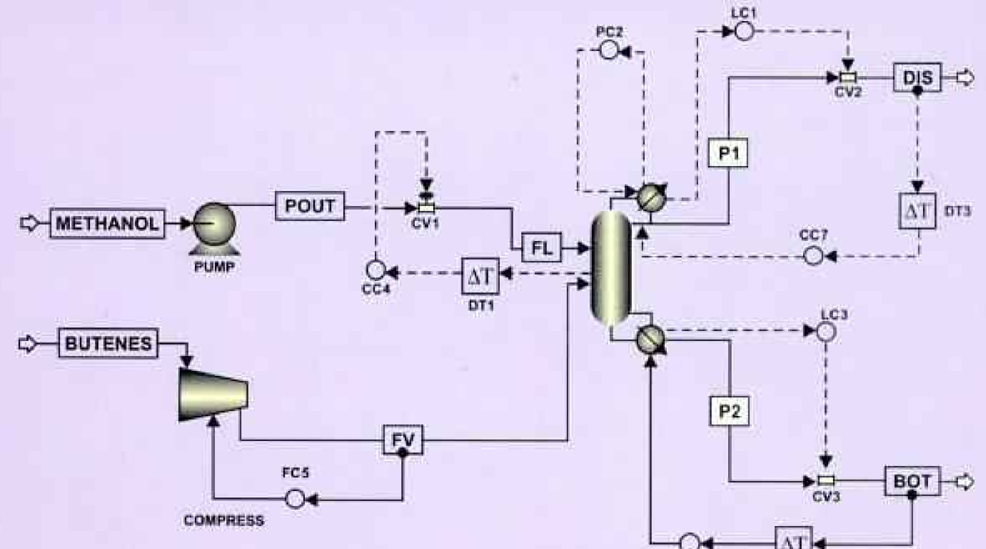
Eastern Economy Edition

PROCESS SIMULATION AND CONTROL USING ASPEN™



PHI

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PROCESS SIMULATION AND CONTROL USING ASPEN™
Amiya K. Jana

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Preface

"The future success of the chemical process industries mostly depends on the ability to design and operate complex, highly interconnected plants that are profitable and that meet quality, safety, environmental and other standards". To achieve this goal, the software tools for process simulation and optimization are increasingly being used in industry.

By developing a computer program, it may be manageable to solve a model structure of a chemical process with a small number of equations. But as the complexity of a plant integrated with several process units increases, the solution becomes a challenge. Under this circumstance, in recent years, we motivate to use the process *flowsheet simulator* to solve the problems faster and more reliably. In this book, the Aspen™ software package has been used for steady state simulation, process optimization, dynamics and closed-loop control.

To improve the design, operability, safety, and productivity of a chemical process with minimizing capital and operating costs, the engineers concerned must have a solid knowledge of the process behaviour. The process dynamics can be predicted by solving the mathematical model equations. Within a short time period, this can be achieved quite accurately and efficiently by using Aspen flowsheet simulator. This software tool is not only useful for plant simulation but can also automatically generate several control structures, suitable for the used process flow diagram. In addition, the control parameters, including the constraints imposed on the controlled as well as manipulated variables, are also provided by Aspen to start the simulation run. However, we have the option to modify or even replace them.

This well organized book is divided into three parts. Part I (Steady State Simulation and Optimization using Aspen Plus™) includes three chapters. Chapter 1 presents the introductory concepts with solving the flash chambers. The computation of bubble point and dew point temperatures is also focused. Chapters 2 and 3 are devoted to simulation of several reactor models and separating column models, respectively.

Part II (Chemical Plant Simulation using Aspen Plus™) consists of only one chapter (Chapter 4). It addresses the steady state simulation of large chemical plants. Several individual processes are interconnected to form the chemical plants. The Aspen Plus™ simulator is used in both Part I and Part II.

The Aspen Dynamics™ package is employed in Part III (Dynamics and Control using Aspen Dynamics™) that comprises Chapters 5 and 6. Chapter 5 is concerned with the dynamics and control of flow-driven chemical processes. In the closed-loop control study, the servo as well as regulatory tests have been conducted. Dynamics and control of pressure-driven processes have been discussed in Chapter 6.

The target readers for this book are undergraduate and postgraduate students of chemical engineering. It will be also helpful to research scientists and practising engineers.

Amiya K. Jana

Acknowledgements

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I am greatly indebted to the editorial staff of PHI Learning Private Limited, for their constant encouragement and unstinted efforts in bringing the book in its present form.

No list would be complete without expressing my thanks to two most important people in my life—my mother and my wife. I have received their consistent encouragement and support throughout the development of this manuscript.

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Part I

Steady State Simulation and Optimization using Aspen Plus™

CHAPTER 1

Introduction and Stepwise Aspen Plus™ Simulation: Flash Drum Examples

1.1 ASPEN: AN INTRODUCTION

By developing a computer program, it may be manageable to solve a model structure of a chemical process with a small number of equations. However, as the complexity of a plant integrated with several process units increases, solving a large equation set becomes a challenge. In this situation, we usually use the process flowsheet simulator, such as Aspen Plus™ (AspenTech), ChemCad™ (Chemstations), HYSYS™ (Hyprotech) and PRO/II™ (SimSci-Esscor). In 2002, Hyprotech was acquired by AspenTech. However, most widely used commercial process simulation software is the Aspen software.

During the 1970s, the researchers have developed a novel technology at the Massachusetts Institute of Technology (MIT) with United States Department of Energy funding. The undertaking, known as the *Advanced System for Process Engineering* (ASPEN) Project, was originally intended to design nonlinear simulation software that could aid in the development of synthetic fuels. In 1981, AspenTech, a publicly traded company, was founded to commercialize the simulation software package. AspenTech went public in October 1994 and has acquired 19 industry-leading companies as part of its mission to offer a complete, integrated solution to the process industries (http://www.aspentech.com/corporate/careers/faqs.cfm#whenAT).

The sophisticated Aspen software tool can simulate large processes with a high degree of accuracy. It has a model library that includes mixers, splitters, phase separators, heat exchangers, distillation columns, reactors, pressure changers, manipulators, etc. By interconnecting several unit operations, we are able to develop a process flow diagram (PFD) for a complete plant. To solve the model structure of either a single unit or a chemical plant, required Fortran codes are built-in in the Aspen simulator. Additionally, we can also use our own subroutine in the Aspen package.

The Aspen simulation package has a large experimental databank for thermodynamic and physical parameters. Therefore, we need to give limited input data for solving even a process plant having a large number of units with avoiding human errors and spending a minimum time.

Aspen simulator has been developed for the simulation of a wide variety of processes, such as chemical and petrochemical, petroleum refining, polymer, and coal-based processes. Previously, this flowsheet simulator was used with limited applications. Nowadays, different Aspen packages are available for simulations with promising performance. Briefly, some of them are presented below.

Aspen Plus—This process simulation tool is mainly used for steady state simulation of chemicals, petrochemicals and petroleum industries. It is also used for performance monitoring, design, optimization and business planning.

Aspen Dynamics—This powerful tool is extensively used for dynamics study and closed-loop control of several process industries. Remember that Aspen Dynamics is integrated with Aspen Plus.

Aspen BatchCAD—This simulator is typically used for batch processing, reactions and distillations. It allows us to derive reaction and kinetic information from experimental data to create a process simulation.

Aspen Chromatography—This is a dynamic simulation software package used for both batch chromatography and chromatographic simulated moving bed processes.

Aspen Properties—It is useful for thermophysical properties calculation.

Aspen Polymers Plus—It is a modelling tool for steady state and dynamic simulation, and optimization of polymer processes. This package is available within Aspen Plus or Aspen Properties rather than via an external menu.

Aspen HYSYS—This process modelling package is typically used for steady state simulation, performance monitoring, design, optimization and business planning for petroleum refining, and oil and gas industries.

It is clear that Aspen *simulates the performance* of the designed process. A solid understanding of the underlying chemical engineering principles is needed to supply reasonable values of input parameters and to analyze the results obtained. For example, a user must have good idea of the distillation column behaviour before attempting to use Aspen for simulating that column. In addition to the process flow diagram, required input information to simulate a process are: setup, components, properties, streams and blocks.

1.2 GETTING STARTED WITH ASPEN PLUS SIMULATION

Aspen Plus is a user-friendly steady state process flowsheet simulator. It is extensively used both in the educational arena and industry to predict the behaviour of a process by using material balance equations, equilibrium relationships, reaction kinetics, etc. Using Aspen Plus, which is a part of Aspen software package, we will mainly perform in this book the steady state simulation and optimization. For process dynamics and closed-loop control, Aspen Dynamics (formerly DynaPLUS) will be used in several subsequent chapters. The standard Aspen notation is used throughout this book. For example, distillation column stages are counted from the top of the column: the condenser is Stage 1 and the reboiler is the last stage.

As we start Aspen Plus from the *Start* menu or by double-clicking the Aspen Plus icon on our desktop, the *Aspen Plus Startup* dialog appears. There are three choices and we can create our work from scratch using a *Blank Simulation*, start from a *Template* or *Open an Existing Simulation*. Let us select the *Blank Simulation* option and click *OK* (see Figure 1.1).

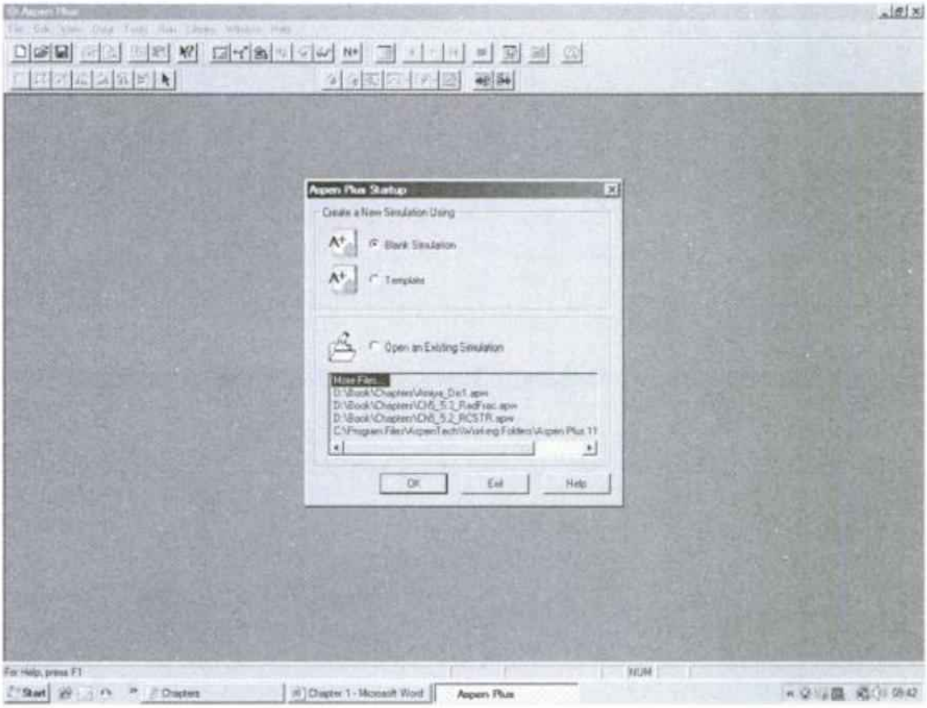

FIGURE 1.1

The simulation engine of Aspen Plus is independent from its Graphical User Interface (GUI). We can create our simulations using the GUI at one computer and run them connecting to the simulation engine at another computer. Here, we will use the simulation engine at 'Local PC'. Default values are *OK*.

Hit *OK* in the *Connect to Engine* dialog (Figure 1.2). Notice that this step is specific to the installation.

The next screen shows a blank *Process Flowsheet Window*. The first step in developing a simulation is to create the process flowsheet. *Process flowsheet* is simply defined as a blueprint of a plant or part of it. It includes all input streams, unit operations, streams that interconnect the unit operations and the output streams. Several process units are listed by category at the bottom of the main window in a toolbar known as the *Model Library*. If we want to know about a model, we can use the Help menu from the menu bar. In the following, different useful items are highlighted briefly (Figure 1.3).

FIGURE 1.2

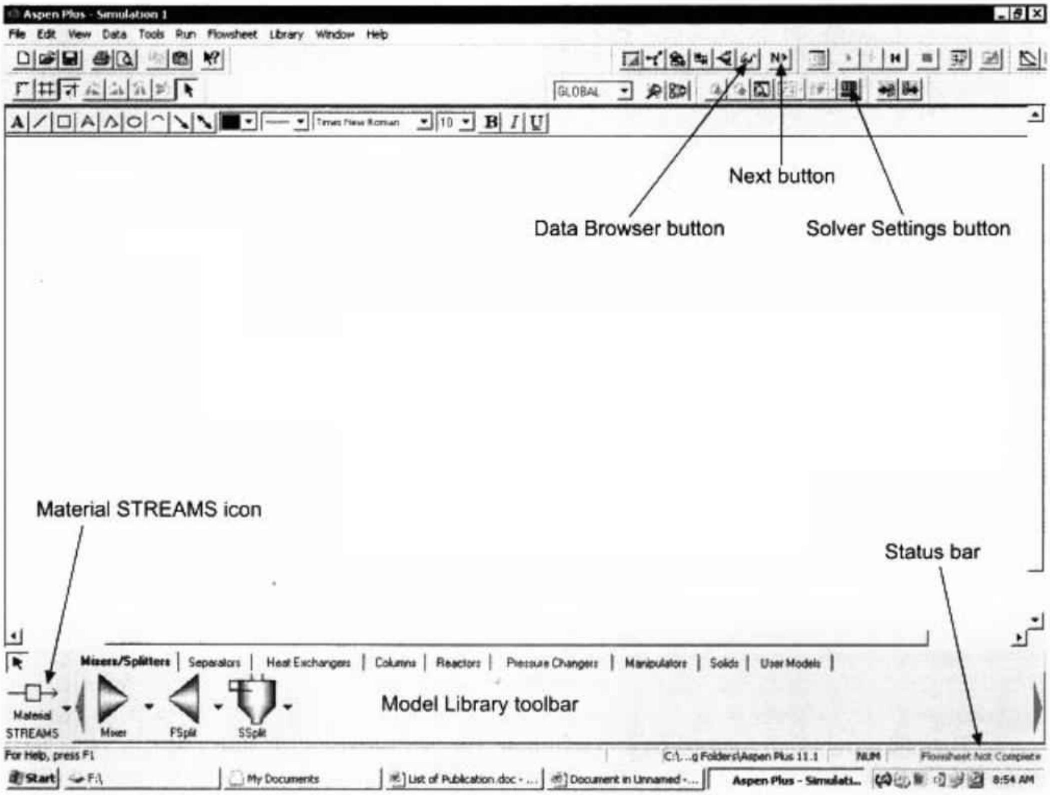

FIGURE 1.3

To develop a flowsheet, first choose a unit operation available in the *Model Library*. Proprietary models can also be included in the flowsheet window using *User Models* option. Excel workbook or Fortran subroutine is required to define the user model. In the subsequent step, using *Material STREAMS* icon, connect the inlet and outlet streams with the process. A process is called as a *block* in Aspen terminology. Notice that clicking on *Material STREAMS*, when we move the cursor into the flowsheet area red and blue arrows appear around the model block. These arrows indicate places to attach streams to the block. Red arrows indicate required streams and blue arrows are optional.

When the flowsheet is completed, the status message changes from *Flowsheet Not Complete* to *Required Input Incomplete*. After providing all required input data using input forms, the status bar shows *Required Input Complete* and then only the simulation results are obtained. In the *Data Browser*, we have to enter information at locations where there are red semicircles. When one has finished a section, a blue checkmark appears. In subsection 1.3.2, a simple problem has been solved, presenting a detailed stepwise simulation procedure in Aspen Plus. In addition, three more problems have also been discussed with their solution approaches subsequently.

1.3 STEPWISE ASPEN PLUS SIMULATION OF FLASH DRUMS

1.3.1 Built-in Flash Drum Models

In the *Model Library*, there are five built-in separators. A brief description of these models is given below.

Flash 2: It is used for equilibrium calculations of two-phase (vapour-liquid) and three-phase (vapour-liquid-liquid) systems. In addition to inlet stream(s), this separator can include three product streams: one liquid stream, one vapour stream and an optional water decant stream. It can be used to model evaporators, flash chambers and other single-stage separation columns.

Flash 3: It is used for equilibrium calculations of a three-phase (vapour-liquid-liquid) system. This separator can handle maximum three outlet streams: two liquid streams and one vapour stream. It can be used to model single-stage separation columns.

Decanter: It is typically used for liquid-liquid distribution coefficient calculations of a two-phase (liquid-liquid) system. This separator includes two outlet liquid streams along with inlet stream(s). It can be used as the separation columns. If there is any tendency of vapour formation with two liquid phases, it is recommended to use Flash3 instead of Decanter.

Sep 1: It is a multi-outlet component separator since two or more outlet streams can be produced from this process unit. It can be used as the component separation columns.

Sep 2: It is a two-outlet component separator since two outlet streams can be withdrawn from this process unit. It is also used as the component separation columns.

At this point it is important to mention that for additional information regarding a built-in model, select that model icon in the *Model Library* toolbar and then press **F1** on the keyboard.

1.3.2 Simulation of a Flash Drum

Problem statement

A 100 kmol/hr feed consisting of 10, 20, 30, and 40 mole% of propane, *n*-butane, *n*-pentane, and *n*-hexane, respectively, enters a flash chamber at 15 psia and 50°F. The flash drum (Flash2) is shown in Figure 1.4 and it operates at 100 psia and 200°F. Applying the SYSOP0 property method, compute the composition of the exit streams.

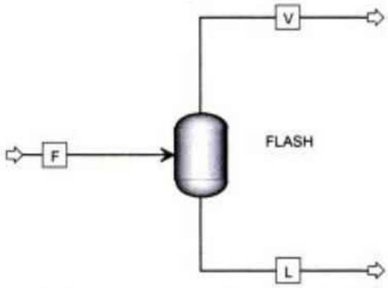

FIGURE 1.4 A flowsheet of a flash drum.

Simulation approach

From the desktop, select *Start* button followed by *Programs*, *AspenTech*, *Aspen Engineering Suite*, *Aspen Plus Version* and *Aspen Plus User Interface*. Then choose *Template* option in the *Aspen Plus Startup* dialog (Figure 1.5).

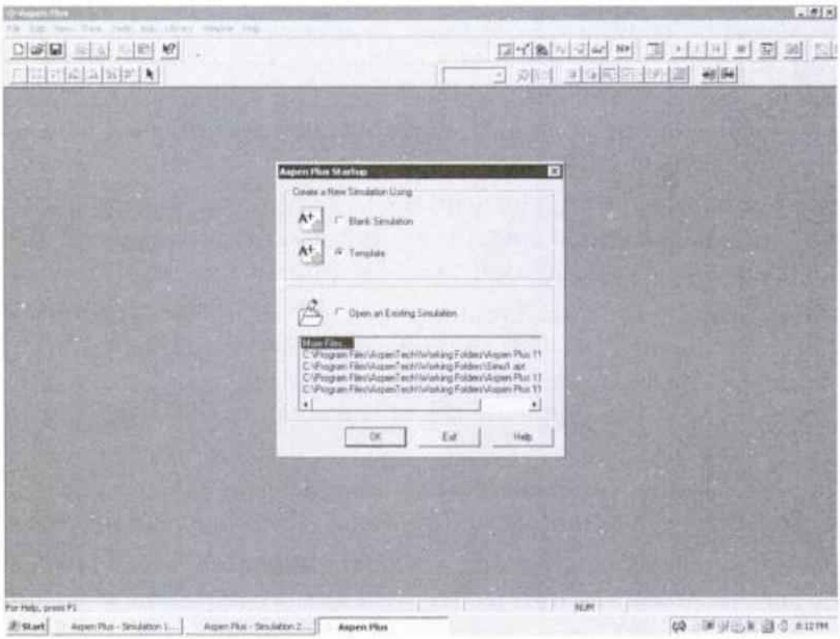

FIGURE 1.5

As the next window appears after hitting *OK* in the above screen, select *General with English Units* (Figure 1.6).

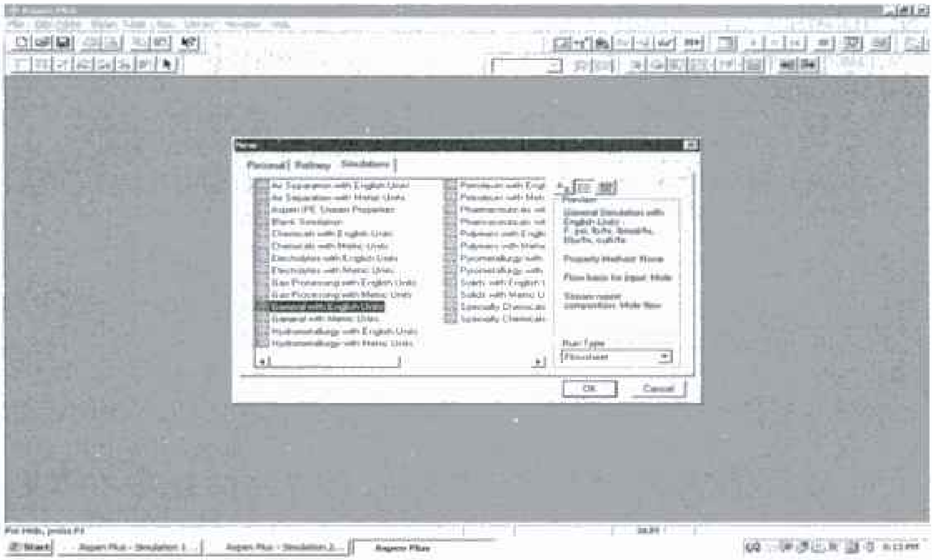

FIGURE 1.6

Then click *OK*. Again, hit *OK* when the Aspen Plus engine window pops up and subsequently, proceed to create the flowsheet.

Creating flowsheet

Select the *Separators* tab from the *Model Library* toolbar. As discussed earlier, there are five built-in models. Among them, select Flash2 and place this model in the window. Now the *Process Flowsheet Window* includes the flash drum as shown in Figure 1.7. By default, the separator is named as B1.

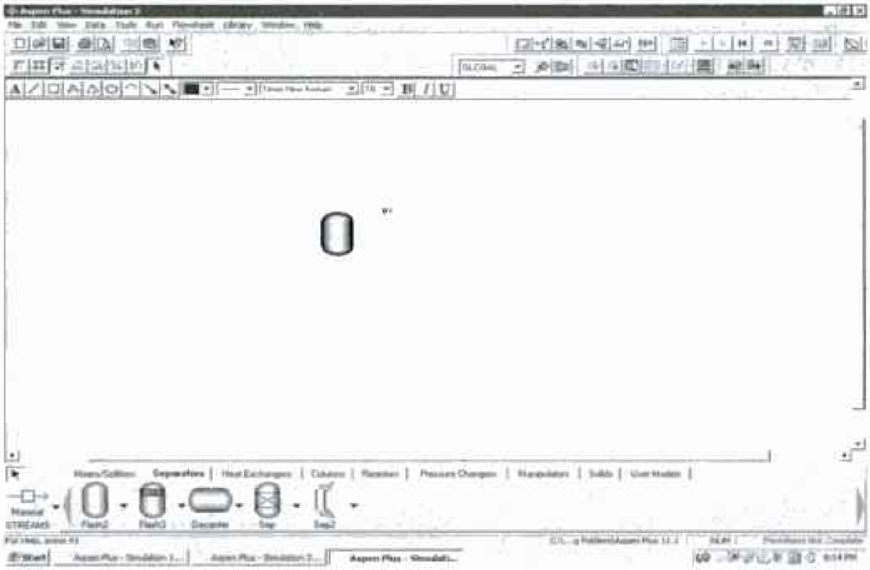

FIGURE 1.7

To add the input and output streams with the block, click on *Streams* section (lower left-hand corner). There are three different stream categories (Material, Heat and Work), as shown in Figure 1.8.

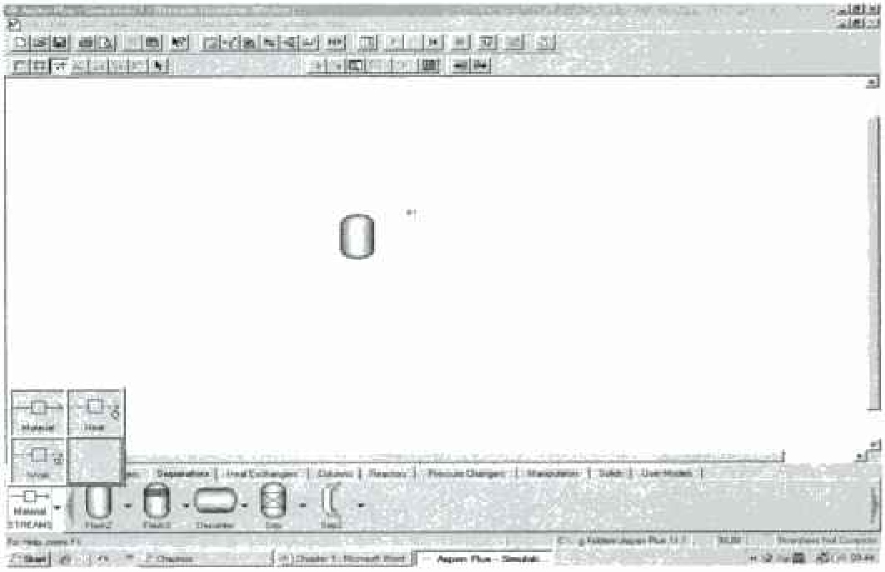

FIGURE 1.8

Block B1 includes three red arrows and one blue arrow as we approach the block after selecting the *Material STREAMS* icon. Now we need to connect the streams with the flash chamber using red arrows and the blue arrow is optional. The connection procedure is presented in Figure 1.9.

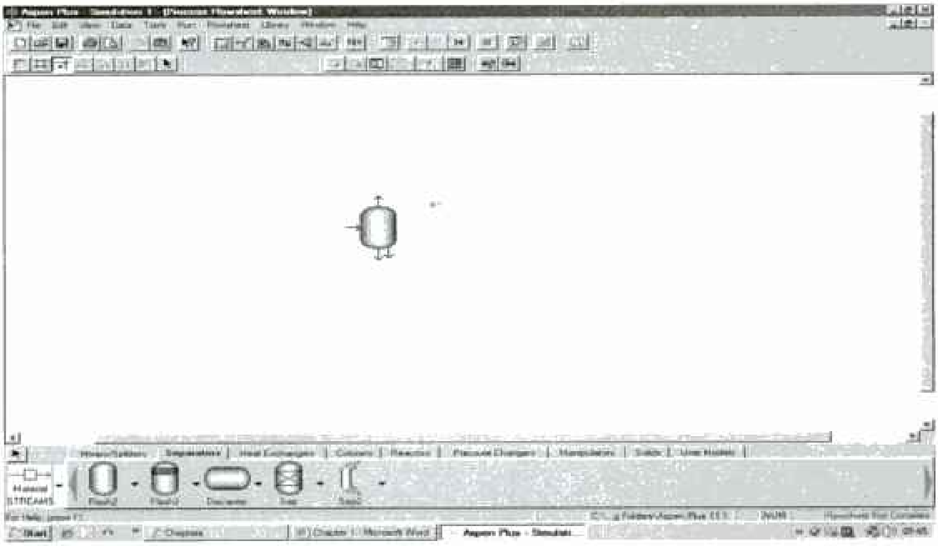

FIGURE 1.9

Clicking on *Material STREAMS*, move the mouse pointer over the red arrow at the inlet of the flash chamber. Click once when the arrow is highlighted and move the cursor so that the stream is in the position we want. Then click once more. We should see a stream labelled 1 entering the drum as a feed stream. Next, click the red arrow coming out at the bottom of the unit and drag the stream away and click. This stream is marked as 2. The same approach has been followed to add the product stream at the top as Stream 3. Now the flowsheet looks like Figure 1.10. Note that in the present case, only the red arrows have been utilized.

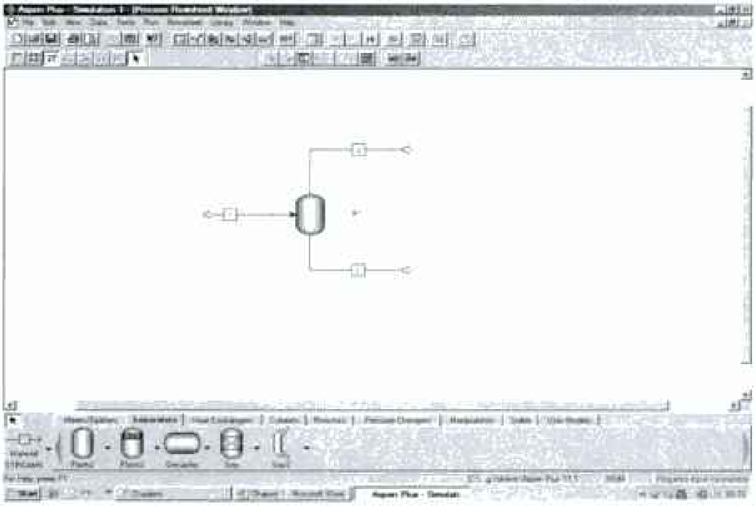

FIGURE 1.10

We can rename the stream(s) and block(s). To do that highlight the object we want to rename and click the right mouse button. Select *Rename Block* and then give a new name, as shown in Figure 1.11 for Block B1.

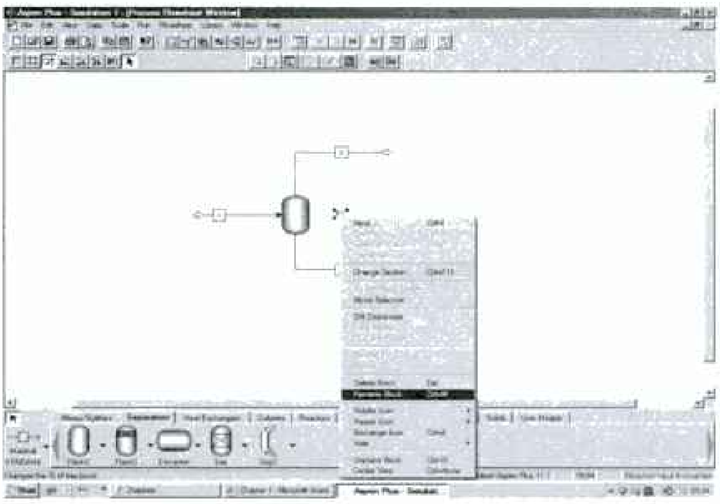

FIGURE 1.11

Alternatively, highlight the object, press Ctrl + M on the keyboard, change the name, and finally hit *Enter* or *OK*. After renaming Stream 1 to F, Stream 2 to L, Stream 3 to V and Block B1 to FLASH, the flowsheet finally resembles Figure 1.12.

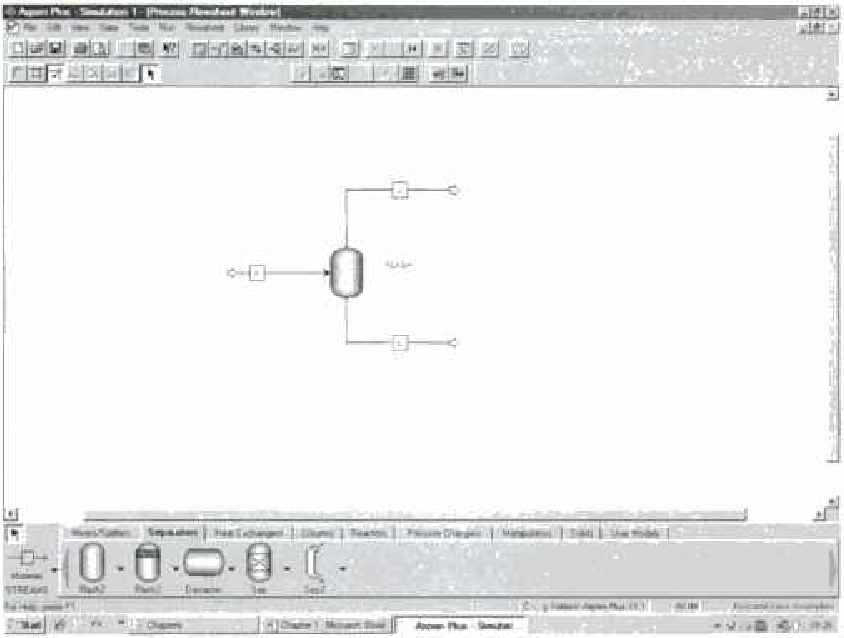

FIGURE 1.12

In order to inspect completeness for the entire process flowsheet, look at the status indicator. If the message includes *Flowsheet Not Complete*, click on *Material STREAMS*. If any red arrow(s) still exists in the flowsheet window, it indicates that the process is not precisely connected with the stream(s). Then we need to try again for proper connection. To find out why the connectivity is not complete, hit the *Next* button on the *Data Browser* toolbar. However, if we made a mistake and want to remove a stream (or block) from the flowsheet, highlight it, right click on it, hit *Delete Stream* (or *Delete Block*), and finally click *OK*.

Anyway, suppose that the flowsheet connectivity is complete. Accordingly, the status message changes from *Flowsheet Not Complete* to *Required Input Incomplete*.

We have defined the unit operation to be simulated and set up the streams into and out of the process. Next we need to enter the rest of the information using several input forms required to complete the simulation. Within Aspen Plus, the easiest way to find the next step is to use one of the followings:

1. click the *Next* button 
2. find *Next* in the *Tools* menu
3. use shortcut key F4

As a consequence, Figure 1.13 appears.

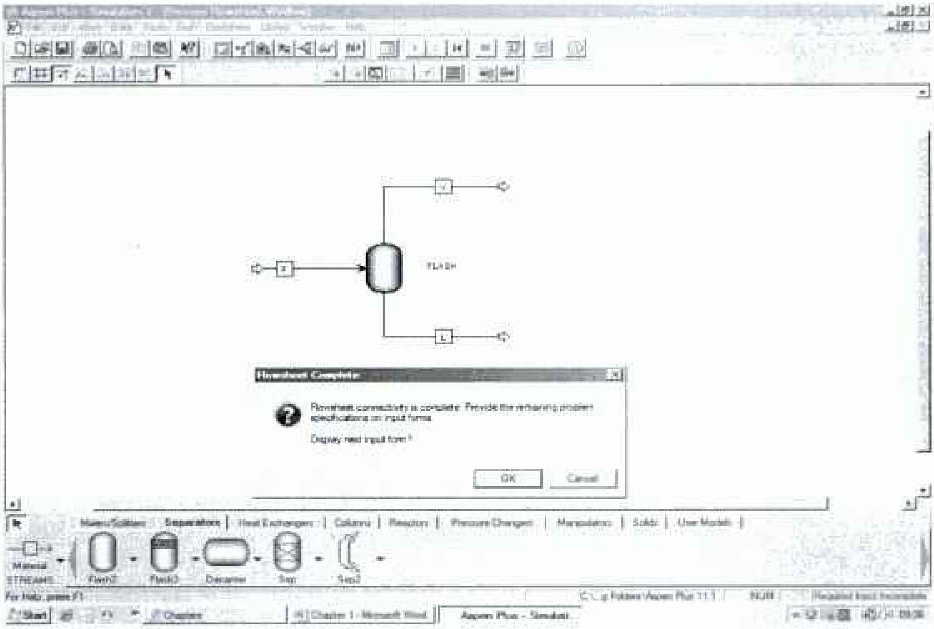

FIGURE 1.13

Configuring settings

As we click *OK* on the message, Aspen Plus opens the *Data Browser* window containing the *Data Browser* menu tree and *Setup/Specifications/Global* sheet.

Alternatively, clicking on *Solver Settings* and then choosing *Setup/Specifications* in the left pane of the *Data Browser* window, we can also obtain this screen (Figure 1.14).

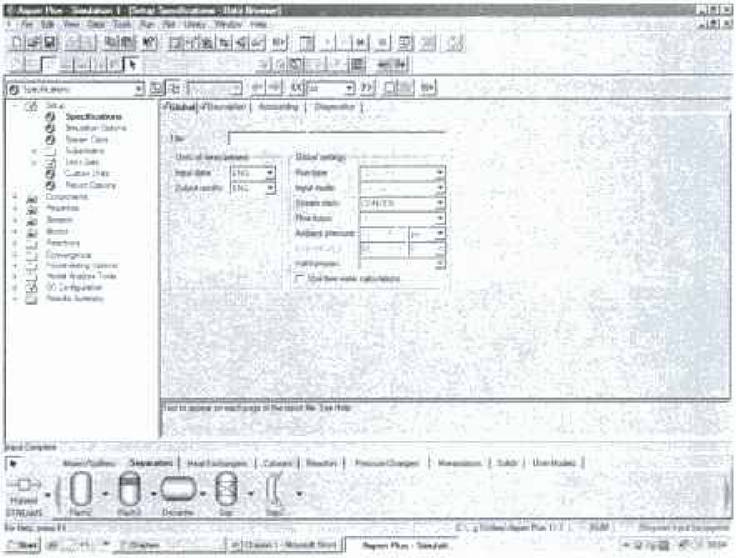

FIGURE 1.14

Although optional, it is a good practice to fill up the above form for our project giving the *Title* (Flash Calculations) and keeping the other items unchanged (Figure 1.15).

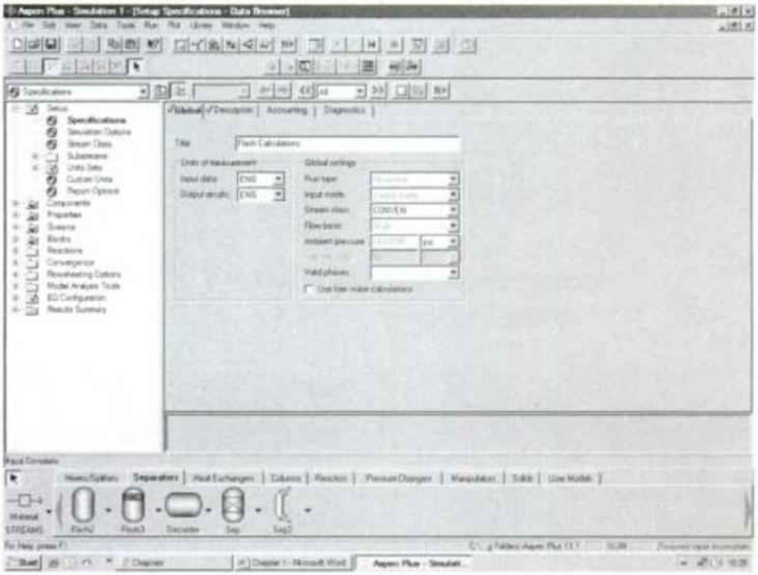

FIGURE 1.15

In the next step (Figure 1.16), we may provide the *Aspen Plus accounting information* (required at some installations). In this regard, a sample copy is given with the followings:

User name: AKJANA
Account number: 1
Project ID: ANYTHING
Project name: AS YOU WISH

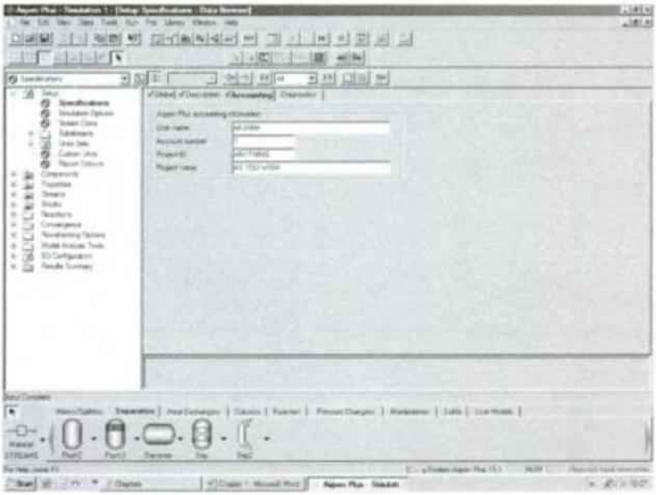

FIGURE 1.16