Finally, computer simulation can be used as a purely exploratory tool. This sound strange. One would be inclined to say that one can not "discover anything by simulation because you can never get out what you have not put in. Computer discoveries, in this respect, are not unlike mathematical discoveries. In fact before computers were actually available this kind of numerical charting of unknown territory was never considered.

The best way to explain it is to give an explicit example. In the mid 1950s, one of the burning questions in statistical mechanics was this can crystals form in a system of spherical particles that have a harsh short range repulsion, but no mutul attraction whatsoever? In a very famous computer simulation, Alder and Wainwrighter and Wood & Jacobson showed that such a system does indeed have a first order freezing transition. This is now accepted wisdom, but at the time it was greeted with skepticism. For instances at a meeting in New Jersey in 1957, a group of some 15 very distinguished scientists (among whom were 2 Nobel laureates) discuss the issue. When a vote was taken as to whether hard spheres can form a stable crystall, it appeared that half the audience simply could not believe this result. Howevere, the work of the past 30 years has shown that harsh repulsive forces really determine the structural properties of a simple liquid and that attractive forces are in a sense of secondary importance.

Keeping the history and versatility of Chemical Engineering in the background, considering the AIChE and working definitions of improved and matured chemical engineering, and being the challenges ahed of a chemical engineer in mind, the complete process design can be viewed as being carried out in the following three stages-

a) Process synthesis

b) Process analysis

c) Optimization

a) Process Synthesis

Process synthesis is the first stage of the process design activity. Flowsheet of the process is constructed including all equipment and their interconnections. For this purpose informations are gathered for both simple and complex design problems.

A systematic procedure has been laid down for screening the alternatives by following five levels of design decision hierarcy. The five levels of decision hierarcy in conceptual design are

1. Batch versus continuous production
2. Input-output structure of the flowsheet
3. Recycle structure of the flowsheet

4. General structure of the separation system
   a) Vapor recovery system
   b) Liquid recovery system
5. Heat-exchanger network synthesis (energy integration)

A beginner can subsitute the evaluation of a number of extra calculations for experience during the development of a conceptual design by following this hierarchical decision procedure. However, the penalty paid in the form of time required to screen more alternatives is not very high, as short-cut calculations are used. As a designer gains experience, it is possible to recognize alternatives that should not be considered for a particular type of process, and thereby improve efficiency.

b) Process Analysis

Process analysis is the 2nd stage in process design after process synthesis. Once the process flowsheet is synthesized, an analysis is required for the following purposes:

- Solving material and energy balances for a steady process
- Sizing and costing the equipment
- Evaluating the worth of the flowsheet

Chemical process simulation, also known as 'flowsheeting', is represented by a mathematical model in order to obtain information about the response of a plant to varius inputs. The salient features and requirements of general purpose simulation are

- Modular approaches (Sequential and simultaneous) to process simulation
- Equation-solving approach (unconstrained and constrained material balances)
- Decomposition of networks (partitioning, tearing algorithms etc)
- Convergence promotion
- Physical and thermodynamic properties
- Specific-purpose simulation and
- Dynamic simulation

c) Optimization

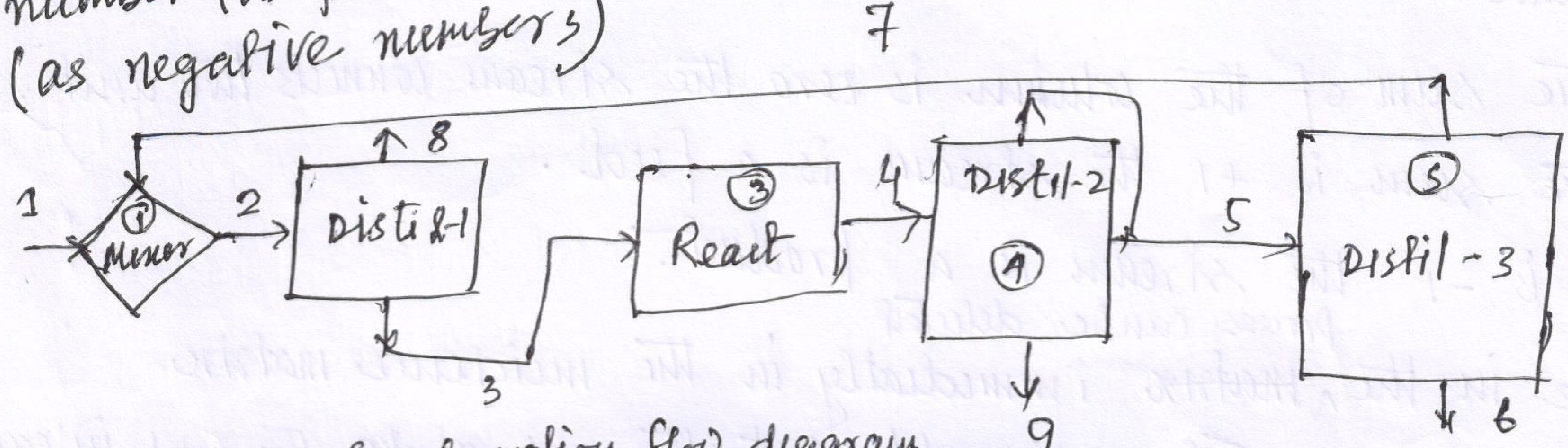
This is the final step in the development of a process flowsheet. Many constrained and unconstrained optimisation techniques are employed for this purpose. Of late nontraditional optimization techniques such as genetic algorithms and differential evolution are being used. All these interrelated activities should obviously lead to an optimal design and safe operation of a chemical plant.

## Conversion of information Diagram into Numerical form

There are four methods
- The process matrix method
- The stream connection matrix method
- The incidence matrix method
- The adjacency matrix method

### The process matrix

- Each unit in the information flow diagram is given one row of the process matrix
- The contents of that row are the number of the particular unit, the name of the unit computation representing the unit and the input stream number (as positive numbers) followed by the output stream number (as negative numbers)




Process Metric of information flow diagram

| unit | unit computation name | Associated streams numbers | | |
|---|---|---|---|---|
| 1 | MIXER | 1 | 7 | -2 |
| 2 | DISTL | 2 | -8 | -3 |
| 3 | REACT | 3 | -4 | |
| 4 | DISTL | 4 | -5 | -9 |
| 5 | DISTL | 5 | -7 | 6 |

- order of the input and output stream numbers are important
- Heat exchanger the first input & output may be the process fluid the second input and output the service fluid
- Distillation unit the first output is overhead and second the bottoms

It reveals the following
- what stream links what units
- what unit computation represents each unit
- the name of the unit computation represents each unit
- the order of the order of the input and output streams of a unit.

### The Stream Connection matrix

The stream connection matrix is an array with these entries per row
The first entry is the stream number and the second and third are the numbers of the equipment units from which that stream comes and to which it goes respectively.

| Stream number | From unit number | to unit number | | | |
|---|---|---|---|---|---|
| 1 | 0 | 1 | 6 | 5 | 0 |
| 2 | 1 | 2 | 7 | 5 | 1 |
| 3 | 2 | 3 | 8 | 2 | 0 |
| 4 | 3 | 4 | 9 | 4 | 0 |
| 5 | 4 | 5 | | | |

## The incidence matrix method

| unit no. | Stream number 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 1 | -1 | | | | | 1 | | |
| 2 | | 1 | -1 | | | | | -1 | |
| 3 | | | 1 | -1 | | | | | |
| 4 | | | | 1 | -1 | | | | -1 |
| 5 | | | | | 1 | -1 | -1 | | |
| sum | 1 | 0 | 0 | 0 | 0 | -1 | 0 | -1 | -1 |

(+1) shows that stream enter the unit

(-1) indicates conversely shows that the stream leaves the equipment.

a Blank or zero shows that the stream does not connect to that equipment.

If the sum of the column is zero the stream connects two units.

If the sum is +1 the stream is a feed.

If it is -1 the stream is a product.

Recycle in the process can be deleted immediately in the incidence matrix

If no rearrangement of rows would put the -1 above the +1 in each column having a zero sum. Thus stream 7 in the following table shows that there is recycle.

The incidence matrix contains the same information as the stream connection and thus has less information than the process matrix

## The Adjacency Metrics Method

| | To unit no. 1 | 2 | 3 | 4 | 5 |
|---|---|---|---|---|---|
| From unit No. 1 | | 1 | | | |
| 2 | | | 1 | | |
| 3 | | | | 1 | |
| 4 | | | | | 1 |
| 5 | 1 | | | | |

Adjancy Metrics of Information Flow diagram.