New Directions in Process Simulation

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ABSTRACT

In today's competitive economy, the engineer must become as productive as possible. One means of increasing productivity is to use process simulation packages and other engineering computer aids to their maximum utility. In addition to increasing the engineer's productivity, process simulation packages may be used to analyze operating problems in existing plants and to design new facilities. In general, the virtues of process simulation have become well recognized in the industry and most process engineers have some type of simulation capability available to them. In the last few years, major emphasis has been placed on increasing the engineer''s productivity with process simulation packages. This includes the "up front" time to learn to use the simulator as well as the time to produce a completed analysis once the engineer has become familiar with the simulator. This need for increased engineering productivity has generated a new type of tool called interactive process simulation.

INTRODUCTION

In today's competitive economy, the engineer must become as productive as possible. One means of increasing productivity is to use process simulation packages and other engineering computer aids to their maximum utility. In addition to increasing the engineer's productivity, process simulation packages may be used to analyze operating problems in existing plants and to design new facilities.

Process simulation has become the primary tool for exploring design alternatives as well as debottlenecking and expanding existing facilities. In general, the virtues of process simulation have become well recognized in the industry and most process engineers have some type of simulation capability available to them.

In the last few years, major emphasis has been placed on increasing the engineer's productivity with process simulation packages. This includes the "up front" time to learn to use the simulator as well as the time to produce a completed analysis once the engineer has become familiar with the simulator. This need for increased engineering productivity has generated a new type of tool called interactive process simulation.

Interactive process simulators are generally referred to as those where the engineer can freely interact with the computer throughout the simulation. The input information is entered in a conversational type mode, the inputs are checked as they are entered and on-line help is available as needed.

In addition, the user is able to direct the computer to perform calculations for any part of the plant at any time during the simulation. Numerous other features of interactive process simulation will be discussed later in the paper.

HISTORICAL PERSPECTIVE OF PROCESS SIMULATION

Of necessity, the early process simulators were used in the batch mode. Since the large mainframes of the late sixties and early seventies were expensive both to purchase and operate, programs run on these machines were designed on the premise that the computer's time was more valuable than that of the engineer. This meant that the engineer was required to produce an input data set for the computer on an off-line device, usually a card punch or paper tape punching teletype.

The resulting simulation input was then submitted to a "batch" processor, which read the entire card deck or paper tape, executed the simulation in a burst, and then printed the results. The operating system was called a batch type system because of the way it selected a given set of input, worked on it exclusively until finished, then selected another input set and so forth.

The batch system uses a computer very efficiently, but frequently leaves users waiting for hours or days before the machine reaches their individual batch job. The cost of an engineer waiting for "turnaround" was expensive, but upgrading the machine to reduce the time was even more expensive.

In the late seventies and early eighties, a new generation of mini and microcomputers which drastically changed the simulation picture began to appear. Because of the low price and high performance of these new computers, an entirely new philosophy of computer operation evolved around these machines. Since a computer could be dedicated to the use of an individual, it was no longer necessary to use the batch philosophy in the operation of the machine.

The computer could afford to sit idle while the user thought about results of a previous operation and then respond instantly to a command entered on the keyboard. This "interactive" environment provided a much more effective use of the engineer's time at the expense of computer efficiency. Fortunately, the driving forces for increased engineering productivity appeared simultaneously with the remarkable developments in computers and software. As a result, a new generation of process simulation software is being developed to serve the engineer instead of the computer.

METHODOLOGY FOR INTERACTIVE PROCESS SIMULATION

Beginning with the premise that the process simulator's purpose is to serve the engineer, several new approaches in methodology are required. The primary emphasis is on the methods of communication between the engineer, the simulator and the computer.

In choosing a communication method, several criteria must be considered. One important criterion is the time required for an engineer to learn to use the simulator. At the same time, experienced users should not be burdened with unnecessary trivial communication. In addition, at least two levels of on-line help should be available. The beginning user needs a very detailed level of help while the experienced user needs only a concise reminder of the proper actions.

In all cases, the communications should allow the engineer to interact fully with the simulator. The user should be able to execute any portion of the plant at any time after the inlet streams and parameters for the appropriate unit operations have been specified. As a result, the engineer can optimize a plant on a unit-operation by unit-operation basis as it is being simulated.

On the other hand, the communications should allow the user to interactively input the data for a complete plant and then execute the entire plant in essentially a batch mode. This capability is needed primarily as an aid in

performing parametric studies. During any simulation, the suitability of the data should be checked by the communications interface. Information on flow rates and properties from any stream and the results from any unit operation should be available for inspection at any time.

The communication methods include interrogative driven, menu driven, command driven and hybrids of these. Each of these methods will be briefly described in this section and examples of their applications will be presented in the next section.

Interrogative Driven

In interrogative driven simulators, questions are presented one at a time, and the user responds to them with either a yes, no or value of some type. The driver begins asking general questions and then narrows down to specific questions about the process.

Interrogative drivers are very straightforward for the beginning user. However, they usually provide limited flexibility and editing capabilities. These drivers are especially advantageous for simulators that are designed for single purpose plants such as gas sweetening with amines and gas dehydration with glycols.

Menu Driven

The menu driven simulators are very easy for the beginning user since essentially every possible option is displayed on the screen. Obviously, this could become particularly burdensome to the experienced user since he or she would be required to pass through all of the details in every simulation. Several variations of menu driven simulators are possible. For example, a mouse may be used to point to particular items from a given menu.

Command Driven

These simulators use a command structure to direct the simulation. In the early versions, the user was required to either remember the command list or consult the manual. This problem has been overcome by having on-line help commands. The better versions of the command driven simulators have two levels of on-line help; an abbreviated version for the experienced user and a detailed version for the beginning user. Other improvements which have been recently realized include the following:

1. When an incorrect command is entered, the simulator will recognize the error and then automatically display the list of commands appropriate to the user's location in the program.
2. When the user requests help, a more detailed version of help appropriate to the user's location is given.
3. By entering one command, the user can create a standard batch type input data set from the interactive data entry.

Hybrids of Interrogative, Menu and Command Driven Simulators

The hybridization of these communication methods offers great potential. Hybridization is in the early developmental stage and several of the major advances depend on improved computer capabilities. One example of a hybrid communication method that is possible at the present time with several mini and microcomputers is the following:

The overall program control could be command driven while the data entry would be of a menu type consisting of "fill in the blank." Data entry for the various unit operations is a prime candidate for a "fill in the blank" application. A full screen editor in the simulator would list the allowable parameters on the screen with blanks for data entry to the right. The cursor on the screen would automatically step from blank to blank with each stroke of the return key or, alternatively, the cursor could be controlled by the cursor control keys, mouse, joystick or other pointing device. This format is particularly convenient for reviewing and updating previously entered data.

Examples of Interactive Process Simulators

Three examples of interactive communications with simulators will be presented. In the first example, an interrogative driver has been developed as a part of a simulator, called TSWEET, which is for gas and/or liquid

sweetening with amines. The generalized flow sheet which may be used with the interactive driver is shown in Fig. 1. The equipment which is represented by dashed lines is optional and may be deleted by answering "no" to the appropriate questions in the flow sheet section. Some examples of the flow sheet questions are as follows:

1. Do you want a flash tank before the cross exchanger?
2. Do you want split flow?
3. Do you want a reclaimer?

After the series of flow sheet questions are answered, the driver automatically numbers the process streams and unit operations.
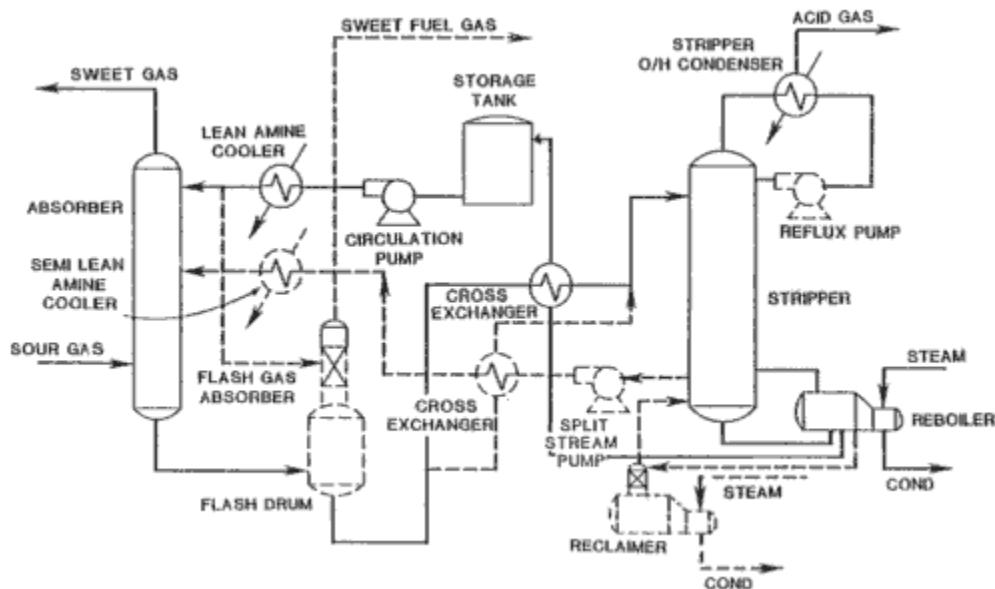
Figure 1. Process flow for sweetening plant.

At the present time, the interactive driver for TSWEET is restricted to the flow sheet options presented in Fig. 1. The driver can be expanded to handle other plant configurations.

The process parameters are also entered in response to a series of questions. Some operating condition questions are:

1. What amine do you wish to use (MEA, DEA, DGA, MDEA, HS-101)?
2. Weight percent amine?
3. Temperature of feed to stripper?

The interactive driver for TSWEET has been well received by both beginning and experienced users. For specialized processes, the interrogative driver is probably the fastest data entry form available. The driver may also be used to edit existing files. The data from the files are automatically loaded into the driver as the default values. Thus, the user can step through the unchanged information by hitting return on the keyboard. Alternatively, the standard data set can be edited directly.

An example of a menu driven program is shown in Fig. 2. The cursor is moved to the desired option by either the arrow keys or a mouse. In this example, Define/Modify Component List was chosen by placing an X on that line. A new menu consisting of a component list is immediately produced. The desired components are chosen in the same manner as before. Several screens are needed to display all of the available components. After the components are chosen, another menu is displayed to prompt the user for flow rate, temperature and pressure.

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MAIN MENU    __EXECUTE BLOCK(S)   __DEFINE/MODIFY STREAM   __DEFINE/MODIFY BI
```

The third example of interactive simulators involves a command driven simulator, called PROSIM, which is for general process simulation of hydrocarbon systems. The primary commands, which are shown in Fig. 3, allow excellent flexibility in using PROSIM. This figure was generated by typing HELP at the command level.

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ENTER COMMAND HELP    USAGE:  HELP     This command provides a list of all    val
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At any time, the user can define input streams, define and specify parameters for unit operations, execute any portion or all of the plant, view the input data and results for any stream or unit operation, obtain on-line help and perform numerous other operations. A WRITE DECK command allows the user to create a standard condensed input deck for the current flowsheet and operating conditions. These input data can be read back into PROSIM with a READ DECK command.

A flow diagram for a simple example plant is shown in Fig. 4 and some of the corresponding interactive communications are shown in Fig. 5. The user inputted commands and responses are denoted by an underline. The at sign, @, denotes hitting the return key on a blank line.
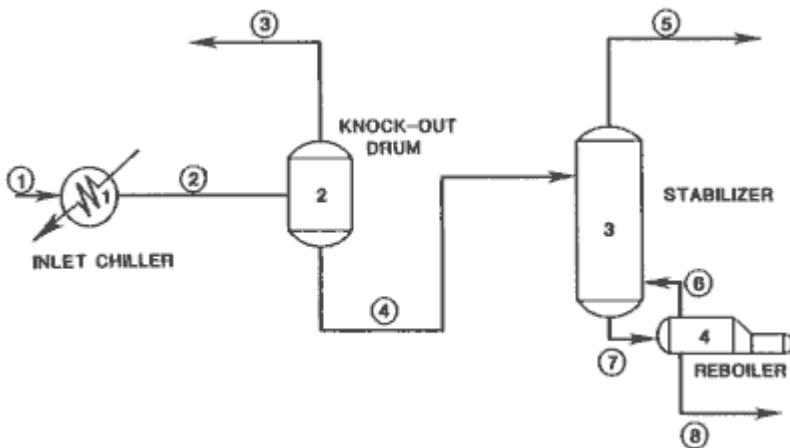
Figure 4. Process flow for stabilizer plant.

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WELCOME TO PROSIM VERSION 85.4     GENERAL PURPOSE PROCESS SIMULATOR     ENTE
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The simulation is begun by defining the input stream. The composition may be entered in any order along with the temperature and pressure. The first unit operation is defined and given a descriptive name. The program, knowing what kind of unit operation is being defined, prompts the user for the appropriate inlet and outlet stream numbers and then provides a list of valid specifications and waits on a command. An outlet temperature of 25°F and pressure drop of 3 psi is input.

The second, third and fourth unit operations are defined likewise with the appropriate prompts from the program and responses by the user. The simulation is then executed from beginning to end and an output is produced by the PRINT command. A condensed input data set is created to be used at a later date. The simulation is then terminated.

By using a system of commands, prompts and on-line help, PROSIM has been able to accommodate the beginning user while also providing the speed and brevity needed for the experienced user. In addition, this type of communications package has permitted PROSIM to be run on mainframe IBM computers as well as on mini and microcomputers.

FUTURE DEVELOPMENTS

The key factor to many of the major future developments in process simulation is expanded computer capabilities. If current price trends continue, desktop computers with speeds equivalent to today's mainframe computer will be available for a few thousand dollars within the next five to six years. Other dramatic computer developments will include low cost, excellent quality graphics and greatly improved user interface.

For example, alternate selection devices such as the joystick, the mouse and possibly the touch screen will probably become recognized as engineering aids and not just toys. Icon-based, multiple-window operating systems such as the Macintosh desktop or Microsoft Windows operating systems will probably become adopted on engineering computers.

With almost limitless computer speed and graphics capabilities, the developments which will occur in process simulation during the next five to ten years will be phenomenal. Due to the computer speed increases, some additional accuracy in the simulation will result due to items like extended equations of state. The increased speeds will also permit extended optimization of the process, equipment sizing and much greater economic evaluations of the plants.

These improvements will be most impressive; however, the major strides in process simulation will be communications. The productivity of the engineer will be the central theme. Improved computers and software will permit rapid construction of process flow diagrams along with the associated numbering of the streams and unit operations. The process simulators will all probably be various hybrids of interrogative, menu and command driven versions.

SUMMARY

In the last few years, interactive process simulation has emerged as a means of increasing the productivity of engineers. Historically, process simulators were of the batch type due to the limitations of computers and their operating systems. In the late 1970's, a new generation of mini and microcomputers was introduced which permitted the development of truly interactive process simulators.

The interactive feature of process simulators emphasizes the communications between the engineer, the simulator and the computer. At the present time, the communications methods include interrogative driven, menu driven, command driven and hybrids of these. In interrogative drivers, the input data is entered in response to a series of questions. In the menu driven simulators, essentially every possible option is displayed on the screen and the user selects those of interest.

In the command driven simulators, the user communicates with the simulator via a series of commands. The ultimate interactive process simulators will probably be a combination of these which readily accommodates both beginning and experienced users. Tremendous advances in interactive process simulation will be made in the next few years due to rapid developments in computers and the communications packages in the process simulators.