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# THE USE OF I/O INFORMATION AT THE PROCESS LEVEL FOR CHEMICAL INDUSTRY PROGRAMMING ON A TIME-SHARED COMPUTER SYSTEM

by

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## 1. INTRODUCTION

The objective of this paper is to define a heuristic, non-optimizing yet efficeint computer-based mode of using process-level I/O information for planning the chemical sector.[1/]

Sectoral planning models using process-level I/O information are typically set up as formal I/O or mathematical programming systems.[2/] Derivation of the inverse matrix or of optimizing and parametrically optimizing solutions is then accomplished by complex algorithms incorporated in large computer programs. Several major problems arise with this approach in concrete applications.

First, it does not permit including in the planning process information that is either qualitative, un-quantified, or quantified in a manner not conforming to model structure. Yet there is increasing evidence that information pertaining to technological capability, institutional structure, system diversification and integration, and the extent and kind of foreign dependency, none of which typically fit into I/O, L/P, or I/P model formats, in many policy problems are of decisive importance. Such considerations often dominate resource allocation decisions around which formal models revolve.

This problem has been encountered in full force in a recent empirical/theoretical investigation of the development of the heavy electrical equipment indus-

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1/For chemical industry planning, see United Nations (1966a, 1967).

2/Recent examples of such work will be found in Goreux and Manne (1973) and Stoutjesdijk and Westphal (1974).

tries in Mexico sponsored by the Development Research Center of the World Bank. As reported in a paper to the last I/O Conference (Vietorisz, 1972), day-to-day operation and technological change are inextricably intertwined in the engineering industries, making formal models or resource allocation at best incomplete and at worst grossly misleading. More recent work on the same project (Vietorisz, 1974) has raised serious doubt about the comparative advantage concept implicit in formal optimizing models, and suggested interfacing such models with information derived from historical development sequences.

A heuristic, non-optimizing approach to sectoral modelling uses process-level I/O data in a step-by-step fashion and thus permits taking into account supplementary information of many kinds as sectoral programs are gradually pieced together.

A second problem with formal models arises from the predetermined categories which are needed for setting them up. Even when full technical information is available and can be fitted into the mathematical structure of the model, doubt often persists about how much detail should be included on individual processes. In concrete applications it is generally not known in advance which detailed item will turn out to be critical. Small amounts of impurities in ethylene or hydrogen feedstocks can be utterly ruinous to some processes and a matter of minor concern to others. Thus the formal model is either defined in tremendous detail most of which will turn out to be redundant, or omits detail which may turn out to be vital. Even worse, detail that is critical for the model may never be identified as such since modelling consists of two non-overlapping phases: information gathering and computation.

Heuristic models avoid the need for gathering all information into a bushel, pouring it into the computer, and sitting back while the pre-set computer program blindly grinds out a solution. Since heuristic models are build up from processes step by step, the procedure is completely transparent, can be followed by engineering specialists, and permits infusing additional qualitative or quantitative technical information as it becomes identified as critical.

A third problem with formal models is that the larger they get, the more their workings take on the nature of a mechanism working inside a black box. Policy makers rightly detest black boxes. The more opaque a large model becomes, the more chance there is for severe distortion arising from undetected keypunching errors, technical mistakes in the definition of a few among the thousands of coefficients, uncontrolled biases inherent in mixing engineering data of various levels or reliability, or failure to include relevant items of information. For example, in L/P models two alternative processes are treated on a par even though the data for one may be derived from past experience while the data for the other may represent unconfirmed engineering estimates. In a large, opaque model biases of this kind are totally impossible to keep track of. Heuristic models, on the other hand, are completely transparent and therefore particulary suited to detecting technical errors as processes are built into programs, adding information as needed, keeping track of the reliability of data, and representing the inner logic of complex process combinations for the appraisal of policymakers.

In this paper the design of a heuristic model-building system for the chemical sector will be discussed which is aimed at taking maximum ad-

vantage of time-shared computer facilities. The heuristic system rests on a data bank that is set up so that it can grow and expand in use.

The principles of organizing such a data bank will be discussed, and its application to heuristic modelling tasks will be laid out. A published data base for the chemical industry (Vietorisz, 1966) will be used for illustrative purposes.

The heuristic method discussed here has been used by the author in an earlier, simpler, less systematic, and far more cumbersome version some years ago to define chemical industry development possibilities in Puerto Rico (Isard, Schooler, and Vietorisz, 1959), and in Latin America (Vietorisz and Szabo, 1959; United Nations, 1963). The main reason for bypassing formal models in these early experiments was the absence of powerful computer programs for the solution of large integer programming problems. With advances in mathematical programming and computing techniques, these problems have become amenable to formal solution. Integer programming models of the chemical sector have been explored in simplified models (Vietorisz and Manne, 1963; Vietorisz, 1964) and lately, in large and complex ones (Goreux and Manne, 1973; Stoutjesdijk and Westphal, 1974).

In the meantime, however, the author's faith in such formal models, and the underlying view of development as resource accumulation, has been severely shaken. If development is viewed as primarily a matter of technological capability, institution building, and the dialectics of foreign dependency, then questions of resource allocation come to be seen as operations-research

problems of second-order significance. Overriding concern with efficiency in resource allocation, which is the motivating force behind formal models, thus gives way to concern for the possibilities of interfacing resource-allocation problems with broader (and more important) questions of technological, institutional, and political strategies of development. Heuristic modelling methods, which offer no guarantee of absolute efficiency but lend themselves beautifully to interfacing, all of a sudden appear highly attractive, and disclose further virtues (some of which have been indicated above) as they are analysed more carefully. The wheel thus swings back to the techniques which have provided the first systematic approach to sectoral planning for the chemical industries.

## 2. ORGANIZATION OF PROCESS-LEVEL I/O DATA

The heuristic approach to modelling the chemical industries rests on organizing process-level I/O data and supplementary information into a data bank. This data bank must be flexible in use, and capable of expansion and growth at the very time that it is being applied to a specific planning problem, because a concrete problem will typically generate new information that has not yet been included in the data bank.

A time-shared computer system offers the needed virtues of rapid information processing capability together with great flexibility of data input and data format modification. The following discussion of heuristic model design will therefore be oriented to such a system.

### The data base needed for sectoral programming

The tasks of sectoral programming are:

-Tracing the most improtant technological and economic linkages between different branches of the chemical sector, regardless of the subdivision of the sector between individual enterprises.

-Tracing the technological and economic linkages between the chemical sector and its supply, raw material, and institutional base.

-Tracing the technological and economic linkages between the chemical sector and its key markets in other domestic sectors and abroad.

The data base required for these tasks must define the I/O structure of processes and products, and must provide complementary information on the local economy: production capacities, imports, prices.

The major components of this data base are discussed in the following sections.

## Organization of the Data Bank: Sources

The organization of the data follows closely the principles set out in "Programming Data Summary for the Chemical Industry," (Vietorisz, 1966). This source contains detailed technical information on 90 processes, organized in a uniform manner. Other sources of chemical process information are: Chemical Engineering (Flowsheet collection, no date) and current issues; Oil and Gas Journal, current issues; Faith, Keyes, and Clark (1965); Hahn (1970), Noyes Development Corporation (Monograph series), Shreve (1956), United Nations (1966 b).

## Directories

Each one of the following directories can be maintained manually as an alphabetic-order card file. In the computerized version, each directory converts into an

array stored in memory:

1) Process codes and names
2) Item codes and names
3) Unit of measurement codes and names.

An example of brief directories of this kind, based on two sample processes, is given at the end of this section. Directories must be updated whenever a process is added to the data bank, modified, or deleted.

Process Bank

The process bank consists of a set of processes; each process has a full name and a process code (maintained in an alphabetical directory).

Two processes which differ in any respect -- e.g., units of measurement used, comments, etc. -- must have separate process codes.

Each individual process is maintained in the process bank in the following format:

Process code
Item code
  Item information
Item code
  Item information
  .....
  .....
  .....

The number of items in each process is open. Thus, a simple process may consist of only six or eight items, a complicated process of twenty or more.

Each process is headed by a process code (PC) which is a string of 8 alphanumeric characters beginning with "0" (zero). The code may terminate in blanks. For example, the process of manufacturing ammonia from natural gas, shown below, is coded as "0A10".

Individual items within a process may be of four kinds:

1) Scale-related resources, or "resources" for short;
2) Indirect inputs;
3) Institutional requirements;
4) General comments on the process as a whole.

Each item is introduced by an item code. This item code consists of a string of 8 alphanumeric characters which may terminate in blanks, with the first character being 1 to 4, depending on the four classes of items specified above. Thus, for example, ammonia may be coded as "1NH3". The initial "1" identifies this item as a resource.

Scale-related resources

These resources are outputs, shown as positive amounts, or inputs, shown as negative amounts. They always vary as a function of the scale of the process as a whole.

The scale of the process is measured by a scaling resource selected for this purpose. For example, in ammonia production, the output of the resource, ammonia, is used to measure the process scale. In petroleum refining, generally, the input of the resource, crude oil, is used as the measure of scale.

Scaling functions

Resource inputs may vary linearly or non-linearly with scale. Four standard functional relationships are specified to record this variation.

1) Proportionality. The amount of the resource X varies proportionally to the scaling resource S:

$$\left(\frac{X}{Xo}\right) = \left(\frac{S}{So}\right)$$

where Xo is the amount of the resource corresponding to the base level,

So, of the scaling resource. (See Figure 1). For example, in the production of ammonia from natural gas, the input of natural gas is proportional to scale. Thus, So = 1 ton of ammonia, Xo = 1,500 $m^3$ of natural gas; therefore X = 1,500 S, where S is measured in tons of ammonia output, and X is measured in $m^3$ of natural gas. If the scale of production is 50,000 tons per year, natural gas input is

(1,500)(50,000) = 75,000,000 $m^3$ per year.

2) Constant elasticity. The amount of the resource X varies as a fixed power, E, of the scaling resource, S:

$$\left(\frac{X}{Xo}\right) = \left(\frac{S}{So}\right)^E \quad ,$$

where Xo and So are interpreted as in the proportional case, and E is a constant exponent, called scale elasticity. (See Figure 2). For example, in the production of ammonia from natural gas, the requirement for plant investment varies non-linearly, with scale. So = 36

Figure 1
SCALING FUNCTIONS: PROPORTIONAL CASE

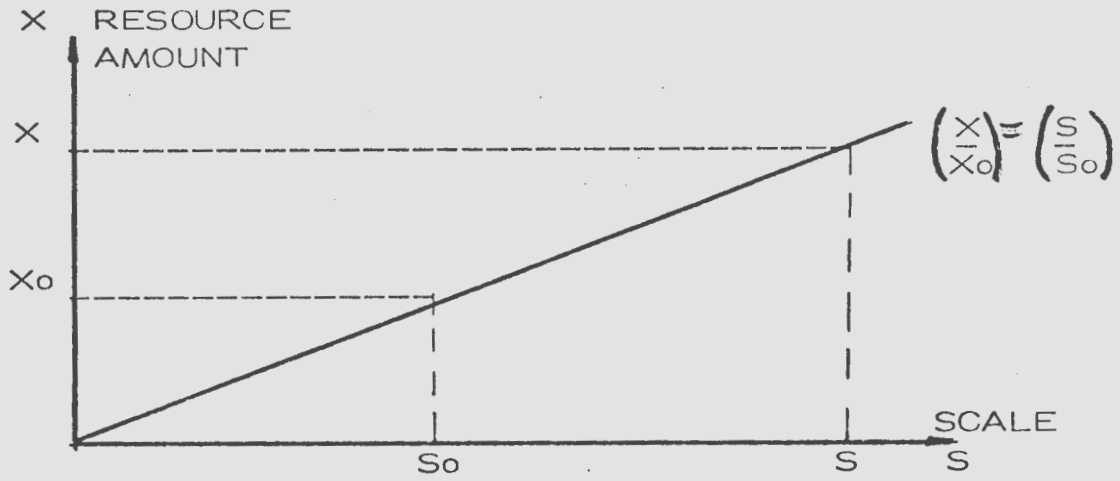
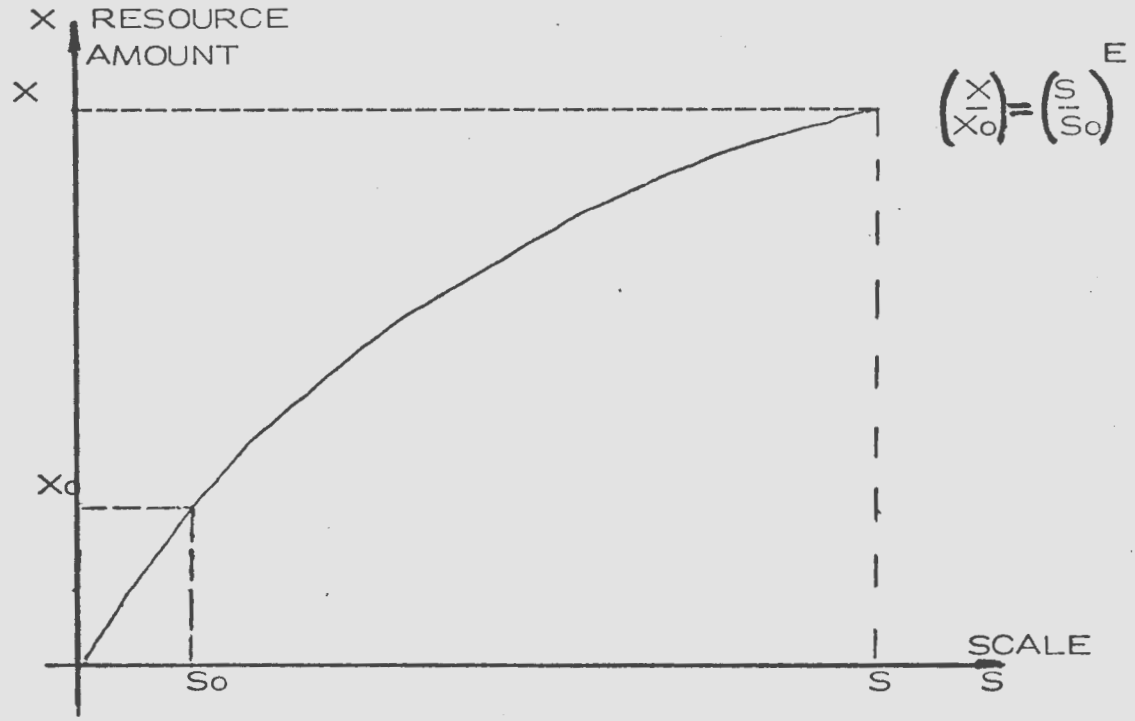



Figure 2
SCALING FUNCTIONS: CONSTANT ELASTICITY CASE



thousand tons per year of ammonia; Xo = 5 million dollars; E = .73. Therefore, $\frac{X}{5} = \left(\frac{S}{36}\right)^{.73}$. If the scale of production is 50 thousand tons per year, $X = 5\left(\frac{50}{36}\right)^{.73} = (5)(1.389)^{.73} = (5)(1.27) = 6.35$.

Note that proportionality can be regarded as a special case of constant elasticity, with E = 1.

3) Step function. The amount of the resource X is constant at Xo, X1, X2, etc., over specified ranges of scale So to S1, S1 to S2, ... etc:

X = Xo when So $\leq$ S < S1

X = X1 when S1 $\leq$ S < S2

X = X2 when S2 $\leq$ S ...

where Xo, X1, X2... etc. are constant resource inputs and So, S1, S2, ... etc., are specified scale levels (see Figure 3).

Figure 3

SCALING FUNCTIONS: STEP FUNCTION CASE

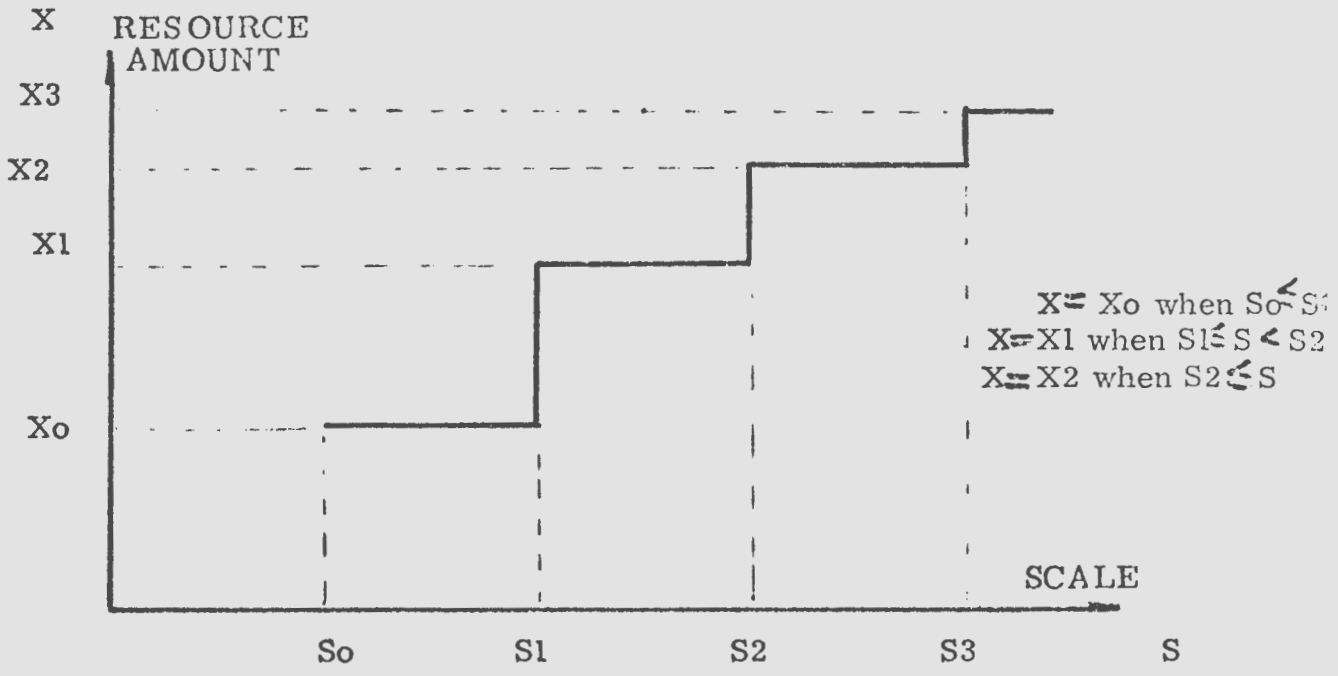
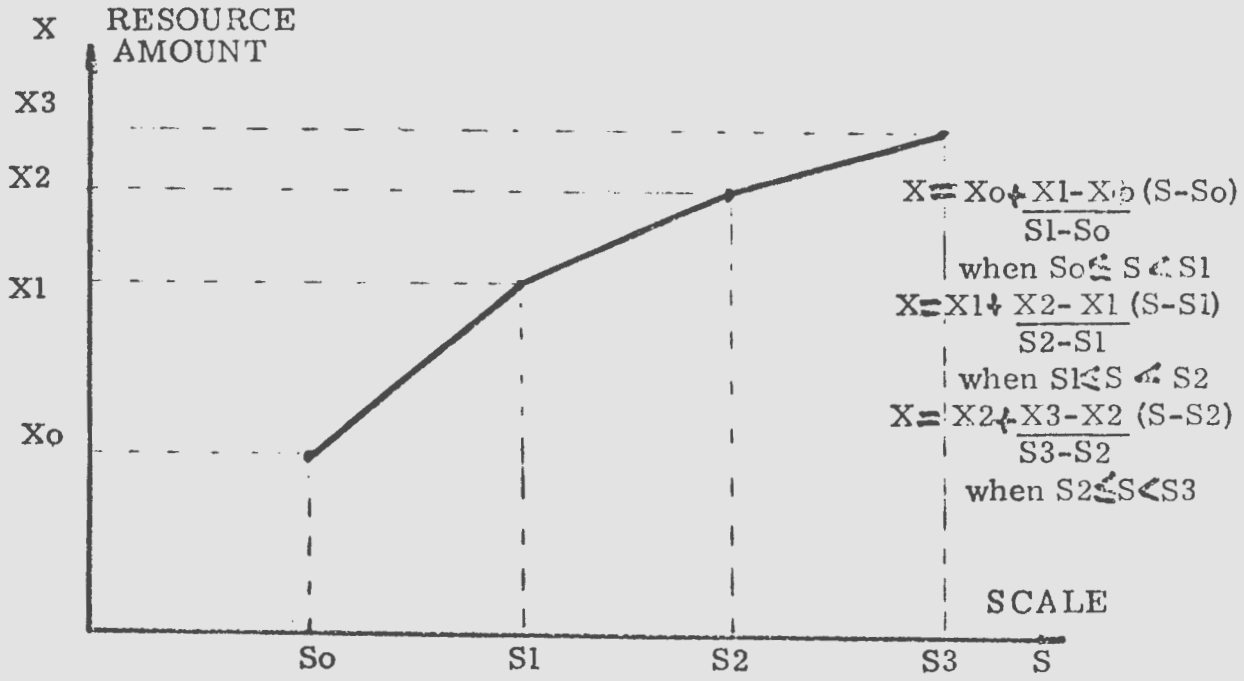



Figure 4

SCALING FUNCTIONS:PIECEWISE LINEAR CASE



For example, in the production of ammonia from natural gas, supervisory staff requirements can be represented by a step function as follows: under 200 tons/day, 2 men/shift; over 200 tons/day, 4 men/shift. Set So = 36 thousand tons/year (as before) and S1 = 66 thousand tons/year (assuming 330 production days per year). Then:

$X = 2$ men/shift when $36 \leq S < 66$

$X = 4$ men/shift when $66 \leq S$,

with S measured in thousands of tons per year.

Note that the step function can be regarded as a special case of constant elasticity within each individual range, with $E = 0$.

4) Piecewise linearity. The change in the amount of the resource X per unit change of scale, $\Delta X/\Delta S$, is constant within specified ranges. (See Figure 4.) The function is specified by giving the resource inputs Xo, X1, X2, ... at the scales So, S1, S2, ... etc.

$$(X-Xo)/(S-So) = (X1-Xo)/(S1-So) \quad \text{when } So \leq S < S1$$

$$(X-X1)/(S-S1) = (X2-X1)/(S2-S1) \quad \text{when } S1 \leq S < S2$$

$$(X-X2)/(S-S2) = (X3-X2)/(S3-S2) \quad \text{when } S2 \leq S < S3, \text{ ... etc.}$$

For example, in the production of ammonia from natural gas, an alternative may be representing plant investment requirements (instead of the

constant-elasticity function given above) is to specify the following:

| | | | |
|---|---|---|---|
| Si, capacity, thousands of tons/year | 36 | 108 | 180 |
| Xi, investment, millions of dollars/year | 5 | 11 | 16 |

Then So = 36, Xo = 5, etc...., and

$(X-5)/(S-36) = (11-5)/(108-36)$ when $36 \leq S \leq 108$

$(X-11)/(S-108) = (16-11)/(180-108)$ when $108 \leq S \leq 180$.

If X = 50 thousand tons per year,

$(X-5)/(50-36) = (11-5)/(108-36)$

$X = 5 + (50-36)\ (11-5)/(108-36) =$

$= 5 + (14)\ (6)/(72)$

$= 5 + 1.167$

$= 6.167$.

Classification of resources.

For purposes of tracing resource balances and building chemical complexes, it is useful to classify resources three ways:

1) Major process inputs and outputs (major resources).

2) Minor process inputs and outputs, such as small amounts of auxiliary chemicals or minor byproducts (minor resources).

3) Common process inputs. These are inputs found in all (or nearly all) processes. They include the utilities: fuel, steam, electric power, and cooling water; labor: direct and supervisory; and plant investment (common resources).

Indirect Inputs

Indirect inputs are estimated, generally in money-value units, not from the process scale, but from two specific resource inputs: direct labor and plant investment. The most important indirect inputs are maintenance, depreciation, and overhead. Maintenance and depreciation are estimated as percentages of plant investment; overhead is estimated as a percentage of direct labor cost plus a percentage per year of plant investment.

For example, if overhead is 80% of direct labor cost plus 11% per year plant investment, then the labor and plant investment requirements for the given scale are first determined; then the labor input is costed out ( by multiplication by the wage rate); and finally the percentages given above are applied to labor cost and to plant investment. Occasionally the percentages vary as a step function of process scale.

Institutional requirements

The chemical industry depends for its technological advance on the presence of supporting institutions. These include: engineering education at the undergraduate and postgraduate levels; research laboratories; development and pilot-plant facilities; consulting engineering firms; professional associations; industry and trade associations; labor

training institutions; productivity institutes; export promotion associations and facilities; and many others.

While it is often not possible to associate the requirements for specific institutions with particular processes, whenever the need for high-level technology or specific institutional support is clear-cut, provision can be made to include this type of information in the data bank. Generally the information is only semi-quantitative: the amount of required service by specific institutions is impossible to establish; therefore the need is registered simply on a O-1 basis: O= no need; 1 = need exists.

General comments

In many cases comments must be attached to the data on given processes. These comments may refer to the grade, purity, etc.of particular resources; in this case they can be included with the item referring to the resource (see below under "information given for individual items"). In other cases, the comments refer to the process as a whole. Each such "general" comment is then given an item code of its own

A process may contain more than one general comment; each of these must have a separate item code.

An important kind of general comment refers to the rang- between minimum and maximum economical scales. Another important kind of general comment gives information for the conversion of units. For example, in order to convert tons/day to tons/year, the number of operating days per year is needed. This information can be given in a general comment. Likewise, information on the number of shifts, e.g., for converting men/shift to manhours/year, can be given in a general comment.

Information given for individual items

The following is a listing of all classes of information that can be recorded for various items. No one item can have every class of information recorded. For example, institutional requirement items omit all but the item code and (possibly) a comment. The classes of information are:

1) Item code (all items).
2) Resource specifications (for resources only).
3) Scaling parameters (for resources only).
4) Indirect parameters (for indirect inputs only).
5) Item comments (any item).

These principles have made it possible to work out a specific coding system for all processes and items in the data bank. The use of such data in heuristic programming models is discussed in the next section.

## 3. PROGRAMMING USE OF PROCESS DATA IN HEURISTIC MODELS

The basic concepts needed for using process data from the process bank in order to prepare heuristic development programs for the chemical industry are the following:

1) process vector;
2) technology tree;
3) program matrix;
4) complex vector;
5) capacity evaluation;
6) cost evaluation.

These concepts will be discussed both in relation to the design of a computerized system and in relation to a simple manual system that can be used for experimentation prior to computerizing the heuristic approach.

### Process vector

The purpose of maintaining a process bank is to be able to rapidly represent (on a CRT display or as a printout) the resource flows, plant investment, indirect input requirements and other relevant information for any processes under two specific conditions:

1) for any desired scale;
2) on an annual basis.

The scale of operation of a process is generally defined by market conditions (for the production of products marketed

outside the chemical industry) or by processing requirements (for intermediate products). Once the scale is known, all resource flows are fixed and can be calculated from the relevant scaling functions. For programming use, quantities given by shift (e.g., labor) or on a daily basis, must be annualized.

For example, the process vector of the ammonia process 0A10, operated at a scale of 36 thousand tons per year, will appear as follows:

| (Process and item codes) | (Unit of measurement codes) | (Amounts) |
|---|---|---|
| 0A10 | | |
| 1NH3 | KTONPY | +36.0 |
| 1NATGAS | MM3PY | -54.0 |
| 1NAOH | KTONPY | -.144 |
| 1CCR | KDOLPY | -72.0 |
| 1ELEC | MWHPY | -4320.0 |
| 1WATER | MM3PY | -.9 |
| 1LABOR | KMHRPY | -56.0 |
| 1SUP | KMHRPY | -16.0 |
| 1PLANT | MDOLLAR | -5.0 |
| 2MAINT | KDOLPY | -150.0 |
| 2DEPREC | KDOLPY | -400.0 |
| 2OHLAB | KMHRPY | -56.0 |
| 2OHKAP | KDOLPY | -550.0 |

The information presented by the computer in the form of a process vector is greatly simplified in comparison with the original process coding. When a process vector is required in the manual system, it must be calculated at the proper scale. In the computerized system, the scaling computerization will be made automatic, and the process vector can be displayed as indicated above, -- ideally, on a cathode ray tube or alternatively, in the form of a printout. In the computerized display of the process vectors the coded comments may be appended as desired.

Note that the following new units of measurement appear above (and have to be included in the directory of units of measurement):

| | |
|---|---|
| MM3PY | MILLIONS M3 PER YEAR |
| KDOLPY | THOUSAND DOLLARS PER YEAR |
| MWHPY | MEGAWATTHOURS PER YEAR |
| KMHRPY | THOUSAND MANHOURS PER YEAR. |

Note also that overhead appears not in one but in two rows. The first is that part which depends on direct labor; it has the units of labor and, for costing purposes, it has to be evaluated as the wage rate of direct labor. The second part depends on capital (plant investment) and is obtained directly in dollars (thousands) per year; for costing purposes, no further operation is required. These overhead concepts are coded as 2OHLAB and 2OHKAP, respectively.

In the manual system it may be convenient to maintain a file of such process vectors at the minimum economic scale, in order to save computations.

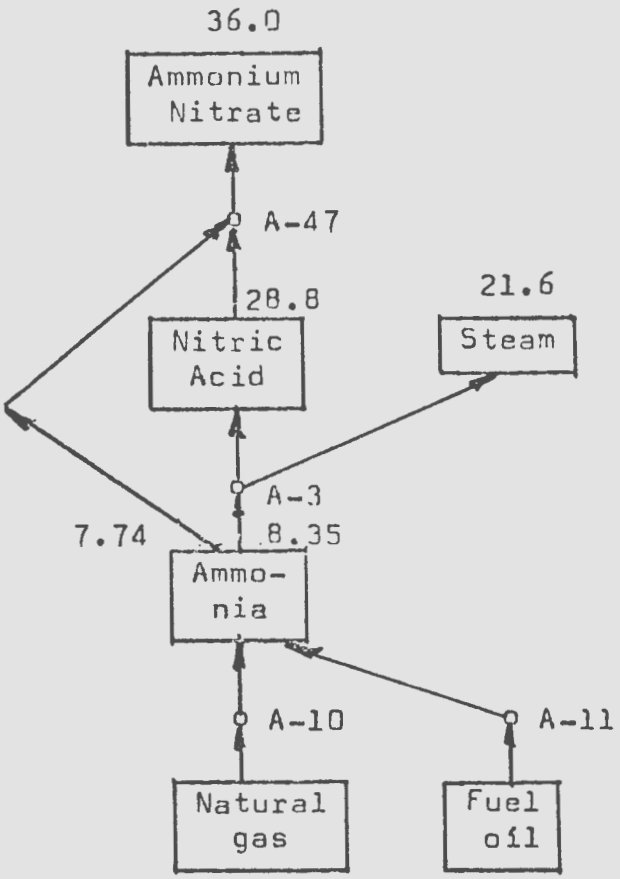
Technology tree

Process vectors can be organized into technology trees by indicating their interrelations in the process of production. For example, the production of ammonium nitrate can be represented by the technology tree shown in Figure 5.

In this tree, ammonia can be produced either from fuel oil or from natural gas. Ammonia, made by process A (see "Programming Data Summary...," op. cit.) converts into nitric acid by process A-3; then ammonia and nitric acid combine (shown by circle) to form ammonium nitrate via process A-4.

Figure 5

Technology Tree for Ammonium Nitrate




UNITS: Kilotons per year combined Ammonia requirement
7.74 8.35 16.09
Minimum ammonia scale 36.0
Minimum nitric acid scale 10.0
PROCESS CODE: Refer to: "Programming Data Summary for The Chemical Industry"

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Quantifying the technology tree

The technology tree can be quantified by choosing a scale, e.g., 36,000 tons per year, for the final output(ammonium nitrate) and producing intermediates (ammonia and nitric acid) in the amounts needed for conversion. The key questions at this stage are:

i) At what scale can the production of the final output be

justified by market conditions;

2) Are the final output and intermediates to be produced at scales exceeding the minimum economic scale?

The information needed to answer these questions is relatively limited. It consists of the input of the major intermediate resources (which generally vary proportionally with scale), and of the minimum economic scales of production of final and intermediate products.

In the illustrative case in Figure 5, the scale of production of the final product, ammonium nitrate, is chosen to correspond to the minimum economic scale. The intermediate, nitric acid, is required well above its minimum economic scale of 10 KTONPY. Ammonia is needed as a direct input (7.74 KTONPY), and indirectly for nitric acid production (8.35KTONPY). The combined amount is 16.09 KTONPY, but the minimum economic scale for ammonia production is 36KTONPY. Consequently, the ammonium nitrate process would have to be operated at a rate of(36.0)(2.24) of 80.64 KTONPY or more before the ammonia intermediate can be produced at the minimum economic scale; provided that there is no other need for ammonia that could use up part of the output of the minimum sized ammonia plant.

With the aid of the process bank, technology trees can be constructed

fast and efficiently, yet a large amount of computation is involved when many alternatives are under consideration. It is worthwhile to computerize these tasks in order to increase efficiency and in order to obtain not only feasibility information based on minimum scales, but also -- and equally rapidly in the computerized system -- costing information that is much more time-consuming to obtain manually.

The reason for this is that the technology tree can be constructed just by concentrating on the most important intermediate inputs, but for costing purposes, more exact computations are needed to obtain every process vector at the precise scale at which it fits into each trial version of each technology tree.

Key interrelationships in the technology tree

Figure 5 shows the five types of key relationships that appear in a technology tree; these are essential for programming the development of the industry:

1) Sequential relations. The output of one process becomes input to another, e.g., the output of the ammonia process A-10 becomes input into the nitric acid process A-3. Such sequential relations are used to trace back intermediates for a final output.

2) Joint intputs. The outputs of two or more processes combine as inputs into another; for example, the ammonia process A-10 and the nitric acid process A-3 produce outputs that combine to produce ammonium nitrate by process A-47. Sequential relations and joint inputs tie together processes into a complex.

3) Alternative sources. Two processes are alternatives when they produce the same output which is needed by another process. For example, the ammonia processes A-10 (from natural gas) and A-11 (from fuel oil) are alternatives for producing nitric acid and ammonium nitrate. Processes providing alternative sources for an input will generally compete with each other but sometimes (especially in cases of raw material shortage) they may supplement eachother.

For most intermediates, imports form an alternative to domestic production. Exceptions exist when the intermediate is difficult or expensive to transport in industrial quantities, e.g., ethylene or acetylene. Imports as an alternative are essential when an input is needed in an amount that is not sufficient to economical-scale domestic production.

In order to distinguish joint inputs from alternative inputs in groups of technology trees, joint inputs are shown as arrows terminating in a circle; an arrow then leads from the circle to the output commodity.

4) Joint outputs. A single process may produce more than one output; the outputs can then connect sequentially to separate processes. An important example is the joint production of caustic (NaOH) and chlorine ($Cl_2$) by electrologists of salt (NaCl). In Figure 5, nitric acid and steam are joint outputs of process A-3; nitric acid then feeds into process A-47.

Joint outputs are shown graphically as originating from a circle which is connected by an arrow (or arrows) to the inputs of the process.

In the programming of chemical industry development, joint outputs often raise problems of economic utilization. Further processes may be added to convert such joint products into marketable end products.

5) Alternative outlets. Two or more processes may form alternative outlets for the output of a given process. For example, in Figure 5, process A-3 and A-47 are alternative outlets for ammonia production.

Alternative outlets may compete with each other for a scarce intermediate product; but more typically in the programming of chemical industry development they will supplement each other in brining a production process up to a more economic scale. Often it is necessary to search for supplementary outlets in order to make a group of processes economical. Then several additional processes are typically included in the complex, in order to convert the

critical intermediate product into other kinds of marketable end-products.

Program matrix.

A program consists of two or more processes, each at a specified scale. The program matrix is a table whose columns are the individual process vectors. For example, the matrix of a program consisting of the production of 36,000 tons per year of ammonia and 10,000 tons per year of nitric acid is shown below; comments are omitted.

| | | 0A01 | 0A03 |
|---|---|---|---|
| 1NH3 | KTONPY | + 36.0 | — 2.9 |
| 1HN03 | KTONPY | ---- | + 10.0 |
| 1 NATGAS | MM3PY | — 54.0 | ---- |
| LNA0H | KTONPY | —.144 | ---- |
| 1CCR | KDOLPY | — 72.0 | ---- |
| 1MR | KDOLPY | ---- | — 60.0 |
| 1STEAM | KTONPY | ---- | + 7.5 |
| 1ELECT | MWHPY | —4320.0 | — 1900.0 |
| 1WATER | MM3PY | — .9 | — .9 |
| 1LABOR | KMHPY | — 56.0 | — 16.0 |
| 1SUP | KMHPY | — 16.0 | — 8.0 |
| 1PLANT | MDOLLAR | — 5.0 | — .65 |
| 2MAINT | KDOLPY | — 150.0 | — 19.5 |
| 2DEPREC | KDOLPY | — 400.0 | — 39.0 |
| 2OHLAB | KMHRPY | — 56.0 | — 16.0 |
| 2OHKAP | KDOLPY | —550.0 | — 58.5 |

In this matrix, 1HN03 stands for nitric acid, and 1MR for miscellaneous and royalties.

In the technology tree (Fig. 5), the ammonia and nitric acid processes are in a sequential relationship; i.e., the output of one (ammonia) becomes input to the other (nitric acid). In the matrix (see 1NH3 row) the corresponding entries are +36.0 and −2.9.

The scales chosen for this program have so far been arbitrary except that in each case the scale chosen has been the minimum economic scale. When two processes in a program are in a sequential relationship, however, it is desirable to balance the connecting resource, in this case, ammonia. This can be done by choosing the scales of the two processes so that the positive ammonia entry for ammonia process will be offset by the negative ammonia entry for the nitric acid process.

For example, if the scale of the ammonia process remains as it is, there is now a large ammonia surplus (+ 36.0 against - 2.9). Now increase the scale of nitric acid production in the ratio 36.0/2.9= 12.414. Then ammonia input into nitric acid will be-36.0, and the matrix will be as follows:

| | | 0A10 | 0A03 | COMPLEX |
|---|---|---|---|---|
| 1NH3 | KTONPY | + 36.0 | - 36.0 | 0. |
| 1HN03 | KTONPY | ---- | + 124.14 | + 124.14 |
| 1NATGAS | MM3PY | - 54.0 | ---- | - 54.0 |
| 1NAOH | KTONPY | - .144 | ---- | - .144 |
| 1CCR | KDOLPY | - 72.0 | ---- | - 72.0 |
| 1MR | KDOLPY | ---- | - 744.84 | - 744.84 |
| 1STEAM | KTONPY | ---- | + 93.105 | + 93.105 |
| 1ELEC | MWHPY | - 4320.0 | - 23586.6 | - 27906.6 |
| 1WATER | MM3PY | - .9 | - 11.173 | - 12.073. |
| 1LABOR | KMHPY | - 56.0 | - 48.0 | - 104.0 |
| 1SUP | KMHPY | - 16.0 | - 48.0 | - 64.0 |
| 1PLANT | MDOLLAR | - 5.0 | - 4.711 | - 9.711 |
| 2 MAINT | KDOLPY | - 150.0 | - 141.3 | - 291.3 |
| 2DEPREC | KDOLPY | - 400.0 | - 282.6 | - 682.6 |
| 2OHLAB | KMHRPY | - 56.0 | - 57.6 | - 113.6 |
| 2OHKAP | KDOLPY | - 550.0 | - 339.2 | - 889.2 |

Complex vector.

A third column of numbers has been introduced to show the algebraic sum of each row item. This column is the complex vector. It treats a group of two or more processes as an integrated chemical-industry complex and represents it by a single set of input and output figures. The complex shown here produces an enormous amount of nitric acid.

The nonlinear items associated with the nitric acid process have been derived by assuming that several near-maximal-size plants are used (the maximum shown in the reference "Programming Data Summary for the Chemical Industry," op. cit., is 46,000 tons/yr). If there were three nitric acid plants, each producing one-third the given output, the scale of each would be 41,380.0 tons per year, -- near the maximum.

In any realistic chemical industry development plan, this amount of nitric acid could rarely be marketed directly. It is therefore necessary to search for other ways of utilizing ammonia. In Figure 5, the ammonium nitrate process is added which uses additional ammonia and also uses up the nitric acid produced.

Choose the scales of ammonium nitrate and nitric acid production so that:

1) ammonia is produced in a minimum-sized plant

(36,000 tons per year);

2) ammonia is balanced;

3) nitric acid is balanced.

Then the scale of the ammonia process will be 36,000 tons per year, the scale of the nitric acid process will be 64,430 tons per year, and the scale of the ammonium nitrate process will be 80,530 tons per year.

These scales are still very large. They can be cut in half if half the ammonia output can be channeled into the production of urea fertilizer; then the scales will be: ammonia, 36,000 tons per year; nitric acid, 32,215 tons per year; ammonium nitrate, 40,265 tons per year; and urea, 31,034 tons per year (see process A-49 for urea in reference cited above). This program matrix and the corresponding complex vector can be readily constructed by the methods discussed above. The corresponding technology tree is also easy to derive; it will have a structure similar to that of Figure 5, but the urea process will be added on as one more arrow leading away from the box representing ammonia.

How complexes are put together

As shown above, putting together candidate complexes for chemical industry development makes use of both technology trees and program matrices. The basic principles of constructing candidate complexes for subsequent evaluation are the following:

1) Start with an end-product whose domestic production is of interest. Fix its scale of production at the projected market size.

2) Work back through intermediate inputs to processes in a sequential relation with the first (see section above:"Key interrelationships in the technology tree"). Fix the scale of each process so as to balance intermediates. Avoid both deficits (which would imply supplementary imports) and surpluses (which would imply a marketing dilemma) whenever possible.

3) When the scales of intermediates are below minimum economic scales, search for additional outlets for these intermediates. Survey processes which use the intermediates and see if these processes can lead via a sequence to marketable end-products.

4) When nothing else helps, a low-scale intermediate can be imported.

5) When joint products appear, search for outlets as under point (3) above.

6) The sequencing steps and outlet-finding steps indicated above will soon give rise to large program matrices with correspondingly complicated technology trees. Alternative processes will further expand the range of possibilities.

7) Evaluate candidate complexes as discussed below.

Capacity evaluation

In evaluating candidate complexes, the first key consideration is the relationship of the complex to existing domestic production capacity. Some of the in-

termediates that are required may already be domestically produced and will often have large excess capacities. If so, the complex will make use of these excess capacities and thereby confer large benefits on domestic industry.

Whenever a process appears in a candidate complex that is not yet used in domestic production, the key consideration in capacity evaluation is the projected scale of production of the process in question, in relation to the minimum economic scale.

In addition, capacity evaluation also takes into account institutional requirements. Since these are registered on a zero-one basis, the question that arises is whether the institutional base needed for the success of a productive process is or is not present in the country. When a particular set of institutions appears again and again as a bottleneck in the development of particular chemical-industry complexes, this constitutes a clear incentive for establishing the missing institutions.

The construction of complexes and capacity evaluation are not independent but interact continually. Instead of starting the programming task with an end-product that appears attractive for import substitution, one might as well start with an intermediate that has a large excess capacity, and proceed as

shown under step (3) of the previous section.

Capacity monitoring

When a task force is assigned the responsibility of continuously monitoring the development of the chemical industry, one of the key tasks is to set up and keep up-to-date two files that are useful in program construction and capacity evaluation. These are:

1) Plant/product capacity file: What is produced, where, in what amounts, and how much excess capacity exists.

2) Domestic market/import file: What major products are now imported, in what amounts, what prices, for what use, and when has the possibility of import substitution been last considered.

Each of these files is the starting point for the construction and evaluation of candidate complexes. This work needs to be undertaken on a continuous basis for the industry as a whole, since individual productive entities typically do not consider the entire range of industry-wide possibilities and opportunities.

Cost evaluation

Cost evaluation consists of applying prices -- either market prices or opportunity costs -- to the input and output items of a complex vector.

Output items multiplied by their prices become revenues of the complex; input items multiplied by their prices become costs. The balance of revenues and costs is the gross profit which must be divided by total investment to arrive at the rate of return of the complex in question.

If all intermediates of a complex are balanced, then the only required prices are those of end-products and of primary inputs. Primary inputs should be costed both at market and at opportunity cost. Raw materials such as sulfur, salt, limestone, phosphate rock, natural gas, coal, oil, or agricultural commodities, often have a substantially higher market price than their opportunity cost. Then a chemical complex based on them can have a large national benefit even in the presence of a modest commercial profitability.

At times certain raw materials appear with extremely high costs based on very limited domestic production. For example, salt may be produced from sea water on a handicraft basis for table use. The cost of this process is clearly no proper basis for evaluating the feasibility of a chlorine-and-caustic process based on salt electrolysis. Whenever such situations arise, it is necessary to add a process to the technology tree that represents the production of the raw material at an industrial scale, using modern technology.

This may carry the representation of technology slightly beyond the bounds of the chemical industry itself, but otherwise represents no drastically new departure as compared with what has been discussed before.

End products and imported intermediates should be accounted for at c.i.f. cost, including import duties for market-price evaluation, but without duties for social cost/benefit evaluation.

Intermediates drawing on excess domestic capacity should be costed both at market price and at marginal cost (for social cost/benefit evaluation).

Computations needed for cost evaluation

The computations needed for cost evaluation are very simple:

1) the construction of the complex vector from individual process vectors; and

2) the multiplication of the complex vector by a price vector.

The first has been extensively discussed before; the second is an item-by-item multiplication followed by one summation. All computations are simple and can in principle be readily performed in the manual system for any single candidate complex. The manual system is, however, not well suited to performing a large number of repetitive calculations for a great variety of candidate complexes based on a extensive data bank.

To cope with these conditions, computerization is required. This task will be discussed in the next section.

Complementary files in the system: Summary.

In addition to the process data bank, the following files form a complementary part of the manual system:

-Directory of items. Resources, indirect inputs, institutions, general-comment items.

-Directory of units of measurement. Includes conversion rules.

-Plant/product capacity file. Organized by product. What is produced, where; total capacity, current production, excess capacity; projection of excess capacity.

-Domestic market/import file. Organized by product. Current imports; projected imports. Destination (use). Has import substitution been considered? When, by whom?

-Import price file for chemical products. Organized by product. C.I.F. price before and after customs duties and other governmental charges. Needed for all chemical products, not only for those now imported.

-Domestic price file. Organized by products, raw materials, and other input and output items. Both market cost and opportunity cost needed. For domestically producted products, the internal transfer price is often a reasonable measure of opportunity cost.

## 4. CONCLUSION: COMPUTERIZATION PROSPECT

Shortcomings of the manual system

The manual system is cumbersone to operate unless it is of very restricted size and unless the number of candidate complexes to be evaluated is very small, for the following reasons:

1) While the computations are simple, they are very numerous.

2) It is difficult to keep track of a large number of alternatives; beyond a certain point, there is a tendency to drown in endless repetitive calculations, and the number of worksheets becomes almost unmanageable.

3) The training and supervision of computing clerks becomes extremely onerous. Unless this is managed exceptionally well, the computations will be subject to errors and risky to use in concrete decisions.

Computerized system capabilities

The computerized system must have the following capabilities:

1) Directories. Assemble and update from process input; modify codes; modify names; sort; convert units of measurement; display.

2) Process bank. Input new processes; modify and erase existing processes; convert units of measurement of existing processes; display a stored process; graphically display the variation of specified inputs with process scale; display a process vector at any scale in any desired units, with or without comments.

3) Technology tree. Find alternative source processes for producing a resource. Find alternative major outlet processes for disposing of a resource. Sequence specificed processes at appropriate scales. Flag process scales that fall outside of economical scale limits. Construct a technology tree corresponding to a specified program matrix. Display a specified technology tree graphically, with or without comments supplied.

4) Program matrix and complex vector. Construct matrix of specified processes at specified scale. Delete a process. Compute complex vector. Display program matrix and complex vector with or without comments.

5) Complex evaluation. Compare a specified complex vector with a list of excess domestic capacities, with a list of available institutions, and with scale limits for potential production. Display results. Find sequences connecting the complex vector with a list of desired import contributions. Display results. Multiply complex vector by a vector of prices to be used for costing purposes. Display revenues and costs item by item, algebraically summed, or as a return on investments (net social benefit ratio when using opportunity costs).

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