Prediction of Variable Process Performance by Stochastic Flow Sheet Simulation

The method of stochastic (Monte Carlo) simulation is employed to determine variable process performance of a 545 Mg/d ammonia plant. Operating conditions and equipment reliability are varied in a flow sheet simulation model of the process. Probability distributions of the plant production capability and failure times are generated. These data agree closely with the operating experience of an actual ammonia plant.

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SCOPE

Flow sheet simulation programs normally employ steady state or average values of the process variables to obtain predictions about the material balance, energy requirements, or economics of chemical processes. This procedure provides a prediction of the average performance of the process but does not provide information on the variability of process behavior caused by equipment malfunction and changing operating conditions. A knowledge of variable process performance should lead to an improved process design and will permit a more accurate analysis of process economics.

The purpose of this study is to demonstrate how variable process performance can be predicted by the technique of stochastic simulation. A standard flow sheet simulation program, CHESS, is employed, with modifications, to model a 545 Mg/d ammonia plant. Equipment failures and operating conditions are represented as random variables and simulated in the computer model to provide variations in the production capability of the process.

CONCLUSIONS AND SIGNIFICANCE

It is shown that flow sheet simulation programs can be adopted to stochastically simulate variable process behavior. Probability distributions of plant production capability and failure times are generated using this procedure. The production capability of the ammonia plant predicted by simulation agreed closely with that of an operating facility.

Furthermore, the plant failure rates predicted by stochastic flow sheet simulation duplicated that of the real plant. These failure rates are considerably higher than those reported in the literature for similar ammonia plants. Simulation might be adopted as a more accurate means of forecasting plant failures. The exponential probability distribution was found to represent the failure times of the ammonia plant studied. This distribution might be used in the future to describe failures in other chemical processes.

The general procedure for the steady state simulation of chemical processes is to model the process flow sheet with a modular computer program which provides material and energy balance data for each stream and equipment module in the process. These data can then be used to size equipment and compute the process economics; or these data might be used to predict the performance of a specified process design. Steady state or average values of the variables in the process are normally employed in these studies; consequently, only a measure of the average plant performance is obtained, as shown for an ammonia plant in the following example.

AMMONIA PLANT SIMULATION

Figure 1 is a typical chemical process flow sheet (Bressler and James, 1965) showing the equipment for production of ammonia by steam reforming of natural gas. Briefly, this process involves the reaction of steam, natural gas, and air in two stages to yield a mixture of N_2, H_2, H_2O, CO, and CO_2. The carbon monoxide is then converted to CO_2 by reaction with steam. The gases from this shift converter are primarily N_2, H_2, and CO_2 with a H_2:N_2 ratio of about 3:1. The CO_2 is removed by absorption with monoethanolamine and final traces of CO and CO_2 are removed by reaction with H_2 over a nickel catalyst. Ammonia is produced by reaction of H_2 and N_2 and the ammonia is recovered by refrigeration. In recent years plants employing the process in Figure 1 have been built in sizes ranging from 545 Mg/d (600 tons/day) to 1,360 Mg/d (1500 tons/day) (Finneran et al., 1968).

CHESS (Chemical Engineering Simulation System), a modular flow sheet simulation program developed at the University of Houston, was used to model the ammonia process of Figure 1. A description of this program and its

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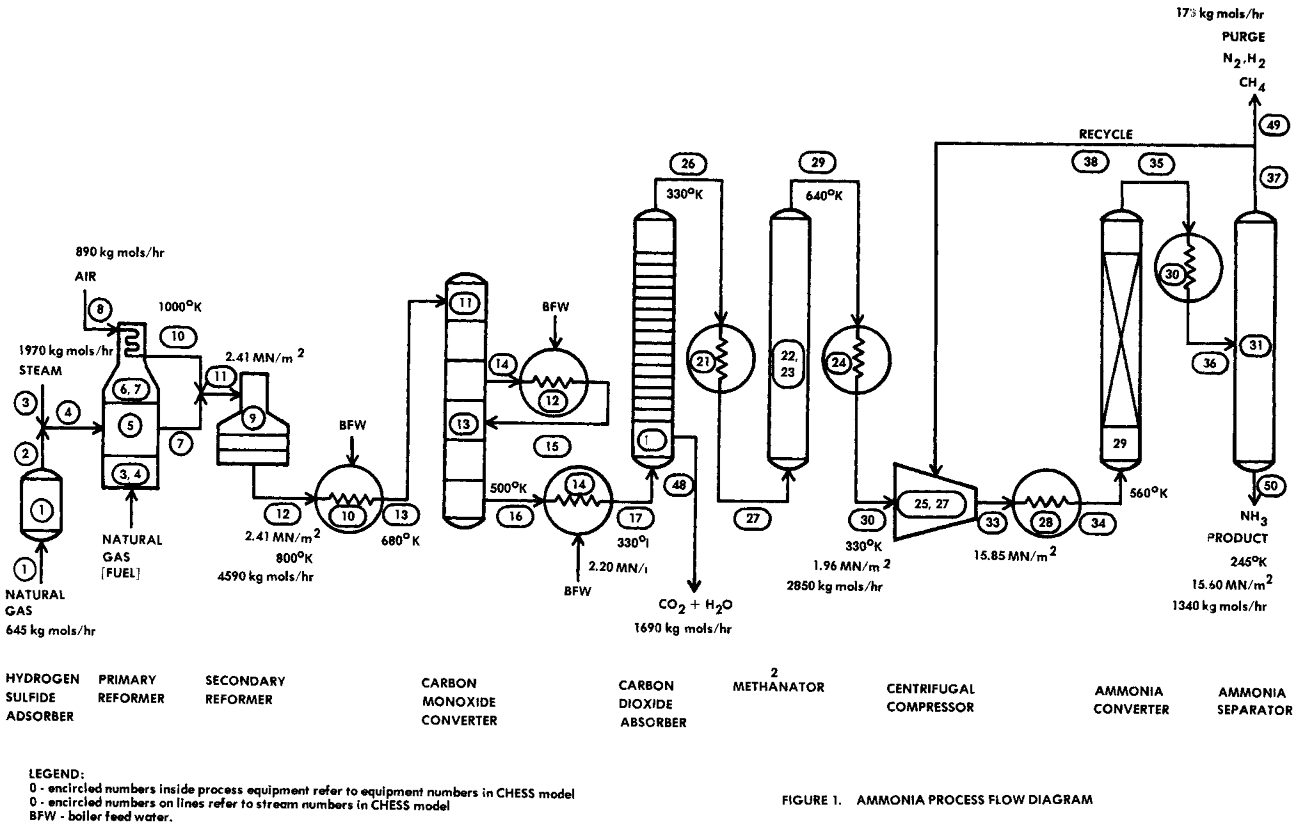

Fig. 1. Ammonia process flow diagram.

use is readily available (Motard et al., 1968) and will not be provided here. Figure 2 shows the CHESS model of the ammonia process. Stream and equipment numbers given in Figure 1 correspond to those in Figure 2.

The results from the CHESS steady state simulation of a 545 Mg/d ammonia plant are shown in part in Figure 1, which gives the temperatures, pressures, and some flow rate data for the various streams in the process. CHESS also provides the stream compositions and enthalpies, and these data are not shown. Stream 50 is the ammonia production rate, shown as 1350 kg moles NH_3/hr or 545 Mg/d, the design (or most probable) on-stream production rate.

In the above CHESS model, the operating conditions in the various process modules were considered constant. For example, in the steam reformer, REAC-9, the conversion of methane was used as 0.92 and this represents the average of a range of possible values of methane conversions that could occur.* Similarly, other variable parameters in this process were also used in the model at their average values. When using these averages, a process simulation produces information only about average plant performance, and, it is assumed that the average simulated plant performance will result from use of averages of the variables.

The performance of a simulated process can be measured by the quantity of product resulting from the calculations in the model. In this discussion, this quantity of product is termed production capability and is defined by Equation (1):

$$PC_i = (1 - f_i)OPC_i \tag{1}$$

* It should be made clear that the variations that are referred to above are those that would occur within a fully instrumented plant, and that this discussion is not concerned with studying instrumentation or process controls.

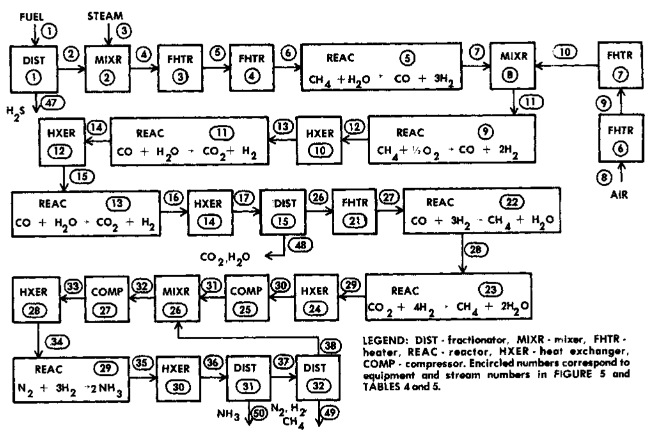

Fig. 2. Chess model of ammonia process.

The on-stream production capability is independent of downtime, and variations in OPC with time are the result of changing operating conditions.

A flow sheet simulation that uses averages of the variables could not be used with Equation (1) to predict variations in production capability with time but would provide the average on-stream production capability $\overline{OPC}$. With this value and an estimate of the average fractional downtime $\bar{f}$, the average production capability $\overline{PC}$ can be computed from Equation (2):

$$\overline{PC} = (1 - \bar{f})\overline{OPC} \tag{2}$$

For the ammonia plant in Figure 1, the average fractional downtime predicted by Piombino (1965) and Bressler and James (1965) is 0.05, or this plant would be expected to be operable 95% of the time. The average on-stream production capability from the CHESS model of Figure 2 is 545 Mg/d. Thus, by Equation (2) the average production capability of a 545 Mg/d ammonia plant would be predicted to be 517 Mg/d (210,000 tons/year).

In certain instances the information from Equation (2) may not be adequate, and it may be desirable to predict how the simulated plant performance varies during each time interval of some future planning period. One such instance might be the prediction of the sales volume when the sales demand is variable with time and, consequently, the variations in production capability become important. The data from this simulation study were used in a broader study (Gaddy, 1972) to compare the economics of large and small ammonia plants, which showed that sales volumes found by simulation could be as much as 10% lower than those predicted from averages.

Other examples of when a knowledge of varying plant performance might be desirable are if the average fractional downtime cannot be estimated or if the average on-stream production capability $\overline{OPC}$ would not be reflected accurately by the average values of the process conditions used in the simulation model. Also, if flow sheet simulation is being used for design purposes, a knowledge of variable behavior is necessary if design criteria are to be satisfied.

STOCHASTIC SIMULATION

In order to predict varying production capability with a flow sheet simulation model, it is necessary to be able to define the variations of failure time or on-stream production capability in Equation (1) for the time intervals of the study. The definition requires a knowledge of the changes in operating conditions within the process, such as equipment malfunctions and catalyst activity. If these variations are random and if the probability distribution of each variable can be defined, the technique of Monte Carlo simulation can be used to vary the operating conditions within the computer model of the process. The Monte Carlo procedure provides values of variable parameters from probability distributions of these parameters by use of random numbers. An explanation of Monte Carlo, or stochastic, simulation is available in the recent literature (Gaddy, 1972; Hertz, 1964, Sprow, 1967; Tayyabkhan and Richardson, 1965) and is beyond the scope of this discussion.

The purpose of this study is to demonstrate how process variables can be manipulated within an ammonia plant CHESS simulation by Monte Carlo procedure to obtain variations in failure time and on-stream production capability. A time interval of one week was used in this simulation. In order to use the stochastic simulation procedure, data for the probability distributions of the weekly failure rates and operating performance of the equipment modules shown in Figure 2 were required. These data were obtained from an operating 545 Mg/d ammonia plant.

Variable Failure Time

In describing the failure time of an item of equipment, it is necessary to consider when that equipment will fail and how long before it is returned to service. Thus, two probability distributions are required: one distribution to define the incidence or frequency of failure and another distribution to describe the length of failure.* These data for the 545 Mg/d ammonia process are shown in Table 1. Discrete distributions were used to describe the frequencies of equipment failures and these are shown in column 3 of Table 1. Triangular distributions were used to describe failure durations. The triangular distribution is defined by minimum, maximum, and most likely values shown in columns 4, 5, and 6. The equipment numbers shown in Table 1 correspond to those in Figures 1 and 2 except for equipment number 1, which refers to all equipment external to the chemical process, such as supply of utilities. Some equipment items in Figure 2 are not shown in Table 1 and this means that these items had not caused a failure in the real plant.

In modifying the CHESS model to determine plant failures from the data of Table 1, two approaches were considered: (1) determine the downtime for each item of equipment as the CHESS system computes the material and energy balances in each equipment module, or (2) determine the downtime prior to the material and energy balance computations. The latter alternative was chosen because when the total plant downtime exceeded the time interval of one week, that is, $f_i = 1$, no product could be produced and the on-stream production capability was superfluous.

Consequently, CHESS was modified so that the first calculations were to find plant failure time, and providing this time exceeded one week, the calculations for that period were terminated. Each item of equipment was sampled* in sequence to determine if that item experienced a failure during the week and, if so, how long the failure lasted. The downtimes for each piece of equipment were added giving the total downtime for the entire plant. Downtimes in excess of seven days were carried over into the subsequent week. If the plant failure time was less than one week, CHESS proceeded to determine the plant on-stream production capability.

Variable Process Conditions

There are many ways in which changing operating conditions could be handled in a CHESS simulation. Each variable in every equipment item (temperature, pressure, etc.) could be simulated using the Monte Carlo technique. However, the simulation can be simplified if the

TABLE 1. FAILURE PROBABILITY DATA FOR EQUIPMENT IN A 545 MG/DAY AMMONIA PLANT

Equip. number	Equip. function	Probability of no failure occurring	Failure duration, days: Minimum	Maximum	Most likely
1	PLANT	0.8218	0.083	0.167	0.083
F-4	FHTR	0.9604	2	6	4
R-5	REAC	0.9802	2	20	8
H-10	HXER	0.9802	3	10	7
R-11	REAC	0.9802	1	3	2
H-12	HXER	0.9934	1	3	2
R-13	REAC	0.9802	1	3	2
D-15	DIST	0.9802	1	8	2
R-23	REAC	0.9934	2	3	2.5
C-27	COMP	0.9208	1	14	4
H-28	HXER	0.9960	2	7	4
R-29	REAC	0.9802	0.083	0.083	0.028
H-30	HXER	0.9802	1	3	2
D-31	DIST	0.9406	0.042	0.042	0.021

* A single distribution might also be utilized by assigning zero failure time to portions of the distribution describing the length of failure.

* The process of sampling from probability distributions using the Monte Carlo method can be briefly exemplified as follows: Obtain a random number between zero and 1; if that number is greater than 0.8218 (the probability of no failure occurring for equipment number 1, Table 1), equipment number 1 failed; and if the number is less than 0.8218, no failure occurred. Similarly, triangular distributions can be sampled to provide failure durations.

TABLE 2. PROBABILITY DISTRIBUTION DATA FOR EQUIPMENT OPERATION IN A 545 MG/DAY AMMONIA PLANT

Equip. no.	Equip. funct.	Variable parameter	Design values of the variable parameter	Triangular distribution data for the variable (fraction of the design value) Min.	Max.	Most likely
D-1	DIST	Fractional H_2S removed	0.0072	0	139.0	1.0
F-4	FHTR	Heat transfer capacity (Gj/hr)	27.60	0.99	1.01	1.0
R-9	REAC	Fractional CH_4 converted	0.92	0.95	1.02	1.0
R-11	REAC	Fractional CO converted	0.80	0.97	1.02	1.0
R-13	REAC	Fractional CO converted	0.92	0.87	1.042	1.0
D-15	DIST	Fractional CO_2 removed	0.9996	0.67	3.3	1.0
R-22	REAC	Fractional CO converted	0.9965	0.9963	1.0018	1.0
R-29	REAC	Fractional H_2 converted	0.1942	0.95	1.02	1.0
D-31	DIST	Fractional NH_3 removed	0.15	0.99	1.01	1.0

variables in each item of equipment can be combined into a single parameter which reflects the overall variation in operation.

In this study, one key parameter was chosen to represent the random behavior of each major piece of equipment, and these parameters and their triangular distribution data are shown in Table 2. The minimum and maximum values are shown as the fractional deviation from the design (or most probable) value.

CHESS was modified so that the determination of process conditions from the probability data of Table 2 was done in each equipment module. As the program proceeded through the material and energy balance calculations to determine the on-stream production capability for that week, the Monte Carlo procedure was used to provide values of the changing operating conditions in each module. Where a module was used to represent more than one item of equipment, the probability data had to be identified by the equipment number. When recycle calculations were involved, only an initial random value of each variable was used.

SIMULATION RESULTS

A sample of the CHESS stochastic simulation of the weekly operation of the 545 Mg/d ammonia plant is shown in Table 3. The on-stream production capability is seen to vary slightly from one week to another according to the operating conditions. The individual item of equipment that failed and its failure time are identified in Table 3. The failure times for the plant as a whole and the fractional weekly failure times are also shown. It will be noted that occasionally the plant is down for the entire week, that is, $f_i = 1.0$. The plant production capability, computed from Equation (1), is seen to vary considerably from week to week, depending primarily upon variations in fractional failure times.

Table 3 represents a prediction of the operation of the ammonia process for a period of 20 weeks. The simulation could be continued to provide predictions of plant performance for several years if desired. However, this might require excessive computer time. Values from Table 3 and additional simulation runs could be arranged into probability distributions which might then be used to simulate future plant performance using the Monte Carlo procedure.

TABLE 3. SAMPLE OF CHESS OUTPUT FOR 545 MG/DAY AMMONIA PLANT

Time period	On-stream production capability Mg/day	Equip. no. failed	Time of failure days	Plant failure time, days	Fractional weekly failure time (f_i)	Production capability (PC) Mg/day
1	540.8	0	0.0	0.0	0.0	540.8
2	539.4	0	0.0	0.0	0.0	539.4
3	536.1	0	0.0	0.0	0.0	536.1
4	540.0	0	0.0	0.0	0.0	540.0
5	531.1	0	0.0	0.0	0.0	531.1
6	544.1	15	1.94	1.94	0.28	393.4
7	538.1	0	0.0	0.0	0.0	538.1
8	0.0	4	4.13	8.30	1.0	0.0
		5	4.17			
9	545.0	0	0.0	1.3	0.19	443.6
10	536.2	1	0.71	0.71	0.10	482.6
11	527.8	0	0.0	0.0	0.0	527.8
12	540.8	0	0.0	0.0	0.0	540.8
13	531.5	0	0.0	0.0	0.0	531.5
14	540.8	27	3.07	3.07	0.44	297.1
15	533.4	0	0.0	0.0	0.0	533.4
16	542.1	0	0.0	0.0	0.0	542.1
17	535.3	0	0.0	0.0	0.0	535.3
18	536.0	0	0.0	0.0	0.0	536.0
19	538.5	31	0.53	4.06	0.58	226.2
		1	3.53			
20	534.0	27	5.54	5.80	0.83	91.5
		1	0.26			

A probability distribution for ammonia plant on-stream production capability is shown in Figure 3. This curve is the result of 500 simulation runs like those in Table 3. The maximum and minimum observed on-stream production capabilities were about 555 and 520 Mg/d respectively. Interestingly, the average on-stream production capability, OPC, from these data was about 535 Mg/d, slightly below the design average of 545 Mg/d. The variations in the simulated on-stream production capability were small, but agreed well with those observed in the actual operating facility.

From the simulation results, probability data can also be compiled for the failure incidence and failure times for the entire ammonia plant. The failure incidence of the plant as a whole was found to be 0.414, or the probability that a plant failure would occur during any given week was 0.414. Figure 4 is the cumulative distribution of the plant failure times for the 545 Mg/d ammonia plant. This figure also shows (dashed line) the theoretical exponential distribution, which is often used to describe equipment service times. The exponential distribution gave a statistically significant fit (at the 99% confidence level) of the simulation data of Figure 9 when an exponent of 3.5 was used. This value of the exponent was the average failure time of the data from Figure 4 and could also be obtained from the data of Table 1. The plant failure times have the exponential memory property, that is, the repair time is independent of the length of service (Hillier and Lieberman, 1967). Thus, the exponential distribution of failure times is reasonable for the data of this study, and, it might be found that this distribution can also be used to forecast other chemical process downtimes in future studies of this type.

The average fractional failure rate $\bar{f}$ compiled from the simulation data was found to be 0.2, considerably above the value usually reported for these plants. This average failure rate agreed identically with that experienced by the actual operating ammonia plant. Using this value of $\bar{f}$, in Equation (2) the average production capability of this ammonia plant is predicted to be only 436 Mg/d (172,000 tons/year), or about 16% less than would be expected when using averages reported in the literature.

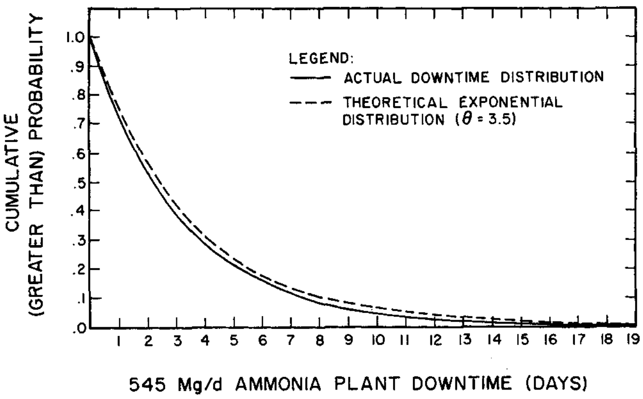

Fig. 3. Cumulative distribution of 545 Mg/day ammonia plant on-stream production capability.

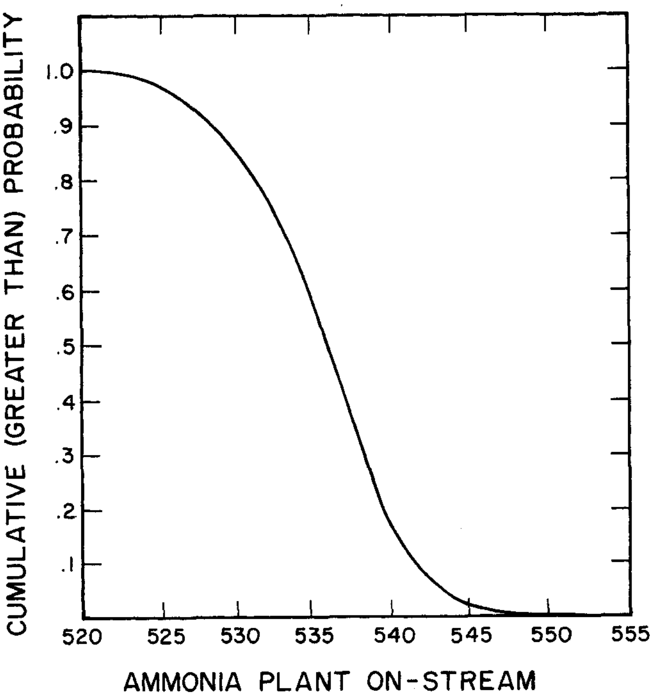

Fig. 4. Cumulative distribution of 545 Mg/day ammonia plant failure time.

SUMMARY

In summary, it can be seen that flow sheet simulation programs can be used to determine varying process behavior using Monte Carlo procedures. This information can be quite useful in design of processes and in predicting economics.

In this study, the behavior predicted by simulation agreed quite well with that of an existing facility. However, the accuracy of stochastic simulation depends upon the accuracy of the probability data. This study used actual plant data; therefore, the simulation results were expected to agree with plant experience. Plant data may not be available for every study. However, if conditions are recognized as variable, it may be better to estimate these variations than to ignore them.

NOTATION

PC_i = production capability of the process during time period i, Mg/d

f_i = fractional downtime caused by equipment failure during time period i

OPC_i = on-stream production capability, the amount of product that the plant can produce while operating or on-stream during time period i, Mg/d

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Manuscript received March 7, 1973; revision received August 13 and accepted August 14, 1973.