV 0.999 COMPS=AC STREAMS=9 BASE-STREAMS=7
   VARY 1 D:F 0.01 0.99
   PROPERTIES UNIQ-RK FREE-WATER=STEAM-TA SOLU-WATER=3  &
      TRUE-COMPS=YES

BLOCK B7 RADFRAC
   PARAM NSTAGE=15 ALGORITHM=STANDARD INIT-OPTION=STANDARD
&
      MAXOL=150 DAMPING=NONE
   COL-CONFIG CONDENSER=PARTIAL-V
   FEEDS 6 7
   PRODUCTS 8 1 V / 7 15 L
   P-SPEC 1 20. / 15 27.
   COL-SPECS D:F=0.8 MOLE-RR=0.4084
   SPEC 1 MOLE-RECOV 0.99 COMPS=AC STREAMS=7
   VARY 1 D:F 0.01 0.99
   PROPERTIES UNIQ-RK FREE-WATER=STEAM-TA SOLU-WATER=3  &
      TRUE-COMPS=YES

BLOCK B10 RADFRAC
   PARAM NSTAGE=10 ALGORITHM=NONIDEAL INIT-OPTION=STANDARD  &
      MAXOL=100 MAXIL=50
   COL-CONFIG CONDENSER=NONE REBOILER=NONE
   FEEDS 18 10 ON-STAGE / 32 1
   PRODUCTS 17 10 L / 16 1 V
   P-SPEC 1 14.7
   COL-SPECS
   T-EST 1 110. / 10 68.
   PROPERTIES ELECNRTL HENRY-COMPS=HENRY CHEMISTRY=HCL  &
      FREE-WATER=STEAM-TA SOLU-WATER=3 TRUE-COMPS=NO

BLOCK B6 RPLUG
   PARAM TYPE=ADIABATIC LENGTH=20. DIAM=6. PRES=40.  &
      INT-TOL=1E-005
   COOLANT MAXIT=50
   PROPERTIES UNIQ-RK FREE-WATER=STEAM-TA SOLU-WATER=3  &
      TRUE-COMPS=YES / SYSOP0
   REACTIONS RXN-IDS=R-1
```

```
BLOCK B4 COMPR
   PARAM TYPE=ASME-POLYTROP PRES=90.
   PROPERTIES UNIQ-RK FREE-WATER=STEAM-TA SOLU-WATER=3  &
      TRUE-COMPS=YES

DESIGN-SPEC FEED
   DEFINE S14 MOLE-FLOW STREAM=14 SUBSTREAM=MIXED  &
      COMPONENT=PROPENE
   SPEC "S14" TO "1000"
   TOL-SPEC "0.01"
   VARY MOLE-FLOW STREAM=1 SUBSTREAM=MIXED
COMPONENT=PROPENE
   LIMITS "5" "1000"

DESIGN-SPEC H20
   DEFINE HCL18 MASS-FLOW STREAM=18 SUBSTREAM=MIXED  &
      COMPONENT=HCL
   DEFINE H2032 MASS-FLOW STREAM=32 SUBSTREAM=MIXED  &
      COMPONENT=H2O
   SPEC "H2032" TO "2.1*HCL18"
   TOL-SPEC ".001"
   VARY STREAM-VAR STREAM=15 SUBSTREAM=MIXED VARIABLE=MASS-
FLOW
   LIMITS "10" "60000"

DESIGN-SPEC RESTM
   DEFINE RESTM BLOCK-VAR BLOCK=B6 VARIABLE=RES-TIME  &
      SENTENCE=PARAM
   SPEC "RESTM" TO "1.11E-3"
   TOL-SPEC ".0001"
   VARY BLOCK-VAR BLOCK=B6 VARIABLE=LENGTH SENTENCE=PARAM
   LIMITS "1" "200"

EO-CONV-OPTI


OPTIMIZATION MAXPROFT
   DEFINE AC9 MASS-FLOW STREAM=9 SUBSTREAM=MIXED
COMPONENT=AC
   DEFINE HCL17 STREAM-VAR STREAM=17 SUBSTREAM=MIXED  &
```

```
    VARIABLE=MASS-FLOW
  DEFINE CL3 MASS-FLOW STREAM=3 SUBSTREAM=MIXED  &
    COMPONENT=CHLORINE
  DEFINE PROP1 MASS-FLOW STREAM=1 SUBSTREAM=MIXED  &
    COMPONENT=PROPENE
  DEFINE H2015 MASS-FLOW STREAM=15 SUBSTREAM=MIXED  &
    COMPONENT=H2O
  DEFINE FDHTR BLOCK-VAR BLOCK=B2 VARIABLE=QCALC  &
    SENTENCE=PARAM
  DEFINE REB1 BLOCK-VAR BLOCK=B7 VARIABLE=REB-DUTY  &
    SENTENCE=RESULTS
  DEFINE REB2 BLOCK-VAR BLOCK=B5 VARIABLE=REB-DUTY  &
    SENTENCE=RESULTS
  DEFINE COMP BLOCK-VAR BLOCK=B4 VARIABLE=BRAKE-POWER  &
    SENTENCE=RESULTS
  DEFINE COOL1 BLOCK-VAR BLOCK=B9 VARIABLE=QCALC  &
    SENTENCE=PARAM
  DEFINE COND1 BLOCK-VAR BLOCK=B7 VARIABLE=COND-DUTY  &
    SENTENCE=RESULTS
  DEFINE COND2 BLOCK-VAR BLOCK=B5 VARIABLE=COND-DUTY  &
    SENTENCE=RESULTS
  DEFINE MASSEP MASS-FLOW STREAM=4 SUBSTREAM=MIXED  &
    COMPONENT=PROPENE
  DEFINE MASSEC MASS-FLOW STREAM=4 SUBSTREAM=MIXED  &
    COMPONENT=CHLORINE
  DEFINE MASSXP MASS-FLOW STREAM=5 SUBSTREAM=MIXED  &
    COMPONENT=PROPENE
  DEFINE MASSXC MASS-FLOW STREAM=5 SUBSTREAM=MIXED  &
    COMPONENT=CHLORINE
  DEFINE DCP10 STREAM-VAR STREAM=10 SUBSTREAM=MIXED  &
    VARIABLE=MASS-FLOW
  DEFINE B6TO BLOCK-VAR BLOCK=B6 VARIABLE=REAC-TEMP  &
    SENTENCE=GENPROF ID1=5
  DEFINE PROFIT LOCAL-PARAM PHYS-QTY=UNIT-PRICE UOM="$/lb"  &
    INIT-VAL=0.
  DEFINE PROP2 MOLE-FLOW STREAM=2 SUBSTREAM=MIXED  &
    COMPONENT=PROPENE
  DEFINE T4 STREAM-VAR STREAM=4 SUBSTREAM=MIXED
VARIABLE=TEMP
  DEFINE CL3M STREAM-VAR STREAM=3 SUBSTREAM=MIXED  &
```

```
      VARIABLE=MOLE-FLOW
   DEFINE AC5 MOLE-FLOW STREAM=5 SUBSTREAM=MIXED
COMPONENT=AC
   DEFINE DC25 MOLE-FLOW STREAM=5 SUBSTREAM=MIXED  &
      COMPONENT=12DCP
   DEFINE DC35 MOLE-FLOW STREAM=5 SUBSTREAM=MIXED  &
      COMPONENT=13DCP-C
   DEFINE MCL4 MASS-FLOW STREAM=4 SUBSTREAM=MIXED  &
      COMPONENT=CHLORINE
   DEFINE MP4 MASS-FLOW STREAM=4 SUBSTREAM=MIXED  &
      COMPONENT=PROPENE
   DEFINE MCL5 MASS-FLOW STREAM=5 SUBSTREAM=MIXED  &
      COMPONENT=CHLORINE
   DEFINE MP5 MASS-FLOW STREAM=5 SUBSTREAM=MIXED  &
      COMPONENT=PROPENE
   DEFINE WST12D MASS-FLOW STREAM=10 SUBSTREAM=MIXED  &
      COMPONENT=12DCP
   DEFINE WST13D MASS-FLOW STREAM=10 SUBSTREAM=MIXED  &
      COMPONENT=13DCP-C
   DEFINE HCL5M MASS-FLOW STREAM=5 SUBSTREAM=MIXED  &
      COMPONENT=HCL
   DEFINE AC5M MASS-FLOW STREAM=5 SUBSTREAM=MIXED
COMPONENT=AC
F    REVAC=.88
F    REVHCL=0.0625
F    CSTCL2=.16
F    CSTPRP=.45
F    WSTC=.0011
F    REVENUE=REVAC*AC9+REVHCL*HCL17
F    RAWCST=CSTCL2*CL3+CSTPRP*PROP1
F    NGCST=FDHTR*.0000117
F    TOTST=REB1+REB2
F    STCST=TOTST*0.00001564
F    HTCST=STCST+NGCST
F    ELECST=0.0417*COMP
F    H20BTU=-(COOL1+COND1+COND2)
F    H2O1=(H20BTU/27)*.454*.016088*.00042
F    DIWCST=H2015*.454*.001
F    H20CST=DIWCST+H201
F    UTLCST=HTCST+ELECST+H20CST
```

```
F    WSTCST=DCP10*WSTC
F    HEALTH=4.6*WST12D+4.8*WST13D
F    MP=(HCL5M+AC5M)/((MP4+MCL4+0.000001)-(MP5+MCl5))
F    PROFIT=REVENUE-RAWCST-UTLCST-WSTCST
F    FR=PROP2/CL3M
   MAXIMIZE  &
      "0.4*(PROFIT/1360)-0.4*(HEALTH/31029)+0.2*(MP/0.63447)"
   VARY BLOCK-VAR BLOCK=B2 VARIABLE=TEMP SENTENCE=PARAM
   LIMITS "500" "900"
   VARY MOLE-FLOW STREAM=3 SUBSTREAM=MIXED
COMPONENT=CHLORINE
   LIMITS "166" "1000"
   VARY BLOCK-VAR BLOCK=B6 VARIABLE=PRES SENTENCE=PARAM
   LIMITS "15" "150"

CONV-OPTIONS
   PARAM OPT-METHOD=SQP SPEC-LOOP=INSIDE USER-LOOP=OUTSIDE
   WEGSTEIN MAXIT=100
   DIRECT MAXIT=100
   SECANT MAXIT=100
   BROYDEN MAXIT=100
   NEWTON MAXIT=100
   SQP MAXIT=200 MAXPASS=1000 TOL=0.005 MAXLSPASS=100  &
      NLIMIT=100 STEP-OPT=VALUE STEP-DIR=NEGATIVE  &
      OPT-METHOD=SQP DERIVATIVE=FORWARD CONST-ITER=200  &
      CONV-TEST=KKT

TEAR
   TEAR 13

STREAM-REPOR MOLEFLOW MOLEFRAC MASSFRAC PROPERTIES=IPE-1 IPE-
2  &
      IPE-3

REACTIONS R-1 POWERLAW
   REAC-DATA 1 PHASE=V
   REAC-DATA 2 PHASE=V
   REAC-DATA 3 PHASE=V
   RATE-CON 1 PRE-EXP=40400000. ACT-ENERGY=74300000. <J/kmol>
   RATE-CON 2 PRE-EXP=2300. ACT-ENERGY=27300000. <J/kmol>
```

```
RATE-CON 3 PRE-EXP=90300000000. ACT-ENERGY=110000000. <J/kmol>
STOIC 1 MIXED PROPENE -1. / CHLORINE -1. / AC 1. /  &
   HCL 1.
STOIC 2 MIXED PROPENE -1. / CHLORINE -1. / 12DCP 1.
STOIC 3 MIXED AC -1. / CHLORINE -1. / 13DCP-C 1. /  &
   HCL 1.
POWLAW-EXP 1 MIXED PROPENE 1. / MIXED CHLORINE 1.
POWLAW-EXP 2 MIXED PROPENE 1. / MIXED CHLORINE 1.
POWLAW-EXP 3 MIXED AC 1. / MIXED CHLORINE 1.
```

OUTPUT STREAM SUMMARY – WEIGHTED OPTIMIZATION-ADIABATIC PFR

	1	2	3	4	5	6	7	8	9
Temperature F	80	654.4	80	624.2	926.6	70	178.1	-43.2	117.9
Pressure psia	74.7	74.7	74.7	74.7	34.72	74.7	27	20	16
Vapor Frac	1	1	1	1	1	0.812	0	1	1
Mole Flow lbmol/hr	135.68	1000.00	166.00	1166.00	1138.15	1138.15	134.90	1003.25	76.65
Mass Flow lb/hr	5709.46	42080.64	11770.30	53850.94	53851.22	53851.22	12383.61	41467.62	5865.64
Mass Flow lb/hr	5709.46	42080.64	11770.30	53850.94	53851.22	39103.09		41467.62	5865.64
Mass Flow lb/hr						14748.14	12383.61		
Volume Flow cuft/hr	9783.43	158935.23	12095.54	180158.79	486931.79	65798.07	204.09	216752.28	28810.46
Volume Flow cuft/hr	9783.43	158935.23	12095.54	180158.79	486931.79	65517.78		216752.28	28810.46
Volume Flow cuft/hr						280.28	204.09		
Enthalpy MMBtu/hr	1.17	20.90	-0.03	20.87	20.87	-2.86	-3.84	0.46	0.03
Mole Flow lbmol/hr									
H2O	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
HCL	0.00	0.00	0.00	0.00	138.15	138.15	0.00	138.15	0.00
PROPENE	135.68	1000.00	0.00	1000.00	864.32	864.32	0.00	864.32	0.00
CHLORINE	0.00	0.00	166.00	166.00	0.00	0.00	0.00	0.00	0.00
AC	0.00	0.00	0.00	0.00	77.50	77.50	76.73	0.78	76.65
12DCP	0.00	0.00	0.00	0.00	27.85	27.85	27.85	0.00	0.00
13DCP-C	0.00	0.00	0.00	0.00	30.33	30.33	30.33	0.00	0.00
13DCP-T	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
H+	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
CL-	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

	10	11	12	13	14	15	16	17	18
Temperature F	246.7	84.2	84.2	268.2	243.6	70	83.6	102.3	-43.2
Pressure psia	25	14.7	14.7	90	74.7	14.7	14.7	14.7	20
Vapor Frac	0	0	1	1	1	0	1	0	1
Mole Flow lbmol/hr	58.25	35.45	864.32	864.32	1000.00	551.71	899.78	689.86	1002.47
Mass Flow lb/hr	6517.97	638.72	36371.18	36371.18	42080.64	9939.19	37009.90	14976.33	41408.31
Mass Flow lb/hr			36371.18	36371.18	42080.64		37009.90		41408.31
Mass Flow lb/hr	6517.97	638.72				9939.19		14976.33	
Volume Flow cuft/hr	99.50	10.34	338755.83	72421.47	97822.17	159.73	352223.69	259.53	216592.34
Volume Flow cuft/hr			338755.83	72421.47	97822.17		352223.69		216592.34
Volume Flow cuft/hr	99.50	10.34				159.73		259.53	
Enthalpy MMBtu/hr	-2.97	-4.35	7.65	10.33	11.50	-67.87	3.96	-75.72	0.47
Mole Flow lbmol/hr									
H2O	0.00	35.45	0.00	0.00	0.00	551.71	35.45	551.71	0.00
HCL	0.00	0.00	0.00	0.00	0.00	0.00	0.00	138.15	138.15
PROPENE	0.00	0.00	864.32	864.32	1000.00	0.00	864.32	0.00	864.32
CHLORINE	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
AC	0.08	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
12DCP	27.85	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
13DCP-C	30.33	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
13DCP-T	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
H+	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
CL-	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

	19	32
Temperature F	-43.2	70.9
Pressure psia	20	14.7
Vapor Frac	0	0
Mole Flow lbmol/hr	0.78	587.16
Mass Flow lb/hr	59.31	10577.91
Mass Flow lb/hr		
Mass Flow lb/hr	59.31	10577.91
Volume Flow cuft/hr	0.94	170.07
Volume Flow cuft/hr		
Volume Flow cuft/hr	0.94	170.07
Enthalpy MMBtu/hr	-0.01	-72.22
Mole Flow lbmol/hr		
H2O	0.00	587.16
HCL	0.00	0.00
PROPENE	0.00	0.00
CHLORINE	0.00	0.00
AC	0.78	0.00
12DCP	0.00	0.00
13DCP-C	0.00	0.00
13DCP-T	0.00	0.00
H+	0.00	0.00
CL-	0.00	0.00

INPUT SUMMARY-CONSTRAINED OPTIMIZATION-ADIABATIC PFR

```
TITLE 'ALLYL CHLORIDE -Adiabatic PFR'
IN-UNITS ENG
DEF-STREAMS CONVEN ALL
SIM-OPTIONS OLD-DATABANK=YES
RUN-CONTROL MAX-TIME=100000. MAX-ERRORS=500
DESCRIPTION "
   General Simulation with English Units :
   F, psi, lb/hr, lbmol/hr, Btu/hr, cuft/hr.
   Property Method: None
   Flow basis for input: Mole
   Stream report composition: Mole flow

DATABANKS ASPENPCD  / AQUEOUS  / SOLIDS  / INORGANIC  /  &
      PURE22  / PURE10

PROP-SOURCES ASPENPCD  / AQUEOUS  / SOLIDS  / INORGANIC  /  &
      PURE22  / PURE10

COMPONENTS
   H2O H2O /
   HCL HCL /
   PROPENE C3H6-2 /
   CHLORINE CL2 /
   AC C3H5CL /
   12DCP C3H6CL2 /
   13DCP-C C3H4CL2-D1 /
   13DCP-T C3H4CL2-D2 /
   H+ H+ /
   CL- CL-

HENRY-COMPS HENRY CHLORINE HCL PROPENE

SOLVE
   RUN-MODE MODE=OPT

CHEMISTRY HCL
   STOIC 1 HCL -1 / H+ 1 / CL- 1
```

```
FLOWSHEET
   BLOCK B2 IN=14 OUT=2
   BLOCK B8 IN=1 13 OUT=14
   BLOCK B3 IN=2 3 OUT=4
   BLOCK B6 IN=4 OUT=5
   BLOCK B9 IN=5 OUT=6
   BLOCK B7 IN=6 OUT=8 7
   BLOCK B5 IN=7 OUT=9 10
   BLOCK B10 IN=18 32 OUT=16 17
   BLOCK B1 IN=16 OUT=12 11
   BLOCK B11 IN=8 OUT=18 19
   BLOCK B4 IN=12 OUT=13
   BLOCK B18 IN=15 11 OUT=32

PROPERTIES SYSOP0
   PROPERTIES ELECNRTL / UNIQ-RK / UNIQUAC

STRUCTURES
   STRUCTURES 13DCP-C CL1 C2 S / C2 C3 D / C3 C4 S /  &
      C4 CL5 S

ESTIMATE ALL

PROP-DATA PCES-1
   IN-UNITS ENG
   PROP-LIST DGAQHG / DHAQHG / S25HG / OMEGHG / DHVLB /  &
      VB / RGYR / VLSTD
   PVAL CHLORINE 2983.662941 / -10060.18917 / 28.90035349 /  &
      -17580.05159 / 8784.000000 / .7262124822 /  &
      3.2391732E-10 / .8579136616
   PROP-LIST DHVLB / VB / RGYR
   PVAL 13DCP-C 14431.51333 / 1.612466586 / 1.11089239E-9

PROP-DATA HENRY-1
   IN-UNITS ENG
   PROP-LIST HENRY
   BPVAL HCL H2O -49.78140336 2186.999983 8.370700000  &
      -5.3294445E-3 -3.999995968 68.00000346 0.0
   BPVAL CHLORINE H2O -116.9781387 4371.515965 19.18540000  &
      -4.9558834E-3 49.73000360 103.7300032 0.0
```

```
   BPVAL HCL 12DCP 10.00798341 -2648.879936 0.0 0.0  &
      -4.269995966 67.73000346 0.0
   BPVAL PROPENE H2O 326.3806995 -28021.26578 -41.73762000 0.0  &
      69.53000344 220.7300022 0.0
   BPVAL PROPENE 12DCP 12.93988341 -3932.459880 0.0 0.0  &
      -4.269995966 67.73000346 0.0

PROP-DATA UNIQ-1
   IN-UNITS ENG
   PROP-LIST UNIQ
   BPVAL H2O AC -4.247000000 2292.652782 0.0 0.0 109.9400031  &
      212.0000023 0.0
   BPVAL AC H2O 15.46800000 -10062.08074 0.0 0.0 109.9400031  &
      212.0000023 0.0
   BPVAL H2O 12DCP 0.0 -539.9468957 0.0 0.0 77.00000338  &
      77.00000338 0.0
   BPVAL 12DCP H2O 0.0 -2498.536780 0.0 0.0 77.00000338  &
      77.00000338 0.0

PROP-DATA VLCLK-1
   IN-UNITS ENG
   PROP-LIST VLCLK
   BPVAL H+ CL- .5534556926 .2140997389

PROP-DATA GMELCC-1
   IN-UNITS ENG
   PROP-LIST GMELCC
   PPVAL H2O ( H+ CL- ) 41.67400000
   PPVAL ( H+ CL- ) H2O -22.15400000
   PPVAL HCL ( H+ CL- ) 1.00000000E-3
   PPVAL ( H+ CL- ) HCL -1.0000000E-3

PROP-DATA GMELCD-1
   IN-UNITS ENG
   PROP-LIST GMELCD
   PPVAL H2O ( H+ CL- ) 9581.579923
   PPVAL ( H+ CL- ) H2O -3967.379968

PROP-DATA GMELCE-1
   IN-UNITS ENG
```

```
   PROP-LIST GMELCE
   PPVAL H2O ( H+ CL- ) -5.404000000
   PPVAL ( H+ CL- ) H2O 5.188000000

PROP-DATA GMELCN-1
   IN-UNITS ENG
   PROP-LIST GMELCN
   PPVAL H2O ( H+ CL- ) .0283500000

PCES-PROP-DATA
   IN-UNITS ENG
   GAMINF H2O 12DCP * * 68 2340 / * * 86 2310 / * *  &
      104 2090

PCES-PROP-DATA
   IN-UNITS ENG
   GAMINF H2O 13DCP-C * * 68 1360 / * * 86 1430 / * *  &
      104 1460

PROP-SET IPE-1 TEMP PRES MASSFLMX VOLFLMX MWMX MASSSFRA  &
      MASSVFRA MASSFLOW SUBSTREAM=ALL PHASE=T

PROP-SET IPE-2 CPMX MWMX MASSFLMX KMX SIGMAMX MUMX VOLFLMX
&
      UNITS='J/kg-K' SUBSTREAM=MIXED PHASE=L

PROP-SET IPE-3 VOLFLMX CPMX MUMX KMX MWMX MASSFLMX UNITS= &
      'J/kg-K' SUBSTREAM=MIXED PHASE=V

STREAM 1
   SUBSTREAM MIXED TEMP=80. PRES=74.7
   MOLE-FLOW PROPENE 1000.

STREAM 3
   SUBSTREAM MIXED TEMP=80. PRES=74.7
   MOLE-FLOW CHLORINE 166.

STREAM 15
   SUBSTREAM MIXED TEMP=70. PRES=14.7
   MOLE-FLOW H2O 325.
```

```
BLOCK B3 MIXER
   PROPERTIES UNIQ-RK FREE-WATER=STEAM-TA SOLU-WATER=3  &
      TRUE-COMPS=YES

BLOCK B8 MIXER
   PROPERTIES UNIQ-RK FREE-WATER=STEAM-TA SOLU-WATER=3  &
      TRUE-COMPS=YES

BLOCK B18 MIXER

BLOCK B1 SEP
   PARAM
   FRAC STREAM=12 SUBSTREAM=MIXED COMPS=PROPENE FRACS=1.
   PROPERTIES UNIQ-RK FREE-WATER=STEAM-TA SOLU-WATER=3  &
      TRUE-COMPS=YES

BLOCK B11 SEP
   PARAM
   FRAC STREAM=18 SUBSTREAM=MIXED COMPS=H2O HCL PROPENE  &
      CHLORINE AC 12DCP 13DCP-C 13DCP-T H+ CL- FRACS=1. 1.  &
      1. 1. 0. 0. 0. 0. 1. 1.
   PROPERTIES UNIQ-RK FREE-WATER=STEAM-TA SOLU-WATER=3  &
      TRUE-COMPS=YES

BLOCK B2 HEATER
   PARAM TEMP=700. PRES=74.7
   PROPERTIES UNIQ-RK FREE-WATER=STEAM-TA SOLU-WATER=3  &
      TRUE-COMPS=YES

BLOCK B9 HEATER
   PARAM TEMP=70. PRES=74.7
   PROPERTIES UNIQ-RK FREE-WATER=STEAM-TA SOLU-WATER=3  &
      TRUE-COMPS=YES

BLOCK B5 RADFRAC
   PARAM NSTAGE=15
   COL-CONFIG CONDENSER=PARTIAL-V
   FEEDS 7 6
   PRODUCTS 9 1 V / 10 15 L
```

```
   P-SPEC 1 16. / 15 25.
   COL-SPECS D:F=0.539038 MOLE-RR=4.02554
   SPEC 1 MOLE-RECOV 0.999 COMPS=AC STREAMS=9 BASE-STREAMS=7
   VARY 1 D:F 0.01 0.99
   PROPERTIES UNIQ-RK FREE-WATER=STEAM-TA SOLU-WATER=3  &
      TRUE-COMPS=YES

BLOCK B7 RADFRAC
   PARAM NSTAGE=15 ALGORITHM=STANDARD INIT-OPTION=STANDARD
&
      MAXOL=150 DAMPING=NONE
   COL-CONFIG CONDENSER=PARTIAL-V
   FEEDS 6 7
   PRODUCTS 8 1 V / 7 15 L
   P-SPEC 1 20. / 15 27.
   COL-SPECS D:F=0.8 MOLE-RR=0.4084
   SPEC 1 MOLE-RECOV 0.99 COMPS=AC STREAMS=7
   VARY 1 D:F 0.01 0.99
   PROPERTIES UNIQ-RK FREE-WATER=STEAM-TA SOLU-WATER=3  &
      TRUE-COMPS=YES

BLOCK B10 RADFRAC
   PARAM NSTAGE=10 ALGORITHM=NONIDEAL INIT-OPTION=STANDARD  &
      MAXOL=100 MAXIL=50
   COL-CONFIG CONDENSER=NONE REBOILER=NONE
   FEEDS 18 10 ON-STAGE / 32 1
   PRODUCTS 17 10 L / 16 1 V
   P-SPEC 1 14.7
   COL-SPECS
   T-EST 1 110. / 10 68.
   PROPERTIES ELECNRTL HENRY-COMPS=HENRY CHEMISTRY=HCL  &
      FREE-WATER=STEAM-TA SOLU-WATER=3 TRUE-COMPS=NO

BLOCK B6 RPLUG
   PARAM TYPE=ADIABATIC LENGTH=20. DIAM=6. PRES=40.  &
      INT-TOL=1E-005
   COOLANT MAXIT=50
   PROPERTIES UNIQ-RK FREE-WATER=STEAM-TA SOLU-WATER=3  &
      TRUE-COMPS=YES / SYSOP0
   REACTIONS RXN-IDS=R-1
```

```
BLOCK B4 COMPR
   PARAM TYPE=ASME-POLYTROP PRES=90.
   PROPERTIES UNIQ-RK FREE-WATER=STEAM-TA SOLU-WATER=3  &
      TRUE-COMPS=YES

DESIGN-SPEC FEED
   DEFINE S14 MOLE-FLOW STREAM=14 SUBSTREAM=MIXED  &
      COMPONENT=PROPENE
   SPEC "S14" TO "1000"
   TOL-SPEC "0.01"
   VARY MOLE-FLOW STREAM=1 SUBSTREAM=MIXED
COMPONENT=PROPENE
   LIMITS "5" "1000"

DESIGN-SPEC H20
   DEFINE HCL18 MASS-FLOW STREAM=18 SUBSTREAM=MIXED  &
      COMPONENT=HCL
   DEFINE H2032 MASS-FLOW STREAM=32 SUBSTREAM=MIXED  &
      COMPONENT=H2O
   SPEC "H2032" TO "2.1*HCL18"
   TOL-SPEC ".001"
   VARY STREAM-VAR STREAM=15 SUBSTREAM=MIXED VARIABLE=MASS-
FLOW
   LIMITS "10" "60000"

DESIGN-SPEC RESTM
   DEFINE RESTM BLOCK-VAR BLOCK=B6 VARIABLE=RES-TIME  &
      SENTENCE=PARAM
   SPEC "RESTM" TO "1.11E-3"
   TOL-SPEC ".0001"
   VARY BLOCK-VAR BLOCK=B6 VARIABLE=LENGTH SENTENCE=PARAM
   LIMITS "1" "200"

EO-CONV-OPTI

CONSTRAINT MP
   DEFINE AC9 MASS-FLOW STREAM=9 SUBSTREAM=MIXED
COMPONENT=AC
   DEFINE HCL17 STREAM-VAR STREAM=17 SUBSTREAM=MIXED  &
```

```
    VARIABLE=MASS-FLOW
  DEFINE CL3 MASS-FLOW STREAM=3 SUBSTREAM=MIXED  &
    COMPONENT=CHLORINE
  DEFINE PROP1 MASS-FLOW STREAM=1 SUBSTREAM=MIXED  &
    COMPONENT=PROPENE
  DEFINE H2015 MASS-FLOW STREAM=15 SUBSTREAM=MIXED  &
    COMPONENT=H2O
  DEFINE FDHTR BLOCK-VAR BLOCK=B2 VARIABLE=QCALC  &
    SENTENCE=PARAM
  DEFINE REB1 BLOCK-VAR BLOCK=B7 VARIABLE=REB-DUTY  &
    SENTENCE=RESULTS
  DEFINE REB2 BLOCK-VAR BLOCK=B5 VARIABLE=REB-DUTY  &
    SENTENCE=RESULTS
  DEFINE COMP BLOCK-VAR BLOCK=B4 VARIABLE=BRAKE-POWER  &
    SENTENCE=RESULTS
  DEFINE COOL1 BLOCK-VAR BLOCK=B9 VARIABLE=QCALC  &
    SENTENCE=PARAM
  DEFINE COND1 BLOCK-VAR BLOCK=B7 VARIABLE=COND-DUTY  &
    SENTENCE=RESULTS
  DEFINE COND2 BLOCK-VAR BLOCK=B5 VARIABLE=COND-DUTY  &
    SENTENCE=RESULTS
  DEFINE MASSEP MASS-FLOW STREAM=4 SUBSTREAM=MIXED  &
    COMPONENT=PROPENE
  DEFINE MASSEC MASS-FLOW STREAM=4 SUBSTREAM=MIXED  &
    COMPONENT=CHLORINE
  DEFINE MASSXP MASS-FLOW STREAM=5 SUBSTREAM=MIXED  &
    COMPONENT=PROPENE
  DEFINE MASSXC MASS-FLOW STREAM=5 SUBSTREAM=MIXED  &
    COMPONENT=CHLORINE
  DEFINE DCP10 STREAM-VAR STREAM=10 SUBSTREAM=MIXED  &
    VARIABLE=MASS-FLOW
  DEFINE B6TO BLOCK-VAR BLOCK=B6 VARIABLE=REAC-TEMP  &
    SENTENCE=GENPROF ID1=5
  DEFINE PROFIT LOCAL-PARAM PHYS-QTY=UNIT-PRICE UOM="$/lb"  &
    INIT-VAL=0.
  DEFINE PROP2 MOLE-FLOW STREAM=2 SUBSTREAM=MIXED  &
    COMPONENT=PROPENE
  DEFINE T4 STREAM-VAR STREAM=4 SUBSTREAM=MIXED
VARIABLE=TEMP
  DEFINE CL3M STREAM-VAR STREAM=3 SUBSTREAM=MIXED  &
```

```
      VARIABLE=MOLE-FLOW
   DEFINE AC5 MOLE-FLOW STREAM=5 SUBSTREAM=MIXED
COMPONENT=AC
   DEFINE DC25 MOLE-FLOW STREAM=5 SUBSTREAM=MIXED  &
      COMPONENT=12DCP
   DEFINE DC35 MOLE-FLOW STREAM=5 SUBSTREAM=MIXED  &
      COMPONENT=13DCP-C
   DEFINE MCL4 MASS-FLOW STREAM=4 SUBSTREAM=MIXED  &
      COMPONENT=CHLORINE
   DEFINE MP4 MASS-FLOW STREAM=4 SUBSTREAM=MIXED  &
      COMPONENT=PROPENE
   DEFINE MCL5 MASS-FLOW STREAM=5 SUBSTREAM=MIXED  &
      COMPONENT=CHLORINE
   DEFINE MP5 MASS-FLOW STREAM=5 SUBSTREAM=MIXED  &
      COMPONENT=PROPENE
   DEFINE WST12D MASS-FLOW STREAM=10 SUBSTREAM=MIXED  &
      COMPONENT=12DCP
   DEFINE WST13D MASS-FLOW STREAM=10 SUBSTREAM=MIXED  &
      COMPONENT=13DCP-C
   DEFINE HCL5M MASS-FLOW STREAM=5 SUBSTREAM=MIXED  &
      COMPONENT=HCL
   DEFINE AC5M MASS-FLOW STREAM=5 SUBSTREAM=MIXED
COMPONENT=AC
F    REVAC=.88
F    REVHCL=0.0625
F    CSTCL2=.16
F    CSTPRP=.45
F    WSTC=.0011
F    REVENUE=REVAC*AC9+REVHCL*HCL17
F    RAWCST=CSTCL2*CL3+CSTPRP*PROP1
F    NGCST=FDHTR*.0000117
F    TOTST=REB1+REB2
F    STCST=TOTST*0.00001564
F    HTCST=STCST+NGCST
F    ELECST=0.0417*COMP
F    H20BTU=-(COOL1+COND1+COND2)
F    H2O1=(H20BTU/27)*.454*.016088*.00042
F    DIWCST=H2015*.454*.001
F    H20CST=DIWCST+H201
F    UTLCST=HTCST+ELECST+H20CST
```

```
F    WSTCST=DCP10*WSTC
F    HEALTH=4.6*WST12D+4.8*WST13D
F    MP=(HCL5M+AC5M)/((MP4+MCL4+0.000001)-(MP5+MCl5))
F    PROFIT=REVENUE-RAWCST-UTLCST-WSTCST
F    FR=PROP2/CL3M
   SPEC "PROFIT" MO "0.6324"
   TOL-SPEC ".1"

CONSTRAINT HEALTH
   DEFINE AC9 MASS-FLOW STREAM=9 SUBSTREAM=MIXED
COMPONENT=AC
   DEFINE HCL17 STREAM-VAR STREAM=17 SUBSTREAM=MIXED  &
      VARIABLE=MASS-FLOW
   DEFINE CL3 MASS-FLOW STREAM=3 SUBSTREAM=MIXED  &
      COMPONENT=CHLORINE
   DEFINE PROP1 MASS-FLOW STREAM=1 SUBSTREAM=MIXED  &
      COMPONENT=PROPENE
   DEFINE H2015 MASS-FLOW STREAM=15 SUBSTREAM=MIXED  &
      COMPONENT=H2O
   DEFINE FDHTR BLOCK-VAR BLOCK=B2 VARIABLE=QCALC  &
      SENTENCE=PARAM
   DEFINE REB1 BLOCK-VAR BLOCK=B7 VARIABLE=REB-DUTY  &
      SENTENCE=RESULTS
   DEFINE REB2 BLOCK-VAR BLOCK=B5 VARIABLE=REB-DUTY  &
      SENTENCE=RESULTS
   DEFINE COMP BLOCK-VAR BLOCK=B4 VARIABLE=BRAKE-POWER  &
      SENTENCE=RESULTS
   DEFINE COOL1 BLOCK-VAR BLOCK=B9 VARIABLE=QCALC  &
      SENTENCE=PARAM
   DEFINE COND1 BLOCK-VAR BLOCK=B7 VARIABLE=COND-DUTY  &
      SENTENCE=RESULTS
   DEFINE COND2 BLOCK-VAR BLOCK=B5 VARIABLE=COND-DUTY  &
      SENTENCE=RESULTS
   DEFINE MASSEP MASS-FLOW STREAM=4 SUBSTREAM=MIXED  &
      COMPONENT=PROPENE
   DEFINE MASSEC MASS-FLOW STREAM=4 SUBSTREAM=MIXED  &
      COMPONENT=CHLORINE
   DEFINE MASSXP MASS-FLOW STREAM=5 SUBSTREAM=MIXED  &
      COMPONENT=PROPENE
   DEFINE MASSXC MASS-FLOW STREAM=5 SUBSTREAM=MIXED  &
```

```
      COMPONENT=CHLORINE
   DEFINE DCP10 STREAM-VAR STREAM=10 SUBSTREAM=MIXED  &
      VARIABLE=MASS-FLOW
   DEFINE B6TO BLOCK-VAR BLOCK=B6 VARIABLE=REAC-TEMP  &
      SENTENCE=GENPROF ID1=5
   DEFINE PROFIT LOCAL-PARAM PHYS-QTY=UNIT-PRICE UOM="$/lb"  &
      INIT-VAL=0.
   DEFINE PROP2 MOLE-FLOW STREAM=2 SUBSTREAM=MIXED  &
      COMPONENT=PROPENE
   DEFINE T4 STREAM-VAR STREAM=4 SUBSTREAM=MIXED
VARIABLE=TEMP
   DEFINE CL3M STREAM-VAR STREAM=3 SUBSTREAM=MIXED  &
      VARIABLE=MOLE-FLOW
   DEFINE AC5 MOLE-FLOW STREAM=5 SUBSTREAM=MIXED
COMPONENT=AC
   DEFINE DC25 MOLE-FLOW STREAM=5 SUBSTREAM=MIXED  &
      COMPONENT=12DCP
   DEFINE DC35 MOLE-FLOW STREAM=5 SUBSTREAM=MIXED  &
      COMPONENT=13DCP-C
   DEFINE MCL4 MASS-FLOW STREAM=4 SUBSTREAM=MIXED  &
      COMPONENT=CHLORINE
   DEFINE MP4 MASS-FLOW STREAM=4 SUBSTREAM=MIXED  &
      COMPONENT=PROPENE
   DEFINE MCL5 MASS-FLOW STREAM=5 SUBSTREAM=MIXED  &
      COMPONENT=CHLORINE
   DEFINE MP5 MASS-FLOW STREAM=5 SUBSTREAM=MIXED  &
      COMPONENT=PROPENE
   DEFINE WST12D MASS-FLOW STREAM=10 SUBSTREAM=MIXED  &
      COMPONENT=12DCP
   DEFINE WST13D MASS-FLOW STREAM=10 SUBSTREAM=MIXED  &
      COMPONENT=13DCP-C
   DEFINE HCL5M MASS-FLOW STREAM=5 SUBSTREAM=MIXED  &
      COMPONENT=HCL
   DEFINE AC5M MASS-FLOW STREAM=5 SUBSTREAM=MIXED
COMPONENT=AC
F    REVAC=.88
F    REVHCL=0.0625
F    CSTCL2=.16
F    CSTPRP=.45
F    WSTC=.0011
```

```
F    REVENUE=REVAC*AC9+REVHCL*HCL17
F    RAWCST=CSTCL2*CL3+CSTPRP*PROP1
F    NGCST=FDHTR*.0000117
F    TOTST=REB1+REB2
F    STCST=TOTST*0.00001564
F    HTCST=STCST+NGCST
F    ELECST=0.0417*COMP
F    H20BTU=-(COOL1+COND1+COND2)
F    H2O1=(H20BTU/27)*.454*.016088*.00042
F    DIWCST=H2015*.454*.001
F    H20CST=DIWCST+H201
F    UTLCST=HTCST+ELECST+H20CST
F    WSTCST=DCP10*WSTC
F    HEALTH=4.6*WST12D+4.8*WST13D
F    MP=(HCL5M+AC5M)/((MP4+MCL4+0.000001)-(MP5+MCl5))
F    PROFIT=REVENUE-RAWCST-UTLCST-WSTCST
F    FR=PROP2/CL3M
   SPEC "HEALTH" EQ "29740.4"
   TOL-SPEC ".1"

OPTIMIZATION MINHEALT
   DEFINE AC9 MASS-FLOW STREAM=9 SUBSTREAM=MIXED
COMPONENT=AC
   DEFINE HCL17 STREAM-VAR STREAM=17 SUBSTREAM=MIXED  &
      VARIABLE=MASS-FLOW
   DEFINE CL3 MASS-FLOW STREAM=3 SUBSTREAM=MIXED  &
      COMPONENT=CHLORINE
   DEFINE PROP1 MASS-FLOW STREAM=1 SUBSTREAM=MIXED  &
      COMPONENT=PROPENE
   DEFINE H2015 MASS-FLOW STREAM=15 SUBSTREAM=MIXED  &
      COMPONENT=H2O
   DEFINE FDHTR BLOCK-VAR BLOCK=B2 VARIABLE=QCALC  &
      SENTENCE=PARAM
   DEFINE REB1 BLOCK-VAR BLOCK=B7 VARIABLE=REB-DUTY  &
      SENTENCE=RESULTS
   DEFINE REB2 BLOCK-VAR BLOCK=B5 VARIABLE=REB-DUTY  &
      SENTENCE=RESULTS
   DEFINE COMP BLOCK-VAR BLOCK=B4 VARIABLE=BRAKE-POWER  &
      SENTENCE=RESULTS
   DEFINE COOL1 BLOCK-VAR BLOCK=B9 VARIABLE=QCALC  &
```

```
      SENTENCE=PARAM
   DEFINE COND1 BLOCK-VAR BLOCK=B7 VARIABLE=COND-DUTY  &
      SENTENCE=RESULTS
   DEFINE COND2 BLOCK-VAR BLOCK=B5 VARIABLE=COND-DUTY  &
      SENTENCE=RESULTS
   DEFINE MASSEP MASS-FLOW STREAM=4 SUBSTREAM=MIXED  &
      COMPONENT=PROPENE
   DEFINE MASSEC MASS-FLOW STREAM=4 SUBSTREAM=MIXED  &
      COMPONENT=CHLORINE
   DEFINE MASSXP MASS-FLOW STREAM=5 SUBSTREAM=MIXED  &
      COMPONENT=PROPENE
   DEFINE MASSXC MASS-FLOW STREAM=5 SUBSTREAM=MIXED  &
      COMPONENT=CHLORINE
   DEFINE DCP10 STREAM-VAR STREAM=10 SUBSTREAM=MIXED  &
      VARIABLE=MASS-FLOW
   DEFINE B6TO BLOCK-VAR BLOCK=B6 VARIABLE=REAC-TEMP  &
      SENTENCE=GENPROF ID1=5
   DEFINE PROFIT LOCAL-PARAM PHYS-QTY=UNIT-PRICE UOM="$/lb"  &
      INIT-VAL=0.
   DEFINE PROP2 MOLE-FLOW STREAM=2 SUBSTREAM=MIXED  &
      COMPONENT=PROPENE
   DEFINE T4 STREAM-VAR STREAM=4 SUBSTREAM=MIXED
VARIABLE=TEMP
   DEFINE CL3M STREAM-VAR STREAM=3 SUBSTREAM=MIXED  &
      VARIABLE=MOLE-FLOW
   DEFINE AC5 MOLE-FLOW STREAM=5 SUBSTREAM=MIXED
COMPONENT=AC
   DEFINE DC25 MOLE-FLOW STREAM=5 SUBSTREAM=MIXED  &
      COMPONENT=12DCP
   DEFINE DC35 MOLE-FLOW STREAM=5 SUBSTREAM=MIXED  &
      COMPONENT=13DCP-C
   DEFINE MCL4 MASS-FLOW STREAM=4 SUBSTREAM=MIXED  &
      COMPONENT=CHLORINE
   DEFINE MP4 MASS-FLOW STREAM=4 SUBSTREAM=MIXED  &
      COMPONENT=PROPENE
   DEFINE MCL5 MASS-FLOW STREAM=5 SUBSTREAM=MIXED  &
      COMPONENT=CHLORINE
   DEFINE MP5 MASS-FLOW STREAM=5 SUBSTREAM=MIXED  &
      COMPONENT=PROPENE
   DEFINE WST12D MASS-FLOW STREAM=10 SUBSTREAM=MIXED  &
```

```
      COMPONENT=12DCP
   DEFINE WST13D MASS-FLOW STREAM=10 SUBSTREAM=MIXED  &
      COMPONENT=13DCP-C
   DEFINE HCL5M MASS-FLOW STREAM=5 SUBSTREAM=MIXED  &
      COMPONENT=HCL
   DEFINE AC5M MASS-FLOW STREAM=5 SUBSTREAM=MIXED
COMPONENT=AC
F    REVAC=.88
F    REVHCL=0.0625
F    CSTCL2=.16
F    CSTPRP=.45
F    WSTC=.0011
F    REVENUE=REVAC*AC9+REVHCL*HCL17
F    RAWCST=CSTCL2*CL3+CSTPRP*PROP1
F    NGCST=FDHTR*.0000117
F    TOTST=REB1+REB2
F    STCST=TOTST*0.00001564
F    HTCST=STCST+NGCST
F    ELECST=0.0417*COMP
F    H20BTU=-(COOL1+COND1+COND2)
F    H2O1=(H20BTU/27)*.454*.016088*.00042
F    DIWCST=H2015*.454*.001
F    H20CST=DIWCST+H201
F    UTLCST=HTCST+ELECST+H20CST
F    WSTCST=DCP10*WSTC
F    HEALTH=4.6*WST12D+4.8*WST13D
F    MP=(HCL5M+AC5M)/((MP4+MCL4+0.000001)-(MP5+MCl5))
F    PROFIT=REVENUE-RAWCST-UTLCST-WSTCST
F    FR=PROP2/CL3M
   MAXIMIZE "PROFIT"
   CONSTRAINTS HEALTH
   VARY BLOCK-VAR BLOCK=B2 VARIABLE=TEMP SENTENCE=PARAM
   LIMITS "500" "900"
   VARY MOLE-FLOW STREAM=3 SUBSTREAM=MIXED
COMPONENT=CHLORINE
   LIMITS "166" "1000"
   VARY BLOCK-VAR BLOCK=B6 VARIABLE=PRES SENTENCE=PARAM
   LIMITS "15" "150"
```

```
CONV-OPTIONS
   PARAM OPT-METHOD=SQP SPEC-LOOP=INSIDE USER-LOOP=OUTSIDE
   WEGSTEIN MAXIT=100
   DIRECT MAXIT=100
   SECANT MAXIT=100
   BROYDEN MAXIT=100
   NEWTON MAXIT=100
   SQP MAXIT=200 MAXPASS=1000 TOL=0.005 MAXLSPASS=100  &
      NLIMIT=100 STEP-OPT=VALUE STEP-DIR=NEGATIVE  &
      OPT-METHOD=SQP DERIVATIVE=FORWARD CONST-ITER=200  &
      CONV-TEST=KKT

TEAR
   TEAR 13

STREAM-REPOR MOLEFLOW MOLEFRAC MASSFRAC PROPERTIES=IPE-1 IPE-
2  &
      IPE-3

REACTIONS R-1 POWERLAW
   REAC-DATA 1 PHASE=V
   REAC-DATA 2 PHASE=V
   REAC-DATA 3 PHASE=V
   RATE-CON 1 PRE-EXP=40400000. ACT-ENERGY=74300000. <J/kmol>
   RATE-CON 2 PRE-EXP=2300. ACT-ENERGY=27300000. <J/kmol>
   RATE-CON 3 PRE-EXP=90300000000. ACT-ENERGY=110000000. <J/kmol>
   STOIC 1 MIXED PROPENE -1. / CHLORINE -1. / AC 1. /  &
      HCL 1.
   STOIC 2 MIXED PROPENE -1. / CHLORINE -1. / 12DCP 1.
   STOIC 3 MIXED AC -1. / CHLORINE -1. / 13DCP-C 1. /  &
      HCL 1.
   POWLAW-EXP 1 MIXED PROPENE 1. / MIXED CHLORINE 1.
   POWLAW-EXP 2 MIXED PROPENE 1. / MIXED CHLORINE 1.
   POWLAW-EXP 3 MIXED AC 1. / MIXED CHLORINE 1.
;
;
;
```

OUTPUT STREAM SUMMARY-CONSTRAINED OPTIMIZATION-ADIABATIC PFR

	1	2	3	4	5	6	7	8	9
Temperature F	80	654.4	80	624.2	926.6	70	178.1	-43.2	117.9
Pressure psia	74.7	74.7	74.7	74.7	34.72	74.7	27	20	16
Vapor Frac	1	1	1	1	1	0.812	0	1	1
Mole Flow lbmol/hr	135.68	1000.00	166.00	1166.00	1138.15	1138.15	134.90	1003.25	76.65
Mass Flow lb/hr	5709.46	42080.64	11770.30	53850.94	53851.22	53851.22	12383.61	41467.62	5865.64
Mass Flow lb/hr	5709.46	42080.64	11770.30	53850.94	53851.22	39103.09		41467.62	5865.64
Mass Flow lb/hr						14748.14	12383.61		
Volume Flow cuft/hr	9783.43	158935.23	12095.54	180158.79	486931.79	65798.07	204.09	216752.28	28810.46
Volume Flow cuft/hr	9783.43	158935.23	12095.54	180158.79	486931.79	65517.78		216752.28	28810.46
Volume Flow cuft/hr						280.28	204.09		
Enthalpy MMBtu/hr	1.17	20.90	-0.03	20.87	20.87	-2.86	-3.84	0.46	0.03
Mole Flow lbmol/hr									
H2O	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
HCL	0.00	0.00	0.00	0.00	138.15	138.15	0.00	138.15	0.00
PROPENE	135.68	1000.00	0.00	1000.00	864.32	864.32	0.00	864.32	0.00
CHLORINE	0.00	0.00	166.00	166.00	0.00	0.00	0.00	0.00	0.00
AC	0.00	0.00	0.00	0.00	77.50	77.50	76.73	0.78	76.65
12DCP	0.00	0.00	0.00	0.00	27.85	27.85	27.85	0.00	0.00
13DCP-C	0.00	0.00	0.00	0.00	30.33	30.33	30.33	0.00	0.00
13DCP-T	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
H+	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
CL-	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

	10	11	12	13	14	15	16	17	18
Temperature F	246.7	84.2	84.2	268.2	243.6	70	83.6	102.3	-43.2
Pressure psia	25	14.7	14.7	90	74.7	14.7	14.7	14.7	20
Vapor Frac	0	0	1	1	1	0	1	0	1
Mole Flow lbmol/hr	58.25	35.45	864.32	864.32	1000.00	551.71	899.78	689.86	1002.47
Mass Flow lb/hr	6517.97	638.72	36371.18	36371.18	42080.64	9939.19	37009.90	14976.33	41408.31
Mass Flow lb/hr \			36371.18	36371.18	42080.64		37009.90		41408.31
Mass Flow lb/hr	6517.97	638.72				9939.19		14976.33	
Volume Flow cuft/hr	99.50	10.34	338755.83	72421.47	97822.17	159.73	352223.69	259.53	216592.34
Volume Flow cuft/hr			338755.83	72421.47	97822.17		352223.69		216592.34
Volume Flow cuft/hr	99.50	10.34				159.73		259.53	
Enthalpy MMBtu/hr	-2.97	-4.35	7.65	10.33	11.50	-67.87	3.96	-75.72	0.47
Mole Flow lbmol/hr									
H2O	0.00	35.45	0.00	0.00	0.00	551.71	35.45	551.71	0.00
HCL	0.00	0.00	0.00	0.00	0.00	0.00	0.00	138.15	138.15
PROPENE	0.00	0.00	864.32	864.32	1000.00	0.00	864.32	0.00	864.32
CHLORINE	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
AC	0.08	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
12DCP	27.85	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
13DCP-C	30.33	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
13DCP-T	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
H+	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
CL-	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

	19	32
Temperature F	-43.2	70.9
Pressure psia	20	14.7
Vapor Frac	0	0
Mole Flow lbmol/hr	0.78	587.16
Mass Flow lb/hr	59.31	10577.91
Mass Flow lb/hr		
Mass Flow lb/hr	59.31	10577.91
Volume Flow cuft/hr	0.94	170.07
Volume Flow cuft/hr		
Volume Flow cuft/hr	0.94	170.07
Enthalpy MMBtu/hr	-0.01	-72.22
Mole Flow lbmol/hr		
H2O	0.00	587.16
HCL	0.00	0.00
PROPENE	0.00	0.00
CHLORINE	0.00	0.00
AC	0.78	0.00
12DCP	0.00	0.00
13DCP-C	0.00	0.00
13DCP-T	0.00	0.00
H+	0.00	0.00
CL-	0.00	0.00

INPUT SUMMARY-BASE CASE-ISOTHERMAL PFR

```
TITLE 'ALLYL CHLORIDE -Adiabatic PFR'
IN-UNITS ENG
DEF-STREAMS CONVEN ALL
SIM-OPTIONS OLD-DATABANK=YES
RUN-CONTROL MAX-TIME=100000. MAX-ERRORS=500

DESCRIPTION "
   General Simulation with English Units :
   F, psi, lb/hr, lbmol/hr, Btu/hr, cuft/hr.
   Property Method: None
   Flow basis for input: Mole
   Stream report composition: Mole flow

DATABANKS ASPENPCD  / AQUEOUS  / SOLIDS  / INORGANIC  /  &
      PURE22  / PURE10

PROP-SOURCES ASPENPCD  / AQUEOUS  / SOLIDS  / INORGANIC  /  &
      PURE22  / PURE10

COMPONENTS
   H2O H2O /
   HCL HCL /
   PROPENE C3H6-2 /
   CHLORINE CL2 /
   AC C3H5CL /
   12DCP C3H6CL2 /
   13DCP-C C3H4CL2-D1 /
   13DCP-T C3H4CL2-D2 /
   H+ H+ /
   CL- CL-

HENRY-COMPS HENRY CHLORINE HCL PROPENE

SOLVE
   RUN-MODE MODE=OPT

CHEMISTRY HCL
   STOIC 1 HCL -1 / H+ 1 / CL- 1

FLOWSHEET
   BLOCK B2 IN=14 OUT=2
   BLOCK B8 IN=1 13 OUT=14
   BLOCK B3 IN=2 3 OUT=4
   BLOCK B6 IN=4 OUT=5
```

```
   BLOCK B9 IN=5 OUT=6
   BLOCK B7 IN=6 OUT=8 7
   BLOCK B5 IN=7 OUT=9 10
   BLOCK B10 IN=18 32 OUT=16 17
   BLOCK B1 IN=16 OUT=12 11
   BLOCK B11 IN=8 OUT=18 19
   BLOCK B4 IN=12 OUT=13
   BLOCK B18 IN=15 11 OUT=32

PROPERTIES SYSOP0
   PROPERTIES ELECNRTL / UNIQ-RK / UNIQUAC

STRUCTURES
   STRUCTURES 13DCP-C CL1 C2 S / C2 C3 D / C3 C4 S /  &
      C4 CL5 S

ESTIMATE ALL

PROP-DATA PCES-1
   IN-UNITS ENG
   PROP-LIST DGAQHG / DHAQHG / S25HG / OMEGHG / DHVLB /  &
      VB / RGYR / VLSTD
   PVAL CHLORINE 2983.662941 / -10060.18917 / 28.90035349 /  &
      -17580.05159 / 8784.000000 / .7262124822 /  &
      3.2391732E-10 / .8579136616
   PROP-LIST DHVLB / VB / RGYR
   PVAL 13DCP-C 14431.51333 / 1.612466586 / 1.11089239E-9

PROP-DATA HENRY-1
   IN-UNITS ENG
   PROP-LIST HENRY
   BPVAL HCL H2O -49.78140336 2186.999983 8.370700000  &
      -5.3294445E-3 -3.999995968 68.00000346 0.0
   BPVAL CHLORINE H2O -116.9781387 4371.515965 19.18540000  &
      -4.9558834E-3 49.73000360 103.7300032 0.0
   BPVAL HCL 12DCP 10.00798341 -2648.879936 0.0 0.0  &
      -4.269995966 67.73000346 0.0
   BPVAL PROPENE H2O 326.3806995 -28021.26578 -41.73762000 0.0  &
      69.53000344 220.7300022 0.0
   BPVAL PROPENE 12DCP 12.93988341 -3932.459880 0.0 0.0  &
      -4.269995966 67.73000346 0.0

PROP-DATA UNIQ-1
   IN-UNITS ENG
   PROP-LIST UNIQ
   BPVAL H2O AC -4.247000000 2292.652782 0.0 0.0 109.9400031  &
```

```
      212.0000023 0.0
   BPVAL AC H2O 15.46800000 -10062.08074 0.0 0.0 109.9400031  &
      212.0000023 0.0
   BPVAL H2O 12DCP 0.0 -539.9468957 0.0 0.0 77.00000338  &
      77.00000338 0.0
   BPVAL 12DCP H2O 0.0 -2498.536780 0.0 0.0 77.00000338  &
      77.00000338 0.0

PROP-DATA VLCLK-1
   IN-UNITS ENG
   PROP-LIST VLCLK
   BPVAL H+ CL- .5534556926 .2140997389

PROP-DATA GMELCC-1
   IN-UNITS ENG
   PROP-LIST GMELCC
   PPVAL H2O ( H+ CL- ) 41.67400000
   PPVAL ( H+ CL- ) H2O -22.15400000
   PPVAL HCL ( H+ CL- ) 1.00000000E-3
   PPVAL ( H+ CL- ) HCL -1.0000000E-3

PROP-DATA GMELCD-1
   IN-UNITS ENG
   PROP-LIST GMELCD
   PPVAL H2O ( H+ CL- ) 9581.579923
   PPVAL ( H+ CL- ) H2O -3967.379968

PROP-DATA GMELCE-1
   IN-UNITS ENG
   PROP-LIST GMELCE
   PPVAL H2O ( H+ CL- ) -5.404000000
   PPVAL ( H+ CL- ) H2O 5.188000000

PROP-DATA GMELCN-1
   IN-UNITS ENG
   PROP-LIST GMELCN
   PPVAL H2O ( H+ CL- ) .0283500000

PCES-PROP-DATA
   IN-UNITS ENG
   GAMINF H2O 12DCP * * 68 2340 / * * 86 2310 / * *  &
      104 2090

PCES-PROP-DATA
   IN-UNITS ENG
   GAMINF H2O 13DCP-C * * 68 1360 / * * 86 1430 / * *  &
```

```
      104 1460

PROP-SET IPE-1 TEMP PRES MASSFLMX VOLFLMX MWMX MASSSFRA  &
      MASSVFRA MASSFLOW SUBSTREAM=ALL PHASE=T

PROP-SET IPE-2 CPMX MWMX MASSFLMX KMX SIGMAMX MUMX VOLFLMX
&
      UNITS='J/kg-K' SUBSTREAM=MIXED PHASE=L

PROP-SET IPE-3 VOLFLMX CPMX MUMX KMX MWMX MASSFLMX UNITS= &
      'J/kg-K' SUBSTREAM=MIXED PHASE=V

STREAM 1
   SUBSTREAM MIXED TEMP=80. PRES=74.7
   MOLE-FLOW PROPENE 1000.

STREAM 3
   SUBSTREAM MIXED TEMP=80. PRES=74.7
   MOLE-FLOW CHLORINE 166.

STREAM 15
   SUBSTREAM MIXED TEMP=70. PRES=14.7
   MOLE-FLOW H2O 325.

BLOCK B3 MIXER
   PROPERTIES UNIQ-RK FREE-WATER=STEAM-TA SOLU-WATER=3  &
      TRUE-COMPS=YES

BLOCK B8 MIXER
   PROPERTIES UNIQ-RK FREE-WATER=STEAM-TA SOLU-WATER=3  &
      TRUE-COMPS=YES

BLOCK B18 MIXER

BLOCK B1 SEP
   PARAM
   FRAC STREAM=12 SUBSTREAM=MIXED COMPS=PROPENE FRACS=1.
   PROPERTIES UNIQ-RK FREE-WATER=STEAM-TA SOLU-WATER=3  &
      TRUE-COMPS=YES

BLOCK B11 SEP
   PARAM
   FRAC STREAM=18 SUBSTREAM=MIXED COMPS=H2O HCL PROPENE  &
      CHLORINE AC 12DCP 13DCP-C 13DCP-T H+ CL- FRACS=1. 1.  &
      1. 1. 0. 0. 0. 0. 1. 1.
   PROPERTIES UNIQ-RK FREE-WATER=STEAM-TA SOLU-WATER=3  &
```

```
      TRUE-COMPS=YES

BLOCK B2 HEATER
   PARAM TEMP=700. PRES=74.7
   PROPERTIES UNIQ-RK FREE-WATER=STEAM-TA SOLU-WATER=3  &
      TRUE-COMPS=YES

BLOCK B9 HEATER
   PARAM TEMP=70. PRES=74.7
   PROPERTIES UNIQ-RK FREE-WATER=STEAM-TA SOLU-WATER=3  &
      TRUE-COMPS=YES

BLOCK B5 RADFRAC
   PARAM NSTAGE=15
   COL-CONFIG CONDENSER=PARTIAL-V
   FEEDS 7 6
   PRODUCTS 9 1 V / 10 15 L
   P-SPEC 1 16. / 15 25.
   COL-SPECS D:F=0.539038 MOLE-RR=4.02554
   SPEC 1 MOLE-RECOV 0.999 COMPS=AC STREAMS=9 BASE-STREAMS=7
   VARY 1 D:F 0.01 0.99
   PROPERTIES UNIQ-RK FREE-WATER=STEAM-TA SOLU-WATER=3  &
      TRUE-COMPS=YES

BLOCK B7 RADFRAC
   PARAM NSTAGE=15 ALGORITHM=STANDARD INIT-OPTION=STANDARD
&
      MAXOL=150 DAMPING=NONE
   COL-CONFIG CONDENSER=PARTIAL-V
   FEEDS 6 7
   PRODUCTS 8 1 V / 7 15 L
   P-SPEC 1 20. / 15 27.
   COL-SPECS D:F=0.8 MOLE-RR=0.4084
   SPEC 1 MOLE-RECOV 0.99 COMPS=AC STREAMS=7
   VARY 1 D:F 0.01 0.99
   PROPERTIES UNIQ-RK FREE-WATER=STEAM-TA SOLU-WATER=3  &
      TRUE-COMPS=YES

BLOCK B10 RADFRAC
   PARAM NSTAGE=10 ALGORITHM=NONIDEAL INIT-OPTION=STANDARD  &
      MAXOL=100 MAXIL=50
   COL-CONFIG CONDENSER=NONE REBOILER=NONE
   FEEDS 18 10 ON-STAGE / 32 1
   PRODUCTS 17 10 L / 16 1 V
   P-SPEC 1 14.7
   COL-SPECS
```

```
   T-EST 1 110. / 10 68.
   PROPERTIES ELECNRTL HENRY-COMPS=HENRY CHEMISTRY=HCL  &
      FREE-WATER=STEAM-TA SOLU-WATER=3 TRUE-COMPS=NO

BLOCK B6 RPLUG
   PARAM TYPE=T-SPEC LENGTH=20. DIAM=6. PRES=40.  &
      INT-TOL=1E-005
   T-SPEC 0.0 510. <C>
   COOLANT MAXIT=50
   PROPERTIES UNIQ-RK FREE-WATER=STEAM-TA SOLU-WATER=3  &
      TRUE-COMPS=YES / SYSOP0
   REACTIONS RXN-IDS=R-1

BLOCK B4 COMPR
   PARAM TYPE=ASME-POLYTROP PRES=90.
   PROPERTIES UNIQ-RK FREE-WATER=STEAM-TA SOLU-WATER=3  &
      TRUE-COMPS=YES

DESIGN-SPEC FEED
   DEFINE S14 MOLE-FLOW STREAM=14 SUBSTREAM=MIXED  &
      COMPONENT=PROPENE
   SPEC "S14" TO "1000"
   TOL-SPEC "0.01"
   VARY MOLE-FLOW STREAM=1 SUBSTREAM=MIXED
COMPONENT=PROPENE
   LIMITS "5" "1000"

DESIGN-SPEC H20
   DEFINE HCL18 MASS-FLOW STREAM=18 SUBSTREAM=MIXED  &
      COMPONENT=HCL
   DEFINE H2032 MASS-FLOW STREAM=32 SUBSTREAM=MIXED  &
      COMPONENT=H2O
   SPEC "H2032" TO "2.1*HCL18"
   TOL-SPEC ".001"
   VARY STREAM-VAR STREAM=15 SUBSTREAM=MIXED VARIABLE=MASS-
FLOW
   LIMITS "10" "60000"

DESIGN-SPEC RESTM
   DEFINE RESTM BLOCK-VAR BLOCK=B6 VARIABLE=RES-TIME  &
      SENTENCE=PARAM
   SPEC "RESTM" TO "1.11E-3"
   TOL-SPEC ".0001"
   VARY BLOCK-VAR BLOCK=B6 VARIABLE=LENGTH SENTENCE=PARAM
   LIMITS "1" "200"
```

```
TEAR
   TEAR 13

STREAM-REPOR MOLEFLOW MOLEFRAC MASSFRAC PROPERTIES=IPE-1 IPE-
2  &
      IPE-3

REACTIONS R-1 POWERLAW
   REAC-DATA 1 PHASE=V
   REAC-DATA 2 PHASE=V
   REAC-DATA 3 PHASE=V
   RATE-CON 1 PRE-EXP=40400000. ACT-ENERGY=74300000. <J/kmol>
   RATE-CON 2 PRE-EXP=2300. ACT-ENERGY=27300000. <J/kmol>
   RATE-CON 3 PRE-EXP=90300000000. ACT-ENERGY=110000000. <J/kmol>
   STOIC 1 MIXED PROPENE -1. / CHLORINE -1. / AC 1. /  &
      HCL 1.
   STOIC 2 MIXED PROPENE -1. / CHLORINE -1. / 12DCP 1.
   STOIC 3 MIXED AC -1. / CHLORINE -1. / 13DCP-C 1. /  &
      HCL 1.
   POWLAW-EXP 1 MIXED PROPENE 1. / MIXED CHLORINE 1.
   POWLAW-EXP 2 MIXED PROPENE 1. / MIXED CHLORINE 1.
   POWLAW-EXP 3 MIXED AC 1. / MIXED CHLORINE 1.
```

OUTPUT STREAM SUMMARY-BASE CASE-ISOTHERMAL PFR

	1	2	3	4	5	6	7	8	9
Temperature F	80.00	700.00	80.00	668.10	959.70	70.00	178.60	-43.50	117.90
Pressure psia	74.70	74.70	74.70	74.70	40.00	74.70	27.00	20.00	16.00
Vapor Frac	1.00	1.00	1.00	1.00	1.00	0.82	0.00	1.00	1.00
Mole Flow lbmol/hr	131.33	1000.00	166.00	1166.00	1144.02	1144.02	130.58	1013.44	73.83
Mass Flow lb/hr	5526.42	42080.64	11770.30	53850.94	53851.85	53851.85	11989.46	41862.39	5649.89
Mass Flow lb/hr	5526.42	42080.64	11770.30	53850.94	53851.85	39703.85		41862.39	5649.89
Mass Flow lb/hr						14148.00	11989.46		
Volume Flow cuft/hr	9469.78	165601.50	12095.54	187657.25	434972.28	66867.62	196.99	218819.11	27750.78
Volume Flow cuft/hr	9469.78	165601.50	12095.54	187657.25	434972.28	66599.96		218819.11	27750.78
Volume Flow cuft/hr						267.66	196.99		
Enthalpy MMBtu/hr	1.13	22.11	-0.03	22.09	22.09	-2.61	-3.45	0.25	0.03
Mole Flow lbmol/hr									
H2O	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
HCL	0.00	0.00	0.00	0.00	144.02	144.02	0.00	144.02	0.00
PROPENE	131.33	1000.00	0.00	1000.00	868.67	868.67	0.00	868.67	0.00
CHLORINE	0.00	0.00	166.00	166.00	0.00	0.00	0.00	0.00	0.00
AC	0.00	0.00	0.00	0.00	74.65	74.65	73.90	0.75	73.83
12DCP	0.00	0.00	0.00	0.00	21.99	21.99	21.99	0.00	0.00
13DCP-C	0.00	0.00	0.00	0.00	34.68	34.68	34.68	0.00	0.00
13DCP-T	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
H+	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
CL-	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

	10	11	12	13	14	15	16	17	18
Temperature F	248.00	85.70	85.70	269.80	245.70	70.00	85.00	104.70	-43.50
Pressure psia	25.00	14.70	14.70	90.00	74.70	14.70	14.70	14.70	20.00
Vapor Frac	0.00	0.00	1.00	1.00	1.00	0.00	1.00	0.00	1.00
Mole Flow lbmol/hr	56.75	37.45	868.67	868.67	1000.00	574.65	906.12	718.67	1012.69
Mass Flow lb/hr	6339.57	674.62	36554.22	36554.22	42080.64	10352.49	37228.85	15603.53	41805.26
Mass Flow lb/hr			36554.22	36554.22	42080.64		37228.85		41805.26
Mass Flow lb/hr	6339.57	674.62				10352.49		15603.53	
Volume Flow cuft/hr	96.32	10.93	341427.76	72961.37	98153.40	166.37	355715.51	271.72	218665.17
Volume Flow cuft/hr			341427.76	72961.37	98153.40		355715.51		218665.17
Volume Flow cuft/hr	96.32	10.93				166.37		271.72	
Enthalpy MMBtu/hr	-2.61	-4.60	7.71	10.41	11.54	-70.69	3.81	-78.84	0.26
Mole Flow lbmol/hr									
H2O	0.00	37.45	0.00	0.00	0.00	574.65	37.45	574.65	0.00
HCL	0.00	0.00	0.00	0.00	0.00	0.00	0.00	144.02	144.02
PROPENE	0.00	0.00	868.67	868.67	1000.00	0.00	868.67	0.00	868.67
CHLORINE	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
AC	0.07	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
12DCP	21.99	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
13DCP-C	34.68	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
13DCP-T	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
H+	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
CL-	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

	19	32
Temperature F	-43.50	71.00
Pressure psia	20.00	14.70
Vapor Frac	0.00	0.00
Mole Flow lbmol/hr	0.75	612.10
Mass Flow lb/hr	57.13	11027.12
Mass Flow lb/hr		
Mass Flow lb/hr	57.13	11027.12
Volume Flow cuft/hr	0.90	177.30
Volume Flow cuft/hr		
Volume Flow cuft/hr	0.90	177.30
Enthalpy MMBtu/hr	-0.01	-75.29
Mole Flow lbmol/hr		
H2O	0.00	612.10
HCL	0.00	0.00
PROPENE	0.00	0.00
CHLORINE	0.00	0.00
AC	0.75	0.00
12DCP	0.00	0.00
13DCP-C	0.00	0.00
13DCP-T	0.00	0.00
H+	0.00	0.00
CL-	0.00	0.00

INPUT SUMMARY-CONSTRAINED OPTIMIZATION-ISOTHERMAL PFR

```
TITLE 'ALLYL CHLORIDE -Adiabatic PFR'
IN-UNITS ENG
DEF-STREAMS CONVEN ALL
SIM-OPTIONS OLD-DATABANK=YES
RUN-CONTROL MAX-TIME=100000. MAX-ERRORS=500
DESCRIPTION "
   General Simulation with English Units :
   F, psi, lb/hr, lbmol/hr, Btu/hr, cuft/hr.
   Property Method: None
   Flow basis for input: Mole
   Stream report composition: Mole flow

DATABANKS ASPENPCD  / AQUEOUS  / SOLIDS  / INORGANIC  /  &
      PURE22  / PURE10

PROP-SOURCES ASPENPCD  / AQUEOUS  / SOLIDS  / INORGANIC  /  &
      PURE22  / PURE10

COMPONENTS
   H2O H2O /
   HCL HCL /
   PROPENE C3H6-2 /
   CHLORINE CL2 /
   AC C3H5CL /
   12DCP C3H6CL2 /
   13DCP-C C3H4CL2-D1 /
   13DCP-T C3H4CL2-D2 /
   H+ H+ /
   CL- CL-

HENRY-COMPS HENRY CHLORINE HCL PROPENE

SOLVE
   RUN-MODE MODE=OPT

CHEMISTRY HCL
   STOIC 1 HCL -1 / H+ 1 / CL- 1

FLOWSHEET
   BLOCK B2 IN=14 OUT=2
   BLOCK B8 IN=1 13 OUT=14
   BLOCK B3 IN=2 3 OUT=4
   BLOCK B6 IN=4 OUT=5
   BLOCK B9 IN=5 OUT=6
```

```
   BLOCK B7 IN=6 OUT=8 7
   BLOCK B5 IN=7 OUT=9 10
   BLOCK B10 IN=18 32 OUT=16 17
   BLOCK B1 IN=16 OUT=12 11
   BLOCK B11 IN=8 OUT=18 19
   BLOCK B4 IN=12 OUT=13
   BLOCK B18 IN=15 11 OUT=32

PROPERTIES SYSOP0
   PROPERTIES ELECNRTL / UNIQ-RK / UNIQUAC

STRUCTURES
   STRUCTURES 13DCP-C CL1 C2 S / C2 C3 D / C3 C4 S /  &
      C4 CL5 S

ESTIMATE ALL

PROP-DATA PCES-1
   IN-UNITS ENG
   PROP-LIST DGAQHG / DHAQHG / S25HG / OMEGHG / DHVLB /  &
      VB / RGYR / VLSTD
   PVAL CHLORINE 2983.662941 / -10060.18917 / 28.90035349 /  &
      -17580.05159 / 8784.000000 / .7262124822 /  &
      3.2391732E-10 / .8579136616
   PROP-LIST DHVLB / VB / RGYR
   PVAL 13DCP-C 14431.51333 / 1.612466586 / 1.11089239E-9

PROP-DATA HENRY-1
   IN-UNITS ENG
   PROP-LIST HENRY
   BPVAL HCL H2O -49.78140336 2186.999983 8.370700000  &
      -5.3294445E-3 -3.999995968 68.00000346 0.0
   BPVAL CHLORINE H2O -116.9781387 4371.515965 19.18540000  &
      -4.9558834E-3 49.73000360 103.7300032 0.0
   BPVAL HCL 12DCP 10.00798341 -2648.879936 0.0 0.0  &
      -4.269995966 67.73000346 0.0
   BPVAL PROPENE H2O 326.3806995 -28021.26578 -41.73762000 0.0  &
      69.53000344 220.7300022 0.0
   BPVAL PROPENE 12DCP 12.93988341 -3932.459880 0.0 0.0  &
      -4.269995966 67.73000346 0.0

PROP-DATA UNIQ-1
   IN-UNITS ENG
   PROP-LIST UNIQ
   BPVAL H2O AC -4.247000000 2292.652782 0.0 0.0 109.9400031  &
      212.0000023 0.0
```

```
   BPVAL AC H2O 15.46800000 -10062.08074 0.0 0.0 109.9400031  &
      212.0000023 0.0
   BPVAL H2O 12DCP 0.0 -539.9468957 0.0 0.0 77.00000338  &
      77.00000338 0.0
   BPVAL 12DCP H2O 0.0 -2498.536780 0.0 0.0 77.00000338  &
      77.00000338 0.0

PROP-DATA VLCLK-1
   IN-UNITS ENG
   PROP-LIST VLCLK
   BPVAL H+ CL- .5534556926 .2140997389

PROP-DATA GMELCC-1
   IN-UNITS ENG
   PROP-LIST GMELCC
   PPVAL H2O ( H+ CL- ) 41.67400000
   PPVAL ( H+ CL- ) H2O -22.15400000
   PPVAL HCL ( H+ CL- ) 1.00000000E-3
   PPVAL ( H+ CL- ) HCL -1.0000000E-3

PROP-DATA GMELCD-1
   IN-UNITS ENG
   PROP-LIST GMELCD
   PPVAL H2O ( H+ CL- ) 9581.579923
   PPVAL ( H+ CL- ) H2O -3967.379968

PROP-DATA GMELCE-1
   IN-UNITS ENG
   PROP-LIST GMELCE
   PPVAL H2O ( H+ CL- ) -5.404000000
   PPVAL ( H+ CL- ) H2O 5.188000000

PROP-DATA GMELCN-1
   IN-UNITS ENG
   PROP-LIST GMELCN
   PPVAL H2O ( H+ CL- ) .0283500000

PCES-PROP-DATA
   IN-UNITS ENG
   GAMINF H2O 12DCP * * 68 2340 / * * 86 2310 / * *  &
      104 2090

PCES-PROP-DATA
   IN-UNITS ENG
   GAMINF H2O 13DCP-C * * 68 1360 / * * 86 1430 / * *  &
      104 1460
```

```
PROP-SET IPE-1 TEMP PRES MASSFLMX VOLFLMX MWMX MASSSFRA  &
      MASSVFRA MASSFLOW SUBSTREAM=ALL PHASE=T

PROP-SET IPE-2 CPMX MWMX MASSFLMX KMX SIGMAMX MUMX VOLFLMX
&
      UNITS='J/kg-K' SUBSTREAM=MIXED PHASE=L

PROP-SET IPE-3 VOLFLMX CPMX MUMX KMX MWMX MASSFLMX UNITS= &
      'J/kg-K' SUBSTREAM=MIXED PHASE=V

STREAM 1
   SUBSTREAM MIXED TEMP=80. PRES=74.7
   MOLE-FLOW PROPENE 1000.

STREAM 3
   SUBSTREAM MIXED TEMP=80. PRES=74.7
   MOLE-FLOW CHLORINE 166.

STREAM 15
   SUBSTREAM MIXED TEMP=70. PRES=14.7
   MOLE-FLOW H2O 325.

BLOCK B3 MIXER
   PROPERTIES UNIQ-RK FREE-WATER=STEAM-TA SOLU-WATER=3  &
      TRUE-COMPS=YES

BLOCK B8 MIXER
   PROPERTIES UNIQ-RK FREE-WATER=STEAM-TA SOLU-WATER=3  &
      TRUE-COMPS=YES

BLOCK B18 MIXER

BLOCK B1 SEP
   PARAM
   FRAC STREAM=12 SUBSTREAM=MIXED COMPS=PROPENE FRACS=1.
   PROPERTIES UNIQ-RK FREE-WATER=STEAM-TA SOLU-WATER=3  &
      TRUE-COMPS=YES

BLOCK B11 SEP
   PARAM
   FRAC STREAM=18 SUBSTREAM=MIXED COMPS=H2O HCL PROPENE  &
      CHLORINE AC 12DCP 13DCP-C 13DCP-T H+ CL- FRACS=1. 1.  &
      1. 1. 0. 0. 0. 0. 1. 1.
   PROPERTIES UNIQ-RK FREE-WATER=STEAM-TA SOLU-WATER=3  &
      TRUE-COMPS=YES
```

```
BLOCK B2 HEATER
   PARAM TEMP=700. PRES=74.7
   PROPERTIES UNIQ-RK FREE-WATER=STEAM-TA SOLU-WATER=3  &
      TRUE-COMPS=YES

BLOCK B9 HEATER
   PARAM TEMP=70. PRES=74.7
   PROPERTIES UNIQ-RK FREE-WATER=STEAM-TA SOLU-WATER=3  &
      TRUE-COMPS=YES

BLOCK B5 RADFRAC
   PARAM NSTAGE=15
   COL-CONFIG CONDENSER=PARTIAL-V
   FEEDS 7 6
   PRODUCTS 9 1 V / 10 15 L
   P-SPEC 1 16. / 15 25.
   COL-SPECS D:F=0.539038 MOLE-RR=4.02554
   SPEC 1 MOLE-RECOV 0.999 COMPS=AC STREAMS=9 BASE-STREAMS=7
   VARY 1 D:F 0.01 0.99
   PROPERTIES UNIQ-RK FREE-WATER=STEAM-TA SOLU-WATER=3  &
      TRUE-COMPS=YES

BLOCK B7 RADFRAC
   PARAM NSTAGE=15 ALGORITHM=STANDARD INIT-OPTION=STANDARD
&
      MAXOL=150 DAMPING=NONE
   COL-CONFIG CONDENSER=PARTIAL-V
   FEEDS 6 7
   PRODUCTS 8 1 V / 7 15 L
   P-SPEC 1 20. / 15 27.
   COL-SPECS D:F=0.8 MOLE-RR=0.4084
   SPEC 1 MOLE-RECOV 0.99 COMPS=AC STREAMS=7
   VARY 1 D:F 0.01 0.99
   PROPERTIES UNIQ-RK FREE-WATER=STEAM-TA SOLU-WATER=3  &
      TRUE-COMPS=YES

BLOCK B10 RADFRAC
   PARAM NSTAGE=10 ALGORITHM=NONIDEAL INIT-OPTION=STANDARD  &
      MAXOL=100 MAXIL=50
   COL-CONFIG CONDENSER=NONE REBOILER=NONE
   FEEDS 18 10 ON-STAGE / 32 1
   PRODUCTS 17 10 L / 16 1 V
   P-SPEC 1 14.7
   COL-SPECS
   T-EST 1 110. / 10 68.
```

```
   PROPERTIES ELECNRTL HENRY-COMPS=HENRY CHEMISTRY=HCL  &
      FREE-WATER=STEAM-TA SOLU-WATER=3 TRUE-COMPS=NO

BLOCK B6 RPLUG
   PARAM TYPE=ADIABATIC LENGTH=20. DIAM=6. PRES=40.  &
      INT-TOL=1E-005
   COOLANT MAXIT=50
   PROPERTIES UNIQ-RK FREE-WATER=STEAM-TA SOLU-WATER=3  &
      TRUE-COMPS=YES / SYSOP0
   REACTIONS RXN-IDS=R-1

BLOCK B4 COMPR
   PARAM TYPE=ASME-POLYTROP PRES=90.
   PROPERTIES UNIQ-RK FREE-WATER=STEAM-TA SOLU-WATER=3  &
      TRUE-COMPS=YES

DESIGN-SPEC FEED
   DEFINE S14 MOLE-FLOW STREAM=14 SUBSTREAM=MIXED  &
      COMPONENT=PROPENE
   SPEC "S14" TO "1000"
   TOL-SPEC "0.01"
   VARY MOLE-FLOW STREAM=1 SUBSTREAM=MIXED
COMPONENT=PROPENE
   LIMITS "5" "1000"

DESIGN-SPEC H20
   DEFINE HCL18 MASS-FLOW STREAM=18 SUBSTREAM=MIXED  &
      COMPONENT=HCL
   DEFINE H2032 MASS-FLOW STREAM=32 SUBSTREAM=MIXED  &
      COMPONENT=H2O
   SPEC "H2032" TO "2.1*HCL18"
   TOL-SPEC ".001"
   VARY STREAM-VAR STREAM=15 SUBSTREAM=MIXED VARIABLE=MASS-
FLOW
   LIMITS "10" "60000"

DESIGN-SPEC RESTM
   DEFINE RESTM BLOCK-VAR BLOCK=B6 VARIABLE=RES-TIME  &
      SENTENCE=PARAM
   SPEC "RESTM" TO "1.11E-3"
   TOL-SPEC ".0001"
   VARY BLOCK-VAR BLOCK=B6 VARIABLE=LENGTH SENTENCE=PARAM
   LIMITS "1" "200"

EO-CONV-OPTI
```

```
CONSTRAINT EMY
   DEFINE AC9 MASS-FLOW STREAM=9 SUBSTREAM=MIXED
COMPONENT=AC
   DEFINE HCL17 STREAM-VAR STREAM=17 SUBSTREAM=MIXED  &
      VARIABLE=MASS-FLOW
   DEFINE CL3 MASS-FLOW STREAM=3 SUBSTREAM=MIXED  &
      COMPONENT=CHLORINE
   DEFINE PROP1 MASS-FLOW STREAM=1 SUBSTREAM=MIXED  &
      COMPONENT=PROPENE
   DEFINE H2015 MASS-FLOW STREAM=15 SUBSTREAM=MIXED  &
      COMPONENT=H2O
   DEFINE FDHTR BLOCK-VAR BLOCK=B2 VARIABLE=QCALC  &
      SENTENCE=PARAM
   DEFINE REB1 BLOCK-VAR BLOCK=B7 VARIABLE=REB-DUTY  &
      SENTENCE=RESULTS
   DEFINE REB2 BLOCK-VAR BLOCK=B5 VARIABLE=REB-DUTY  &
      SENTENCE=RESULTS
   DEFINE COMP BLOCK-VAR BLOCK=B4 VARIABLE=BRAKE-POWER  &
      SENTENCE=RESULTS
   DEFINE COOL1 BLOCK-VAR BLOCK=B9 VARIABLE=QCALC  &
      SENTENCE=PARAM
   DEFINE COND1 BLOCK-VAR BLOCK=B7 VARIABLE=COND-DUTY  &
      SENTENCE=RESULTS
   DEFINE COND2 BLOCK-VAR BLOCK=B5 VARIABLE=COND-DUTY  &
      SENTENCE=RESULTS
   DEFINE MASSEP MASS-FLOW STREAM=4 SUBSTREAM=MIXED  &
      COMPONENT=PROPENE
   DEFINE MASSEC MASS-FLOW STREAM=4 SUBSTREAM=MIXED  &
      COMPONENT=CHLORINE
   DEFINE MASSXP MASS-FLOW STREAM=5 SUBSTREAM=MIXED  &
      COMPONENT=PROPENE
   DEFINE MASSXC MASS-FLOW STREAM=5 SUBSTREAM=MIXED  &
      COMPONENT=CHLORINE
   DEFINE DCP10 STREAM-VAR STREAM=10 SUBSTREAM=MIXED  &
      VARIABLE=MASS-FLOW
   DEFINE B6TO BLOCK-VAR BLOCK=B6 VARIABLE=REAC-TEMP  &
      SENTENCE=GENPROF ID1=5
   DEFINE PROFIT LOCAL-PARAM PHYS-QTY=UNIT-PRICE UOM="$/lb"  &
      INIT-VAL=0.
   DEFINE PROP2 MOLE-FLOW STREAM=2 SUBSTREAM=MIXED  &
      COMPONENT=PROPENE
   DEFINE T4 STREAM-VAR STREAM=4 SUBSTREAM=MIXED
VARIABLE=TEMP
   DEFINE CL3M STREAM-VAR STREAM=3 SUBSTREAM=MIXED  &
      VARIABLE=MOLE-FLOW
```

```
   DEFINE AC5 MOLE-FLOW STREAM=5 SUBSTREAM=MIXED
COMPONENT=AC
   DEFINE DC25 MOLE-FLOW STREAM=5 SUBSTREAM=MIXED  &
      COMPONENT=12DCP
   DEFINE DC35 MOLE-FLOW STREAM=5 SUBSTREAM=MIXED  &
      COMPONENT=13DCP-C
   DEFINE MCL4 MASS-FLOW STREAM=4 SUBSTREAM=MIXED  &
      COMPONENT=CHLORINE
   DEFINE MP4 MASS-FLOW STREAM=4 SUBSTREAM=MIXED  &
      COMPONENT=PROPENE
   DEFINE MCL5 MASS-FLOW STREAM=5 SUBSTREAM=MIXED  &
      COMPONENT=CHLORINE
   DEFINE MP5 MASS-FLOW STREAM=5 SUBSTREAM=MIXED  &
      COMPONENT=PROPENE
   DEFINE WST12D MASS-FLOW STREAM=10 SUBSTREAM=MIXED  &
      COMPONENT=12DCP
   DEFINE WST13D MASS-FLOW STREAM=10 SUBSTREAM=MIXED  &
      COMPONENT=13DCP-C
   DEFINE HCL5M MASS-FLOW STREAM=5 SUBSTREAM=MIXED  &
      COMPONENT=HCL
   DEFINE AC5M MASS-FLOW STREAM=5 SUBSTREAM=MIXED
COMPONENT=AC
F    REVAC=.88
F    REVHCL=0.0625
F    CSTCL2=.16
F    CSTPRP=.45
F    WSTC=.0011
F    REVENUE=REVAC*AC9+REVHCL*HCL17
F    RAWCST=CSTCL2*CL3+CSTPRP*PROP1
F    NGCST=FDHTR*.0000117
F    TOTST=REB1+REB2
F    STCST=TOTST*0.00001564
F    HTCST=STCST+NGCST
F    ELECST=0.0417*COMP
F    H20BTU=-(COOL1+COND1+COND2)
F    H2O1=(H20BTU/27)*.454*.016088*.00042
F    DIWCST=H2015*.454*.001
F    H20CST=DIWCST+H201
F    UTLCST=HTCST+ELECST+H20CST
F    WSTCST=DCP10*WSTC
F    HEALTH=4.6*WST12D+4.8*WST13D
F    EMY=(HCL5M+AC5M)/((MP4+MCL4+0.000001)-(MP5+MCl5))
F    PROFIT=REVENUE-RAWCST-UTLCST-WSTCST
F    FR=PROP2/CL3M
   SPEC "MP" EQ "0.6324"
   TOL-SPEC ".1"
```

```
CONSTRAINT HEALTH
   DEFINE AC9 MASS-FLOW STREAM=9 SUBSTREAM=MIXED
COMPONENT=AC
   DEFINE HCL17 STREAM-VAR STREAM=17 SUBSTREAM=MIXED  &
      VARIABLE=MASS-FLOW
   DEFINE CL3 MASS-FLOW STREAM=3 SUBSTREAM=MIXED  &
      COMPONENT=CHLORINE
   DEFINE PROP1 MASS-FLOW STREAM=1 SUBSTREAM=MIXED  &
      COMPONENT=PROPENE
   DEFINE H2015 MASS-FLOW STREAM=15 SUBSTREAM=MIXED  &
      COMPONENT=H2O
   DEFINE FDHTR BLOCK-VAR BLOCK=B2 VARIABLE=QCALC  &
      SENTENCE=PARAM
   DEFINE REB1 BLOCK-VAR BLOCK=B7 VARIABLE=REB-DUTY  &
      SENTENCE=RESULTS
   DEFINE REB2 BLOCK-VAR BLOCK=B5 VARIABLE=REB-DUTY  &
      SENTENCE=RESULTS
   DEFINE COMP BLOCK-VAR BLOCK=B4 VARIABLE=BRAKE-POWER  &
      SENTENCE=RESULTS
   DEFINE COOL1 BLOCK-VAR BLOCK=B9 VARIABLE=QCALC  &
      SENTENCE=PARAM
   DEFINE COND1 BLOCK-VAR BLOCK=B7 VARIABLE=COND-DUTY  &
      SENTENCE=RESULTS
   DEFINE COND2 BLOCK-VAR BLOCK=B5 VARIABLE=COND-DUTY  &
      SENTENCE=RESULTS
   DEFINE MASSEP MASS-FLOW STREAM=4 SUBSTREAM=MIXED  &
      COMPONENT=PROPENE
   DEFINE MASSEC MASS-FLOW STREAM=4 SUBSTREAM=MIXED  &
      COMPONENT=CHLORINE
   DEFINE MASSXP MASS-FLOW STREAM=5 SUBSTREAM=MIXED  &
      COMPONENT=PROPENE
   DEFINE MASSXC MASS-FLOW STREAM=5 SUBSTREAM=MIXED  &
      COMPONENT=CHLORINE
   DEFINE DCP10 STREAM-VAR STREAM=10 SUBSTREAM=MIXED  &
      VARIABLE=MASS-FLOW
   DEFINE B6TO BLOCK-VAR BLOCK=B6 VARIABLE=REAC-TEMP  &
      SENTENCE=GENPROF ID1=5
   DEFINE PROFIT LOCAL-PARAM PHYS-QTY=UNIT-PRICE UOM="$/lb"  &
      INIT-VAL=0.
   DEFINE PROP2 MOLE-FLOW STREAM=2 SUBSTREAM=MIXED  &
      COMPONENT=PROPENE
   DEFINE T4 STREAM-VAR STREAM=4 SUBSTREAM=MIXED
VARIABLE=TEMP
   DEFINE CL3M STREAM-VAR STREAM=3 SUBSTREAM=MIXED  &
```

```
      VARIABLE=MOLE-FLOW
   DEFINE AC5 MOLE-FLOW STREAM=5 SUBSTREAM=MIXED
COMPONENT=AC
   DEFINE DC25 MOLE-FLOW STREAM=5 SUBSTREAM=MIXED  &
      COMPONENT=12DCP
   DEFINE DC35 MOLE-FLOW STREAM=5 SUBSTREAM=MIXED  &
      COMPONENT=13DCP-C
   DEFINE MCL4 MASS-FLOW STREAM=4 SUBSTREAM=MIXED  &
      COMPONENT=CHLORINE
   DEFINE MP4 MASS-FLOW STREAM=4 SUBSTREAM=MIXED  &
      COMPONENT=PROPENE
   DEFINE MCL5 MASS-FLOW STREAM=5 SUBSTREAM=MIXED  &
      COMPONENT=CHLORINE
   DEFINE MP5 MASS-FLOW STREAM=5 SUBSTREAM=MIXED  &
      COMPONENT=PROPENE
   DEFINE WST12D MASS-FLOW STREAM=10 SUBSTREAM=MIXED  &
      COMPONENT=12DCP
   DEFINE WST13D MASS-FLOW STREAM=10 SUBSTREAM=MIXED  &
      COMPONENT=13DCP-C
   DEFINE HCL5M MASS-FLOW STREAM=5 SUBSTREAM=MIXED  &
      COMPONENT=HCL
   DEFINE AC5M MASS-FLOW STREAM=5 SUBSTREAM=MIXED
COMPONENT=AC
F    REVAC=.88
F    REVHCL=0.0625
F    CSTCL2=.16
F    CSTPRP=.45
F    WSTC=.0011
F    REVENUE=REVAC*AC9+REVHCL*HCL17
F    RAWCST=CSTCL2*CL3+CSTPRP*PROP1
F    NGCST=FDHTR*.0000117
F    TOTST=REB1+REB2
F    STCST=TOTST*0.00001564
F    HTCST=STCST+NGCST
F    ELECST=0.0417*COMP
F    H20BTU=-(COOL1+COND1+COND2)
F    H2O1=(H20BTU/27)*.454*.016088*.00042
F    DIWCST=H2015*.454*.001
F    H20CST=DIWCST+H201
F    UTLCST=HTCST+ELECST+H20CST
F    WSTCST=DCP10*WSTC
F    HEALTH=4.6*WST12D+4.8*WST13D
F    EMY=(HCL5M+AC5M)/((MP4+MCL4+0.000001)-(MP5+MCl5))
F    PROFIT=REVENUE-RAWCST-UTLCST-WSTCST
F    FR=PROP2/CL3M
   SPEC "HEALTH" EQ "29740.4"
```

```
   TOL-SPEC ".1"

OPTIMIZATION MAXPROFIT
   DEFINE AC9 MASS-FLOW STREAM=9 SUBSTREAM=MIXED
COMPONENT=AC
   DEFINE HCL17 STREAM-VAR STREAM=17 SUBSTREAM=MIXED  &
      VARIABLE=MASS-FLOW
   DEFINE CL3 MASS-FLOW STREAM=3 SUBSTREAM=MIXED  &
      COMPONENT=CHLORINE
   DEFINE PROP1 MASS-FLOW STREAM=1 SUBSTREAM=MIXED  &
      COMPONENT=PROPENE
   DEFINE H2015 MASS-FLOW STREAM=15 SUBSTREAM=MIXED  &
      COMPONENT=H2O
   DEFINE FDHTR BLOCK-VAR BLOCK=B2 VARIABLE=QCALC  &
      SENTENCE=PARAM
   DEFINE REB1 BLOCK-VAR BLOCK=B7 VARIABLE=REB-DUTY  &
      SENTENCE=RESULTS
   DEFINE REB2 BLOCK-VAR BLOCK=B5 VARIABLE=REB-DUTY  &
      SENTENCE=RESULTS
   DEFINE COMP BLOCK-VAR BLOCK=B4 VARIABLE=BRAKE-POWER  &
      SENTENCE=RESULTS
   DEFINE COOL1 BLOCK-VAR BLOCK=B9 VARIABLE=QCALC  &
      SENTENCE=PARAM
   DEFINE COND1 BLOCK-VAR BLOCK=B7 VARIABLE=COND-DUTY  &
      SENTENCE=RESULTS
   DEFINE COND2 BLOCK-VAR BLOCK=B5 VARIABLE=COND-DUTY  &
      SENTENCE=RESULTS
   DEFINE MASSEP MASS-FLOW STREAM=4 SUBSTREAM=MIXED  &
      COMPONENT=PROPENE
   DEFINE MASSEC MASS-FLOW STREAM=4 SUBSTREAM=MIXED  &
      COMPONENT=CHLORINE
   DEFINE MASSXP MASS-FLOW STREAM=5 SUBSTREAM=MIXED  &
      COMPONENT=PROPENE
   DEFINE MASSXC MASS-FLOW STREAM=5 SUBSTREAM=MIXED  &
      COMPONENT=CHLORINE
   DEFINE DCP10 STREAM-VAR STREAM=10 SUBSTREAM=MIXED  &
      VARIABLE=MASS-FLOW
   DEFINE B6TO BLOCK-VAR BLOCK=B6 VARIABLE=REAC-TEMP  &
      SENTENCE=GENPROF ID1=5
   DEFINE PROFIT LOCAL-PARAM PHYS-QTY=UNIT-PRICE UOM="$/lb"  &
      INIT-VAL=0.
   DEFINE PROP2 MOLE-FLOW STREAM=2 SUBSTREAM=MIXED  &
      COMPONENT=PROPENE
   DEFINE T4 STREAM-VAR STREAM=4 SUBSTREAM=MIXED
VARIABLE=TEMP
   DEFINE CL3M STREAM-VAR STREAM=3 SUBSTREAM=MIXED  &
```

```
      VARIABLE=MOLE-FLOW
   DEFINE AC5 MOLE-FLOW STREAM=5 SUBSTREAM=MIXED
COMPONENT=AC
   DEFINE DC25 MOLE-FLOW STREAM=5 SUBSTREAM=MIXED  &
      COMPONENT=12DCP
   DEFINE DC35 MOLE-FLOW STREAM=5 SUBSTREAM=MIXED  &
      COMPONENT=13DCP-C
   DEFINE MCL4 MASS-FLOW STREAM=4 SUBSTREAM=MIXED  &
      COMPONENT=CHLORINE
   DEFINE MP4 MASS-FLOW STREAM=4 SUBSTREAM=MIXED  &
      COMPONENT=PROPENE
   DEFINE MCL5 MASS-FLOW STREAM=5 SUBSTREAM=MIXED  &
      COMPONENT=CHLORINE
   DEFINE MP5 MASS-FLOW STREAM=5 SUBSTREAM=MIXED  &
      COMPONENT=PROPENE
   DEFINE WST12D MASS-FLOW STREAM=10 SUBSTREAM=MIXED  &
      COMPONENT=12DCP
   DEFINE WST13D MASS-FLOW STREAM=10 SUBSTREAM=MIXED  &
      COMPONENT=13DCP-C
   DEFINE HCL5M MASS-FLOW STREAM=5 SUBSTREAM=MIXED  &
      COMPONENT=HCL
   DEFINE AC5M MASS-FLOW STREAM=5 SUBSTREAM=MIXED
COMPONENT=AC
F    REVAC=.88
F    REVHCL=0.0625
F    CSTCL2=.16
F    CSTPRP=.45
F    WSTC=.0011
F    REVENUE=REVAC*AC9+REVHCL*HCL17
F    RAWCST=CSTCL2*CL3+CSTPRP*PROP1
F    NGCST=FDHTR*.0000117
F    TOTST=REB1+REB2
F    STCST=TOTST*0.00001564
F    HTCST=STCST+NGCST
F    ELECST=0.0417*COMP
F    H20BTU=-(COOL1+COND1+COND2)
F    H2O1=(H20BTU/27)*.454*.016088*.00042
F    DIWCST=H2015*.454*.001
F    H20CST=DIWCST+H201
F    UTLCST=HTCST+ELECST+H20CST
F    WSTCST=DCP10*WSTC
F    HEALTH=4.6*WST12D+4.8*WST13D
F    EMY=(HCL5M+AC5M)/((MP4+MCL4+0.000001)-(MP5+MCl5))
F    PROFIT=REVENUE-RAWCST-UTLCST-WSTCST
F    FR=PROP2/CL3M
   MAXIMIZE "PROFIT"
```

```
   CONSTRAINTS HEALTH
   VARY BLOCK-VAR BLOCK=B2 VARIABLE=TEMP SENTENCE=PARAM
   LIMITS "500" "900"
   VARY MOLE-FLOW STREAM=3 SUBSTREAM=MIXED
COMPONENT=CHLORINE
   LIMITS "166" "1000"
   VARY BLOCK-VAR BLOCK=B6 VARIABLE=PRES SENTENCE=PARAM
   LIMITS "15" "150"

CONV-OPTIONS
   PARAM OPT-METHOD=SQP SPEC-LOOP=INSIDE USER-LOOP=OUTSIDE
   WEGSTEIN MAXIT=100
   DIRECT MAXIT=100
   SECANT MAXIT=100
   BROYDEN MAXIT=100
   NEWTON MAXIT=100
   SQP MAXIT=200 MAXPASS=1000 TOL=0.005 MAXLSPASS=100  &
      NLIMIT=100 STEP-OPT=VALUE STEP-DIR=NEGATIVE  &
      OPT-METHOD=SQP DERIVATIVE=FORWARD CONST-ITER=200  &
      CONV-TEST=KKT

TEAR
   TEAR 13

STREAM-REPOR MOLEFLOW MOLEFRAC MASSFRAC PROPERTIES=IPE-1 IPE-
2  &
      IPE-3

REACTIONS R-1 POWERLAW
   REAC-DATA 1 PHASE=V
   REAC-DATA 2 PHASE=V
   REAC-DATA 3 PHASE=V
   RATE-CON 1 PRE-EXP=40400000. ACT-ENERGY=74300000. <J/kmol>
   RATE-CON 2 PRE-EXP=2300. ACT-ENERGY=27300000. <J/kmol>
   RATE-CON 3 PRE-EXP=90300000000. ACT-ENERGY=110000000. <J/kmol>
   STOIC 1 MIXED PROPENE -1. / CHLORINE -1. / AC 1. /  &
      HCL 1.
   STOIC 2 MIXED PROPENE -1. / CHLORINE -1. / 12DCP 1.
   STOIC 3 MIXED AC -1. / CHLORINE -1. / 13DCP-C 1. /  &
      HCL 1.
   POWLAW-EXP 1 MIXED PROPENE 1. / MIXED CHLORINE 1.
   POWLAW-EXP 2 MIXED PROPENE 1. / MIXED CHLORINE 1.
   POWLAW-EXP 3 MIXED AC 1. / MIXED CHLORINE 1.
```

OUTPUT STREAM SUMMARY-CONSTRAINED OPTIMIZATION-ISOTHERMAL PFR

	1	2	3	4	5	6	7	8	9
Temperature F	80.00	900.00	80.00	856.30	1148.50	70.00	192.30	-45.30	117.90
Pressure psia	74.70	74.70	74.70	74.70	37.46	74.70	27.00	20.00	16.00
Vapor Frac	1.00	1.00	1.00	1.00	1.00	0.83	0.00	1.00	1.00
Mole Flow lbmol/hr	126.09	1000.00	188.80	1188.80	1180.41	1180.41	125.54	1054.87	54.39
Mass Flow lb/hr	5306.06	42080.70	13386.62	55467.31	55467.39	55467.39	12072.79	43394.59	4162.40
Mass Flow lb/hr	5306.06	42080.70	13386.62	55467.31	55467.39	41035.39		43394.59	4162.40
Mass Flow lb/hr						14432.00	12072.79		
Volume Flow cuft/hr	9092.18	194740.93	13756.52	223952.84	543450.08	69847.08	191.81	226856.46	20444.61
Volume Flow cuft/hr	9092.18	194740.93	13756.52	223952.84	543450.08	69584.72		226856.46	20444.61
Volume Flow cuft/hr						262.36	191.81		
Enthalpy MMBtu/hr	1.09	27.79	-0.03	27.76	27.76	-3.48	-2.84	-1.21	0.02
Mole Flow lbmol/hr									
H2O	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
HCL	0.00	0.00	0.00	0.00	180.41	180.41	0.00	180.41	0.00
PROPENE	126.09	1000.00	0.00	1000.00	873.91	873.91	0.00	873.91	0.00
CHLORINE	0.00	0.00	188.80	188.80	0.00	0.00	0.00	0.00	0.00
AC	0.00	0.00	0.00	0.00	55.00	55.00	54.45	0.55	54.39
12DCP	0.00	0.00	0.00	0.00	8.39	8.39	8.39	0.00	0.00
13DCP-C	0.00	0.00	0.00	0.00	62.71	62.71	62.71	0.00	0.00
13DCP-T	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
H+	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
CL-	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

	10	11	12	13	14	15	16	17	18
Temperature F	252.20	94.50	94.50	279.10	255.00	70.00	93.80	119.00	-45.30
Pressure psia	25.00	14.70	14.70	90.00	74.70	14.70	14.70	14.70	20.00
Vapor Frac	0.00	0.00	1.00	1.00	1.00	0.00	1.00	0.00	1.00
Mole Flow lbmol/hr	71.15	50.30	873.91	873.91	1000.00	716.46	924.21	896.87	1054.32
Mass Flow lb/hr	7910.39	906.21	36774.69	36774.64	42080.70	12907.16	37680.90	19484.97	43352.51
Mass Flow lb/hr			36774.69	36774.64	42080.70		37680.90		43352.51
Mass Flow lb/hr	7910.39	906.21				12907.16		19484.97	
Volume Flow cuft/hr	118.55	14.76	349221.54	74440.76	99570.19	207.42	368884.38	355.09	226743.59
Volume Flow cuft/hr			349221.54	74440.76	99570.19		368884.38		226743.59
Volume Flow cuft/hr	118.55	14.76				207.42		355.09	
Enthalpy MMBtu/hr	-2.19	-6.17	7.88	10.63	11.72	-88.14	2.64	-98.15	-1.21
Mole Flow lbmol/hr									
H2O	0.00	50.30	0.00	0.00	0.00	716.46	50.30	716.46	0.00
HCL	0.00	0.00	0.00	0.00	0.00	0.00	0.00	180.41	180.41
PROPENE	0.00	0.00	873.91	873.91	1000.00	0.00	873.91	0.00	873.91
CHLORINE	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
AC	0.05	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
12DCP	8.39	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
13DCP-C	62.71	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
13DCP-T	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
H+	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
CL-	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

	19	32
Temperature F	-45.30	71.60
Pressure psia	20.00	14.70
Vapor Frac	0.00	0.00
Mole Flow lbmol/hr	0.55	766.76
Mass Flow lb/hr	42.09	13813.37
Mass Flow lb/hr		
Mass Flow lb/hr	42.09	13813.37
Volume Flow cuft/hr	0.67	222.18
Volume Flow cuft/hr		
Volume Flow cuft/hr	0.67	222.18
Enthalpy MMBtu/hr	-0.01	-94.30
Mole Flow lbmol/hr		
H2O	0.00	766.76
HCL	0.00	0.00
PROPENE	0.00	0.00
CHLORINE	0.00	0.00
AC	0.55	0.00
12DCP	0.00	0.00
13DCP-C	0.00	0.00
13DCP-T	0.00	0.00
H+	0.00	0.00
CL-	0.00	0.00

INPUT SUMMARY-WEIGHTED OPTIMIZATION-ISOTHERMAL PFR

```
TITLE 'ALLYL CHLORIDE -Adiabatic PFR'
IN-UNITS ENG
DEF-STREAMS CONVEN ALL
SIM-OPTIONS OLD-DATABANK=YES
RUN-CONTROL MAX-TIME=100000. MAX-ERRORS=500
DESCRIPTION "
   General Simulation with English Units :
   F, psi, lb/hr, lbmol/hr, Btu/hr, cuft/hr.
   Property Method: None
   Flow basis for input: Mole
   Stream report composition: Mole flow

DATABANKS ASPENPCD  / AQUEOUS  / SOLIDS  / INORGANIC  /  &
      PURE22  / PURE10

PROP-SOURCES ASPENPCD  / AQUEOUS  / SOLIDS  / INORGANIC  /  &
      PURE22  / PURE10

COMPONENTS
   H2O H2O /
   HCL HCL /
   PROPENE C3H6-2 /
   CHLORINE CL2 /
   AC C3H5CL /
   12DCP C3H6CL2 /
   13DCP-C C3H4CL2-D1 /
   13DCP-T C3H4CL2-D2 /
   H+ H+ /
   CL- CL-

HENRY-COMPS HENRY CHLORINE HCL PROPENE

SOLVE
   RUN-MODE MODE=OPT

CHEMISTRY HCL
   STOIC 1 HCL -1 / H+ 1 / CL- 1

FLOWSHEET
   BLOCK B2 IN=14 OUT=2
   BLOCK B8 IN=1 13 OUT=14
   BLOCK B3 IN=2 3 OUT=4
   BLOCK B6 IN=4 OUT=5
   BLOCK B9 IN=5 OUT=6
```

```
   BLOCK B7 IN=6 OUT=8 7
   BLOCK B5 IN=7 OUT=9 10
   BLOCK B10 IN=18 32 OUT=16 17
   BLOCK B1 IN=16 OUT=12 11
   BLOCK B11 IN=8 OUT=18 19
   BLOCK B4 IN=12 OUT=13
   BLOCK B18 IN=15 11 OUT=32

PROPERTIES SYSOP0
   PROPERTIES ELECNRTL / UNIQ-RK / UNIQUAC

STRUCTURES
   STRUCTURES 13DCP-C CL1 C2 S / C2 C3 D / C3 C4 S /  &
      C4 CL5 S

ESTIMATE ALL

PROP-DATA PCES-1
   IN-UNITS ENG
   PROP-LIST DGAQHG / DHAQHG / S25HG / OMEGHG / DHVLB /  &
      VB / RGYR / VLSTD
   PVAL CHLORINE 2983.662941 / -10060.18917 / 28.90035349 /  &
      -17580.05159 / 8784.000000 / .7262124822 /  &
      3.2391732E-10 / .8579136616
   PROP-LIST DHVLB / VB / RGYR
   PVAL 13DCP-C 14431.51333 / 1.612466586 / 1.11089239E-9

PROP-DATA HENRY-1
   IN-UNITS ENG
   PROP-LIST HENRY
   BPVAL HCL H2O -49.78140336 2186.999983 8.370700000  &
      -5.3294445E-3 -3.999995968 68.00000346 0.0
   BPVAL CHLORINE H2O -116.9781387 4371.515965 19.18540000  &
      -4.9558834E-3 49.73000360 103.7300032 0.0
   BPVAL HCL 12DCP 10.00798341 -2648.879936 0.0 0.0  &
      -4.269995966 67.73000346 0.0
   BPVAL PROPENE H2O 326.3806995 -28021.26578 -41.73762000 0.0  &
      69.53000344 220.7300022 0.0
   BPVAL PROPENE 12DCP 12.93988341 -3932.459880 0.0 0.0  &
      -4.269995966 67.73000346 0.0

PROP-DATA UNIQ-1
   IN-UNITS ENG
   PROP-LIST UNIQ
   BPVAL H2O AC -4.247000000 2292.652782 0.0 0.0 109.9400031  &
      212.0000023 0.0
```

```
   BPVAL AC H2O 15.46800000 -10062.08074 0.0 0.0 109.9400031  &
      212.0000023 0.0
   BPVAL H2O 12DCP 0.0 -539.9468957 0.0 0.0 77.00000338  &
      77.00000338 0.0
   BPVAL 12DCP H2O 0.0 -2498.536780 0.0 0.0 77.00000338  &
      77.00000338 0.0

PROP-DATA VLCLK-1
   IN-UNITS ENG
   PROP-LIST VLCLK
   BPVAL H+ CL- .5534556926 .2140997389

PROP-DATA GMELCC-1
   IN-UNITS ENG
   PROP-LIST GMELCC
   PPVAL H2O ( H+ CL- ) 41.67400000
   PPVAL ( H+ CL- ) H2O -22.15400000
   PPVAL HCL ( H+ CL- ) 1.00000000E-3
   PPVAL ( H+ CL- ) HCL -1.0000000E-3

PROP-DATA GMELCD-1
   IN-UNITS ENG
   PROP-LIST GMELCD
   PPVAL H2O ( H+ CL- ) 9581.579923
   PPVAL ( H+ CL- ) H2O -3967.379968

PROP-DATA GMELCE-1
   IN-UNITS ENG
   PROP-LIST GMELCE
   PPVAL H2O ( H+ CL- ) -5.404000000
   PPVAL ( H+ CL- ) H2O 5.188000000

PROP-DATA GMELCN-1
   IN-UNITS ENG
   PROP-LIST GMELCN
   PPVAL H2O ( H+ CL- ) .0283500000

PCES-PROP-DATA
   IN-UNITS ENG
   GAMINF H2O 12DCP * * 68 2340 / * * 86 2310 / * *  &
      104 2090

PCES-PROP-DATA
   IN-UNITS ENG
   GAMINF H2O 13DCP-C * * 68 1360 / * * 86 1430 / * *  &
      104 1460
```

```
PROP-SET IPE-1 TEMP PRES MASSFLMX VOLFLMX MWMX MASSSFRA  &
     MASSVFRA MASSFLOW SUBSTREAM=ALL PHASE=T

PROP-SET IPE-2 CPMX MWMX MASSFLMX KMX SIGMAMX MUMX VOLFLMX
&
     UNITS='J/kg-K' SUBSTREAM=MIXED PHASE=L

PROP-SET IPE-3 VOLFLMX CPMX MUMX KMX MWMX MASSFLMX UNITS= &
     'J/kg-K' SUBSTREAM=MIXED PHASE=V

STREAM 1
   SUBSTREAM MIXED TEMP=80. PRES=74.7
   MOLE-FLOW PROPENE 1000.

STREAM 3
   SUBSTREAM MIXED TEMP=80. PRES=74.7
   MOLE-FLOW CHLORINE 166.

STREAM 15
   SUBSTREAM MIXED TEMP=70. PRES=14.7
   MOLE-FLOW H2O 325.

BLOCK B3 MIXER
   PROPERTIES UNIQ-RK FREE-WATER=STEAM-TA SOLU-WATER=3  &
     TRUE-COMPS=YES

BLOCK B8 MIXER
   PROPERTIES UNIQ-RK FREE-WATER=STEAM-TA SOLU-WATER=3  &
     TRUE-COMPS=YES

BLOCK B18 MIXER

BLOCK B1 SEP
   PARAM
   FRAC STREAM=12 SUBSTREAM=MIXED COMPS=PROPENE FRACS=1.
   PROPERTIES UNIQ-RK FREE-WATER=STEAM-TA SOLU-WATER=3  &
     TRUE-COMPS=YES

BLOCK B11 SEP
   PARAM
   FRAC STREAM=18 SUBSTREAM=MIXED COMPS=H2O HCL PROPENE  &
     CHLORINE AC 12DCP 13DCP-C 13DCP-T H+ CL- FRACS=1. 1.  &
     1. 1. 0. 0. 0. 0. 1. 1.
   PROPERTIES UNIQ-RK FREE-WATER=STEAM-TA SOLU-WATER=3  &
     TRUE-COMPS=YES
```

```
BLOCK B2 HEATER
   PARAM TEMP=700. PRES=74.7
   PROPERTIES UNIQ-RK FREE-WATER=STEAM-TA SOLU-WATER=3  &
      TRUE-COMPS=YES

BLOCK B9 HEATER
   PARAM TEMP=70. PRES=74.7
   PROPERTIES UNIQ-RK FREE-WATER=STEAM-TA SOLU-WATER=3  &
      TRUE-COMPS=YES

BLOCK B5 RADFRAC
   PARAM NSTAGE=15
   COL-CONFIG CONDENSER=PARTIAL-V
   FEEDS 7 6
   PRODUCTS 9 1 V / 10 15 L
   P-SPEC 1 16. / 15 25.
   COL-SPECS D:F=0.539038 MOLE-RR=4.02554
   SPEC 1 MOLE-RECOV 0.999 COMPS=AC STREAMS=9 BASE-STREAMS=7
   VARY 1 D:F 0.01 0.99
   PROPERTIES UNIQ-RK FREE-WATER=STEAM-TA SOLU-WATER=3  &
      TRUE-COMPS=YES

BLOCK B7 RADFRAC
   PARAM NSTAGE=15 ALGORITHM=STANDARD INIT-OPTION=STANDARD
&
      MAXOL=150 DAMPING=NONE
   COL-CONFIG CONDENSER=PARTIAL-V
   FEEDS 6 7
   PRODUCTS 8 1 V / 7 15 L
   P-SPEC 1 20. / 15 27.
   COL-SPECS D:F=0.8 MOLE-RR=0.4084
   SPEC 1 MOLE-RECOV 0.99 COMPS=AC STREAMS=7
   VARY 1 D:F 0.01 0.99
   PROPERTIES UNIQ-RK FREE-WATER=STEAM-TA SOLU-WATER=3  &
      TRUE-COMPS=YES

BLOCK B10 RADFRAC
   PARAM NSTAGE=10 ALGORITHM=NONIDEAL INIT-OPTION=STANDARD  &
      MAXOL=100 MAXIL=50
   COL-CONFIG CONDENSER=NONE REBOILER=NONE
   FEEDS 18 10 ON-STAGE / 32 1
   PRODUCTS 17 10 L / 16 1 V
   P-SPEC 1 14.7
   COL-SPECS
   T-EST 1 110. / 10 68.
```

```
   PROPERTIES ELECNRTL HENRY-COMPS=HENRY CHEMISTRY=HCL  &
      FREE-WATER=STEAM-TA SOLU-WATER=3 TRUE-COMPS=NO

BLOCK B6 RPLUG
   PARAM TYPE=ADIABATIC LENGTH=20. DIAM=6. PRES=40.  &
      INT-TOL=1E-005
   COOLANT MAXIT=50
   PROPERTIES UNIQ-RK FREE-WATER=STEAM-TA SOLU-WATER=3  &
      TRUE-COMPS=YES / SYSOP0
   REACTIONS RXN-IDS=R-1

BLOCK B4 COMPR
   PARAM TYPE=ASME-POLYTROP PRES=90.
   PROPERTIES UNIQ-RK FREE-WATER=STEAM-TA SOLU-WATER=3  &
      TRUE-COMPS=YES

DESIGN-SPEC FEED
   DEFINE S14 MOLE-FLOW STREAM=14 SUBSTREAM=MIXED  &
      COMPONENT=PROPENE
   SPEC "S14" TO "1000"
   TOL-SPEC "0.01"
   VARY MOLE-FLOW STREAM=1 SUBSTREAM=MIXED
COMPONENT=PROPENE
   LIMITS "5" "1000"

DESIGN-SPEC H20
   DEFINE HCL18 MASS-FLOW STREAM=18 SUBSTREAM=MIXED  &
      COMPONENT=HCL
   DEFINE H2032 MASS-FLOW STREAM=32 SUBSTREAM=MIXED  &
      COMPONENT=H2O
   SPEC "H2032" TO "2.1*HCL18"
   TOL-SPEC ".001"
   VARY STREAM-VAR STREAM=15 SUBSTREAM=MIXED VARIABLE=MASS-
FLOW
   LIMITS "10" "60000"

DESIGN-SPEC RESTM
   DEFINE RESTM BLOCK-VAR BLOCK=B6 VARIABLE=RES-TIME  &
      SENTENCE=PARAM
   SPEC "RESTM" TO "1.11E-3"
   TOL-SPEC ".0001"
   VARY BLOCK-VAR BLOCK=B6 VARIABLE=LENGTH SENTENCE=PARAM
   LIMITS "1" "200"


EO-CONV-OPTI
```

```
OPTIMIZATION MAXPROFT
   DEFINE AC9 MASS-FLOW STREAM=9 SUBSTREAM=MIXED
COMPONENT=AC
   DEFINE HCL17 STREAM-VAR STREAM=17 SUBSTREAM=MIXED  &
      VARIABLE=MASS-FLOW
   DEFINE CL3 MASS-FLOW STREAM=3 SUBSTREAM=MIXED  &
      COMPONENT=CHLORINE
   DEFINE PROP1 MASS-FLOW STREAM=1 SUBSTREAM=MIXED  &
      COMPONENT=PROPENE
   DEFINE H2015 MASS-FLOW STREAM=15 SUBSTREAM=MIXED  &
      COMPONENT=H2O
   DEFINE FDHTR BLOCK-VAR BLOCK=B2 VARIABLE=QCALC  &
      SENTENCE=PARAM
   DEFINE REB1 BLOCK-VAR BLOCK=B7 VARIABLE=REB-DUTY  &
      SENTENCE=RESULTS
   DEFINE REB2 BLOCK-VAR BLOCK=B5 VARIABLE=REB-DUTY  &
      SENTENCE=RESULTS
   DEFINE COMP BLOCK-VAR BLOCK=B4 VARIABLE=BRAKE-POWER  &
      SENTENCE=RESULTS
   DEFINE COOL1 BLOCK-VAR BLOCK=B9 VARIABLE=QCALC  &
      SENTENCE=PARAM
   DEFINE COND1 BLOCK-VAR BLOCK=B7 VARIABLE=COND-DUTY  &
      SENTENCE=RESULTS
   DEFINE COND2 BLOCK-VAR BLOCK=B5 VARIABLE=COND-DUTY  &
      SENTENCE=RESULTS
   DEFINE MASSEP MASS-FLOW STREAM=4 SUBSTREAM=MIXED  &
      COMPONENT=PROPENE
   DEFINE MASSEC MASS-FLOW STREAM=4 SUBSTREAM=MIXED  &
      COMPONENT=CHLORINE
   DEFINE MASSXP MASS-FLOW STREAM=5 SUBSTREAM=MIXED  &
      COMPONENT=PROPENE
   DEFINE MASSXC MASS-FLOW STREAM=5 SUBSTREAM=MIXED  &
      COMPONENT=CHLORINE
   DEFINE DCP10 STREAM-VAR STREAM=10 SUBSTREAM=MIXED  &
      VARIABLE=MASS-FLOW
   DEFINE B6TO BLOCK-VAR BLOCK=B6 VARIABLE=REAC-TEMP  &
      SENTENCE=GENPROF ID1=5
   DEFINE PROFIT LOCAL-PARAM PHYS-QTY=UNIT-PRICE UOM="$/lb"  &
      INIT-VAL=0.
   DEFINE PROP2 MOLE-FLOW STREAM=2 SUBSTREAM=MIXED  &
      COMPONENT=PROPENE
   DEFINE T4 STREAM-VAR STREAM=4 SUBSTREAM=MIXED
VARIABLE=TEMP
   DEFINE CL3M STREAM-VAR STREAM=3 SUBSTREAM=MIXED  &
```

```
      VARIABLE=MOLE-FLOW
   DEFINE AC5 MOLE-FLOW STREAM=5 SUBSTREAM=MIXED
COMPONENT=AC
   DEFINE DC25 MOLE-FLOW STREAM=5 SUBSTREAM=MIXED  &
      COMPONENT=12DCP
   DEFINE DC35 MOLE-FLOW STREAM=5 SUBSTREAM=MIXED  &
      COMPONENT=13DCP-C
   DEFINE MCL4 MASS-FLOW STREAM=4 SUBSTREAM=MIXED  &
      COMPONENT=CHLORINE
   DEFINE MP4 MASS-FLOW STREAM=4 SUBSTREAM=MIXED  &
      COMPONENT=PROPENE
   DEFINE MCL5 MASS-FLOW STREAM=5 SUBSTREAM=MIXED  &
      COMPONENT=CHLORINE
   DEFINE MP5 MASS-FLOW STREAM=5 SUBSTREAM=MIXED  &
      COMPONENT=PROPENE
   DEFINE WST12D MASS-FLOW STREAM=10 SUBSTREAM=MIXED  &
      COMPONENT=12DCP
   DEFINE WST13D MASS-FLOW STREAM=10 SUBSTREAM=MIXED  &
      COMPONENT=13DCP-C
   DEFINE HCL5M MASS-FLOW STREAM=5 SUBSTREAM=MIXED  &
      COMPONENT=HCL
   DEFINE AC5M MASS-FLOW STREAM=5 SUBSTREAM=MIXED
COMPONENT=AC
F    REVAC=.88
F    REVHCL=0.0625
F    CSTCL2=.16
F    CSTPRP=.45
F    WSTC=.0011
F    REVENUE=REVAC*AC9+REVHCL*HCL17
F    RAWCST=CSTCL2*CL3+CSTPRP*PROP1
F    NGCST=FDHTR*.0000117
F    TOTST=REB1+REB2
F    STCST=TOTST*0.00001564
F    HTCST=STCST+NGCST
F    ELECST=0.0417*COMP
F    H20BTU=-(COOL1+COND1+COND2)
F    H2O1=(H20BTU/27)*.454*.016088*.00042
F    DIWCST=H2015*.454*.001
F    H20CST=DIWCST+H201
F    UTLCST=HTCST+ELECST+H20CST
F    WSTCST=DCP10*WSTC
F    HEALTH=4.6*WST12D+4.8*WST13D
F    EMY=(HCL5M+AC5M)/((MP4+MCL4+0.000001)-(MP5+MCl5))
F    PROFIT=REVENUE-RAWCST-UTLCST-WSTCST
F    FR=PROP2/CL3M
   MAXIMIZE  &
```

```
      "0.4*(PROFIT/1360)-0.4*(HEALTH/31029)+0.2*(EMY/0.63447)"
   VARY BLOCK-VAR BLOCK=B2 VARIABLE=TEMP SENTENCE=PARAM
   LIMITS "500" "900"
   VARY MOLE-FLOW STREAM=3 SUBSTREAM=MIXED
COMPONENT=CHLORINE
   LIMITS "166" "1000"
   VARY BLOCK-VAR BLOCK=B6 VARIABLE=PRES SENTENCE=PARAM
   LIMITS "15" "150"

CONV-OPTIONS
   PARAM OPT-METHOD=SQP SPEC-LOOP=INSIDE USER-LOOP=OUTSIDE
   WEGSTEIN MAXIT=100
   DIRECT MAXIT=100
   SECANT MAXIT=100
   BROYDEN MAXIT=100
   NEWTON MAXIT=100
   SQP MAXIT=200 MAXPASS=1000 TOL=0.005 MAXLSPASS=100  &
      NLIMIT=100 STEP-OPT=VALUE STEP-DIR=NEGATIVE  &
      OPT-METHOD=SQP DERIVATIVE=FORWARD CONST-ITER=200  &
      CONV-TEST=KKT

TEAR
   TEAR 13

STREAM-REPOR MOLEFLOW MOLEFRAC MASSFRAC PROPERTIES=IPE-1 IPE-
2  &
      IPE-3

REACTIONS R-1 POWERLAW
   REAC-DATA 1 PHASE=V
   REAC-DATA 2 PHASE=V
   REAC-DATA 3 PHASE=V
   RATE-CON 1 PRE-EXP=40400000. ACT-ENERGY=74300000. <J/kmol>
   RATE-CON 2 PRE-EXP=2300. ACT-ENERGY=27300000. <J/kmol>
   RATE-CON 3 PRE-EXP=90300000000. ACT-ENERGY=110000000. <J/kmol>
   STOIC 1 MIXED PROPENE -1. / CHLORINE -1. / AC 1. /  &
      HCL 1.
   STOIC 2 MIXED PROPENE -1. / CHLORINE -1. / 12DCP 1.
   STOIC 3 MIXED AC -1. / CHLORINE -1. / 13DCP-C 1. /  &
      HCL 1.
   POWLAW-EXP 1 MIXED PROPENE 1. / MIXED CHLORINE 1.
   POWLAW-EXP 2 MIXED PROPENE 1. / MIXED CHLORINE 1.
   POWLAW-EXP 3 MIXED AC 1. / MIXED CHLORINE 1.
```

OUTPUT STREAM SUMMARY-WEIGHTED OPTIMIZATION-ISOTHERMAL PFR

	1	2	3	4	5	6	7	8	9
Temperature F	80.00	661.30	80.00	632.40	1164.70	70.00	208.10	-48.80	117.90
Pressure psia	74.70	74.70	74.70	74.70	37.42	74.70	27.00	20.00	16.00
Vapor Frac	1.00	1.00	1.00	1.00	1.00	0.73	0.00	1.00	1.00
Mole Flow lbmol/hr	379.70	1166.00	166.00	1332.00	1300.47	1300.47	213.07	1087.40	63.19
Mass Flow lb/hr	20763.05	53850.94	11770.30	65621.23	65621.29	65621.29	21529.39	44091.90	4835.54
Mass Flow lb/hr	20763.05	53850.94	11770.30	65621.23	65621.29	39095.63		44091.90	4835.54
Mass Flow lb/hr						26525.66	21529.39		
Volume Flow cuft/hr	27509.92	186504.06	12095.54	207415.93	605390.62	68403.81	335.73	232329.87	23751.04
Volume Flow cuft/hr	27509.92	186504.06	12095.54	207415.93	605390.62	67945.66		232329.87	23751.04
Volume Flow cuft/hr						458.15	335.73		
Enthalpy MMBtu/hr	1.82	21.90	-0.03	21.87	21.87	-13.21	-6.17	-6.74	0.03
Mole Flow lbmol/hr									
H2O	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
HCL	0.00	0.00	0.00	0.00	300.47	300.47	0.00	300.47	0.00
PROPENE	213.70	1000.00	0.00	1000.00	786.29	786.29	0.00	786.29	0.00
CHLORINE	166.00	166.00	166.00	332.00	0.00	0.00	0.00	0.00	0.00
AC	0.00	0.00	0.00	0.00	63.89	63.89	63.25	0.64	63.18
12DCP	0.00	0.00	0.00	0.00	31.53	31.53	31.53	0.00	0.00
13DCP-C	0.00	0.00	0.00	0.00	118.29	118.29	118.29	0.00	0.00
13DCP-T	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
H+	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
CL-	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

	10	11	12	13	14	15	16	17	18
Temperature F	250.90	118.20	118.20	304.30	247.10	70.00	117.60	154.90	-48.80
Pressure psia	25.00	14.70	14.70	90.00	74.70	14.70	14.70	14.70	20.00
Vapor Frac	0.00	0.00	1.00	1.00	1.00	0.00	1.00	0.00	1.00
Mole Flow lbmol/hr	149.88	96.43	786.29	786.30	1166.00	1180.62	882.71	1481.09	1086.76
Mass Flow lb/hr	16693.85	1737.13	33087.61	33087.89	53850.94	21269.12	34824.63	32224.63	44043.01
Mass Flow lb/hr			33087.61	33087.89	53850.94		34824.63		44043.01
Mass Flow lb/hr	16693.85	1737.13				21269.12		32224.63	
Volume Flow cuft/hr	251.34	28.67	328115.59	69492.79	114764.24	341.80	367961.23	662.45	232199.82
Volume Flow cuft/hr			328115.59	69492.79	114764.24		367961.23		232199.82
Volume Flow cuft/hr	251.34	28.67				341.80		662.45	
Enthalpy MMBtu/hr	-5.40	-11.78	7.39	9.97	11.78	-145.24	-2.62	-161.13	-6.74
Mole Flow lbmol/hr									
H2O	0.00	96.43	0.00	0.00	0.00	1180.62	96.42	1180.62	0.00
HCL	0.00	0.00	0.00	0.00	0.00	0.00	0.00	300.47	300.47
PROPENE	0.00	0.00	786.29	786.30	1000.00	0.00	786.29	0.00	786.29
CHLORINE	0.00	0.00	0.00	0.00	166.00	0.00	0.00	0.00	0.00
AC	0.06	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
12DCP	31.53	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
13DCP-C	118.29	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
13DCP-T	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
H+	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
CL-	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

	19	32
Temperature F	-48.80	73.70
Pressure psia	20.00	14.70
Vapor Frac	0.00	0.00
Mole Flow lbmol/hr	0.64	1277.04
Mass Flow lb/hr	48.89	23006.25
Mass Flow lb/hr		
Mass Flow lb/hr	48.89	23006.25
Volume Flow cuft/hr	0.77	370.45
Volume Flow cuft/hr		
Volume Flow cuft/hr	0.77	370.45
Enthalpy MMBtu/hr	-0.01	-157.02
Mole Flow lbmol/hr		
H2O	0.00	1277.04
HCL	0.00	0.00
PROPENE	0.00	0.00
CHLORINE	0.00	0.00
AC	0.64	0.00
12DCP	0.00	0.00
13DCP-C	0.00	0.00
13DCP-T	0.00	0.00
H+	0.00	0.00
CL-	0.00	0.00

VITA

Anand Govindarajan

Candidate for the Degree of

Master of Science

Thesis: OPTIMIZATION OF PROCESSES FOR SUSTAINABILITY

Major Field: Chemical Engineering

Biographical:

Education:

Completed the requirements for the Master of Science in Chemical Engineering at Oklahoma State University, Stillwater, Oklahoma in May , 2011.

Completed the requirements for the Bachelor of Technology in Chemical Engineering at Anna University (Sri Sivasubramaniya Nadar College of Engineering), Chennai, Tamil Nadu/India in 2011.

Experience:

Graduate Engineer Trainee with VA Tech WABAG-India (June-October 2008) ,
Research Associate with SSN Research Centre-India (November 2008 to July 2009),
Internship with Sun to Market Solutions (Summer 2010).
Graduate Teaching Assistant-Communications-School of Chemical Engineering, Oklahoma State University (Aug 2009 to May 2011)

Professional Memberships:

International Society of Automation and Omega Chi Epsilon

Name: Anand Govindarajan Date of Degree: May, 2011

Institution: Oklahoma State University Location: Stillwater, Oklahoma

Title of Study: OPTIMIZATION OF PROCESSES FOR SUSTAINABILITY

Pages in Study: 151 Candidate for the Degree of Master of Science

Major Field: Chemical Engineering

Scope and Method of Study: This research is focused on developing a methodology to optimize processes for sustainability. To design a sustainable process that addresses economic, environmental and social concerns is a complex multiobjective problem. Current state of research is restricted to optimizing processes for profit while satisfying environmental regulations and/or measuring the sustainability of the process using already developed tools. There is no methodology that optimizes a process for being sustainable. There is an increasing need to fill the gap between solving a complicated multiobjective problem for sustainability concerns and a simple single objective problem of profit. This research therefore converts the multiobjective problem of designing processes for being sustainable into a single objective problem by using a method of constraints and a method of weights to combine the objective functions. The methodology combines information from an OSU developed SUSTAINABILITY EVALUATOR and uses a commercially available sequential modular simulator Aspen Plus to optimize processes.

Findings and Conclusions: The base case of a process is simulated in Aspen Plus and evaluated using the SUSTAINABILITY EVALUATOR. A sensitivity analysis is conducted to determine the variables affecting the product yields, health impact, mass productivity and profit. . A FORTRAN code is written to define the objectives in Aspen Plus. A payoff table was generated by optimizing the three individual objectives of profit, health impact and mass productivity. As a next step a multiobjective optimization problem was formulated these three objectives. This was reduced to a single objective problem by using a method of constraints and a method of weights. The constraints are determined using information from the payoff table. The weights were varied from 0 to 1 for each of the objectives. This single objective problem was solved using readily available commercial process simulators such as Aspen Plus. Only the non-dominated set of solutions is presented to a decision maker for choice. The selected solution is compared with a base case using an amoeba chart. By converting a multiobjective problem to a single objective problem a tradeoff between effort and result is achieved. The above methodology is implemented on an Allyl Chloride manufacturing process.

ADVISER'S APPROVAL: Dr. Karen A. High