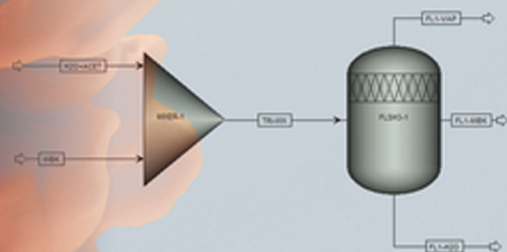


**KAMAL I.M. AL-MALAH**



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## Chemical Engineering Applications

**KAMAL I.M. AL-MALAH**

Department of Chemical Engineering

Higher Colleges of Technology, Ruwais, United Arab Emirates

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*To my creator who taught humans things they did not know before;  
To the last prophet Mohammad and to the preceding prophets, peace be upon all of them;  
To my first lovely teachers in this life: mom and dad;  
To my wife (Fadia), daughters (Anwar and Lama), and sons (Abdallah and Mohammad);  
To my biological brothers and sisters;  
To my first class teacher (Mr Raslan Al-Malah), mercy be upon him;  
To my succeeding teachers and professors between the first class and until I got my Ph.D.  
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To SPi Global, book production team.  
Finally to my brothers and sisters in humanity worldwide;  
To the first, I say: I owe you everything and you are the first and last.  
To the rest, I say: my sincere and warm greetings to all of you.*





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# PREFACE

Aspen Plus<sup>®</sup> is a process flowsheet simulator. A flowsheet simulator is a computer software that is used to quantitatively model a chemical processing plant. In general, a chemical processing plant is comprised of the core reactor unit and different additional unit operations, in the form of pre- and post-treatment steps, as well.

In this regard, Aspen Plus is a very powerful tool that can be used to tackle different chemical process and unit operation calculation-based tasks, in the form of modeling, simulation, optimization, data regression, design specifications, sensitivity analysis, solids handling, dynamics and control, energy saving, safety compliance, and finally process economic analysis.

The book comprises 18 chapters. Each chapter, except the last chapter, constitutes a running tutorial that mainly covers one or more of common unit operations or chemical processes found in chemical industries. Moreover, the book has end-of-chapter contextual problems. The last chapter contains comprehensive problems (or term projects) that require an extensive knowledge of Aspen Plus features and tools that are already explained in previous chapters.

Overall, the book reflects the full-fledge nature of Aspen Plus implementation to versatile chemical process industries.



# THE BOOK THEME

Let me briefly visualize my endeavor or approach in writing this book.

I am acting as the car-driving trainer and I have the student as the trainee who will be prepared to get the driving license.

The training quality (or quality training) on my behalf (as a trainer) is merely governed by two important factors: the first is the car itself, which includes all built-in electromechanical features that will help the trainer and later the driver to carry out their mission, and the second is the high-caliber skilled trainer who knows well what he/she presents to the trainee so that both can maximize their performance and that of the car.

On behalf of the trainee (student), the process of mastering car driving is to maintain the burning desire to love and not fear of driving in parallel with the internal burning/combustion of the car itself, without overburdening the learner's shoulders by the intricate details of how a car starts/stops, moves fast/slowly, forward/backward, and right/left.

The sophisticated car in our case is the Aspen Plus® full-fledge package. Humbly speaking, I am the trainer and I am presenting the training material in a very simplified way (a text in parallel with image) to let the trainee grasp and grab the training courseware real fast with a minimum yet persistent effort. At the same time, I do not really have to compromise the genuineness of both the Aspen Plus package itself and chemical engineering fundamentals.



## ABOUT THE AUTHOR

Kamal I.M. Al-Malah, Professor of Chemical Engineering, graduate of Oregon State University, is currently at Higher Colleges of Technology, Abu-Dhabi, United Arab Emirates. Professor Al-Malah is Windows-based software developer (<https://sites.google.com/site/almalahweb/software>) and MATLAB<sup>®</sup> book author (<http://mhprofessional.com/product.php?isbn=0071831282>).





## WHAT DO YOU GET OUT OF THIS BOOK?

The goal of writing this book is to get you started using Aspen Plus® successfully and fast. I pinpoint the parts of Aspen Plus, which you need to know without overwhelming details. I do my best to avoid presenting cumbersome Aspen Plus features. In each chapter, I demonstrate an Aspen Plus-based, running tutorial that you can refer to when you are doing your own homework, classwork, term project, or even your own project. When you are done with this recipe textbook, you will be able to efficiently use Aspen Plus. You will also be ready to explore more of Aspen Plus features on your own. You might not be an Aspen Plus expert when you finish this textbook, but you will be prepared to become one – if that is what you like and persist to be. I hope you are probably more interested in being an expert at your own specialty, as a professional chemical engineer. This textbook is designed to help you become a proficient Aspen Plus user as quickly as possible and, toward the end of our virtual journey, you will be able to examine different profitability indices of an investment project related to chemical industries.



## WHO SHOULD READ THIS BOOK?

The book is primarily written for Chemical Engineering students, who plan to have a course in computer-aided design (CAD) or what is called virtual simulation (i.e., dry lab). Nevertheless, the book is expanded to reflect the broad-spectrum nature of Chemical Engineering realm in terms of courses being taught and applications being tackled. The virtual journey starts at the main station of basic principles of Chemical Engineering, while it passes through transit stations of transport phenomena, thermodynamics, chemical reaction engineering, process modeling, optimization, and simulation, the “love boat” glides down at the final stations of process dynamics and control, energy saving scenarios and safety measures, and finally process economic analysis, which declares the end of the journey.

As far as applications are concerned, in addition to classical chemical processes and unit operations, special processes are also discussed in the book, namely electrolytes, polymerization, drug characterization, and solids handling.

Professional chemical engineers can also benefit from the book as it gives them an opportunity to replenish their skills in mastering a powerful tool, such as Aspen Plus®, and stay updated at the same time. Keep in mind that Aspen Plus technology is progressively used in petroleum, petrochemical, and chemical industries, at large. Moreover, the developers of Aspen Plus keep augmenting their software with new features that will help the chemical engineer better achieve his/her mission at a pace of the speed of light compared with the manual (decrepit) mode of any calculation-based model testing or case study. Once the chemical engineer masters such a powerful tool, he/she can use it in his/her daily professional life. The book can be recommended to all chemical engineering unions, chapters, and organizations.

Aspen Plus is a full-fledge package and appears cumbersome for beginners; we need to facilitate the process of learning and later master such a powerful tool in a very short time without really making their life miserable. This textbook is recipe or cookbook type and the solution for the problem in hand is algorithmically presented via successive images (i.e., snapshots for the relevant Aspen Plus platform) in parallel with the textual explanation.



# NOTES FOR INSTRUCTORS

For me, who has been spending his life digging in and pondering on chemical engineering pathways, while passing from student to instructor side, where I have been learning and teaching at different schools in the Middle East and the United States, I found that the typical classical undergraduate chemical engineering fundamental course ends up with design-oriented chapters. Toward the end of the semester (or a quarter/dime), the instructor will find it difficult to elaborate on the direct application(s) of what the student learns in the first few chapters. My recommendation is that it is time to make a gearshift and make use of CAD flowsheet simulators, such as Aspen Plus®, and have it customized to fit the instructor's needs, starting from the basic principles all the way up to the capstone design or senior project course. Many chapters of this textbook can be tuned-up to serve different fundamental chemical engineering courses, in addition to the computer-aided design course itself.

Bear in mind that the first three chapters of this textbook serve as introductory chapters for those who never used Aspen Plus technology before. I would recommend that the instructor goes first over the first three chapters before he/she moves to upcoming chapters. The instructor has to familiarize himself/herself with the new platforms of Aspen Plus, and their newly added features, which definitely look different from previous versions of Aspen Plus.

The book has contextual problems at the end of each chapter and one last dedicated chapter that encompasses term project problems. In addition, there will be additional problems for the instructor where the instructor can adjust numbers in exam/quiz problems such that each student will have his/her own version. This will minimize the process of cheating or the convective, illegal knowledge transfer among students should the instructor attempt to ask the students to solve problems in a computer lab using Aspen Plus software. For example, the first or last five numbers of a student's ID (alternatively, the national ID or social security number) can be taken as an input, in the form of *abcde*, and plugged in the question statement such that each student ends up with his/her own version.



## ACKNOWLEDGMENT

I would like to thank Aspen Technology, Inc. for their support and co-operation. It should be emphasized that screen images of Aspen Plus<sup>®</sup>, Aspen Plus Dynamics, Aspen Properties<sup>®</sup>, Aspen Energy Analyzer, and Aspen Process Economic Analyzer are reprinted with permission by Aspen Technology, Inc. AspenTech<sup>®</sup>, aspenONE<sup>®</sup>, Aspen Plus<sup>®</sup>, Aspen Properties<sup>®</sup>, and the AspenTech leaf logo are trademarks of Aspen Technology, Inc. All rights reserved.

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## **ABOUT THE COMPANION WEBSITE**

This book is accompanied by a companion website:  
[www.wiley.com/go/Al-Malah/AspenPlusApplications](http://www.wiley.com/go/Al-Malah/AspenPlusApplications)

The website includes:

- Exam and quiz problems for instructors only
- Solution manual for instructors only



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# 1

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## INTRODUCING ASPEN PLUS

### 1.1 WHAT DOES ASPEN STAND FOR?

**ASPEN** is an acronym of **A**dvanced **S**ystem for **P**rocess **E**ngineering. It is based on a flowsheet simulation. Notice that **Aspen** was replaced by **Aspen Plus**<sup>®</sup> in latest versions. A flowsheet simulation is a computer software that is used to quantitatively model a chemical processing plant, which, in addition to the core reactor unit, also includes pre- and post-treatment steps. Thus, simulation of an entire chemical process, starting from the raw material to the final finished product, is symbolically represented by different icons where each icon stands for a unit operation, chemical process, input/output material stream, input/output energy stream, or input/output electric/pneumatic signal. In terms of Aspen Plus flowsheet notation, there will be a block icon and stream icon. The iconic flowsheet simulator, such as Aspen Plus, allows us to predict the behavior of a process using basic engineering relationships. As taught in process modeling and simulation course that we describe a given physical (i.e., real) process by a set of linearly independent algebraic/differential equations such that the number of written equations will be equal to the number of variables (or unknown quantities) and the physical process as such is said to be specified or described by an equivalent mathematical portrayal. In general, writing such equations stems from

- balance equations of extensive thermodynamic properties, such as mass, mole, and energy;
- thermodynamic relationships for reacting and non-reacting medium, such as phase and chemical equilibrium;
- rate correlations for momentum, heat, and mass transfer;
- reaction stoichiometry and kinetic data;
- physical constraints imposed on the process.

Given reliable thermodynamic data, sensible operating conditions, and rigorous equipment models, Aspen Plus can simulate actual plant behavior. Aspen Plus flowsheet simulation enables us to run many tasks, such as

- conduct “what if” tests;
- design specification (plant configuration) checks;
- carry out “de-bottlenecking of constricting parts of a process” studies;
- perform sensitivity analyses;
- run optimization investigations.

With Aspen Plus process simulator, we can design better plants and increase profitability in existing plants. Aspen Plus flowsheet simulation is useful throughout the entire lifecycle of a process, starting from a rough R&D concept/idea and zooming to a refined projected idea with a different level of details, including conceptual engineering, basic engineering, detailed engineering, and finally plant operations and revamps.

## 1.2 WHAT IS ASPEN PLUS PROCESS SIMULATION MODEL?

In general, a chemical process consists of chemical components, or different species, that are subject to physical or chemical treatment, or both. The goal of applying such treatment steps is basically to add a value or convert the raw, cheap material(s) into valuable, final finished products (gold). The physical treatment steps may include mixing, separation (de-mixing), such as absorption, distillation, and extraction, and heating/cooling with or without a phase change. On the other hand, the chemical treatment step involves a single or set of parallel, series, or mixed reactions, which results in a change of chemical identity of each of reacting species. Such treatment steps are visualized in the flowsheet simulator as components being transported from a unit (or block) to another through process streams.

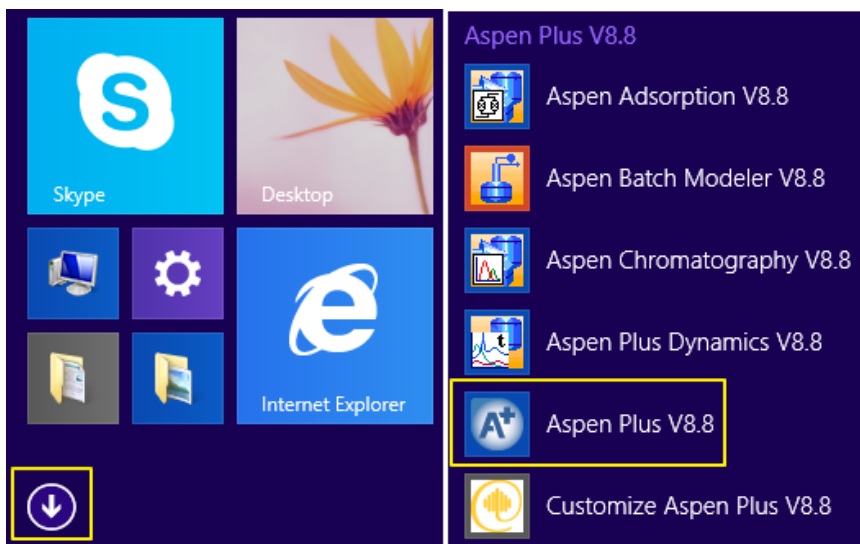
We can translate a process into an Aspen Plus process simulation model by performing the following skeletal necessary steps:

1. Specify the chemical components in the process. We can fetch these components from Aspen Plus databanks, or we can introduce them to Aspen Plus platform.
2. Specify thermodynamic models to represent the physical properties of the components and mixtures in the process. These models are built into Aspen Plus.
3. Define the process flowsheet:
  - Define the unit operations in the process.
  - Define the process streams that flow into and out of the unit operations.
  - Select models from Aspen Plus Model Library to describe each unit operation or chemical synthesis and place them onto the process flowsheet.
  - Label each unit operation model (i.e., block) as part of the process flowsheet and connect the blocks via process streams.
4. Specify the component flow rates and the thermodynamic conditions (temperature, pressure, and composition) of all feed streams.
5. Specify the operating conditions for the unit operation models (i.e., blocks).

We can deliberately change any of the specifications listed in steps 1–5, such as flow-sheet scheme, operating conditions, and feed compositions, run the show, compare the new results with the old (previous) results, and then decide whether to accept or reject new process alternatives. Keep in mind that changing the list of components means that we, in general, test for a new, alternative process type rather than simply a modified version of the same process, in terms of the type and number of physical and/or chemical treatment steps, needed to end up with the same final, finished product.

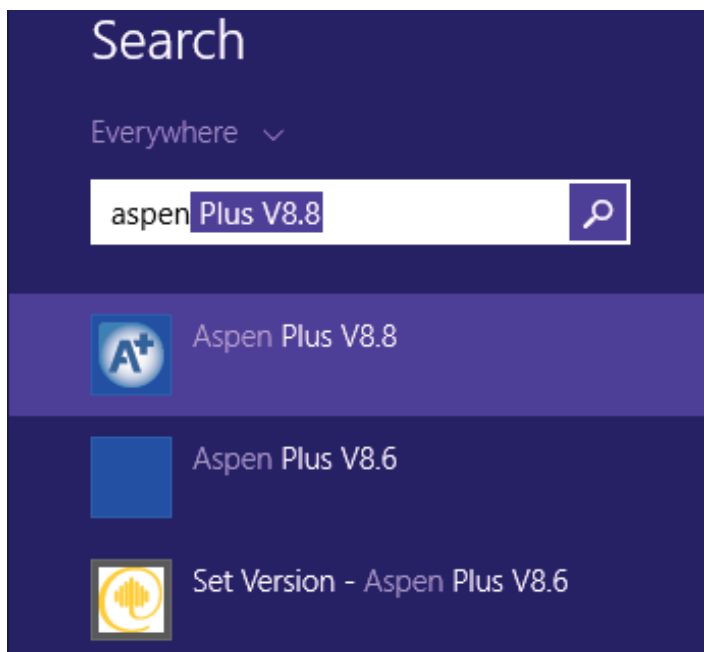
### 1.3 LAUNCHING ASPEN PLUS V8.8

Figure 1.1 shows where to look up Aspen Plus through Windows 8.1 Startup menu. First, click on the Windows icon keyboard button (or click on the bottom left Windows screen icon) to bring the first tile-based interface (the Metro UI) and second, on the down arrow to help the user bring the second tile-based interface to front, where it shows Aspen Plus V8.8 icon.



**Figure 1.1** Go to Windows 8.1 Startup menu, click on the down arrow key icon (*left*), and look for “Aspen Plus V8.8” icon (*right*).

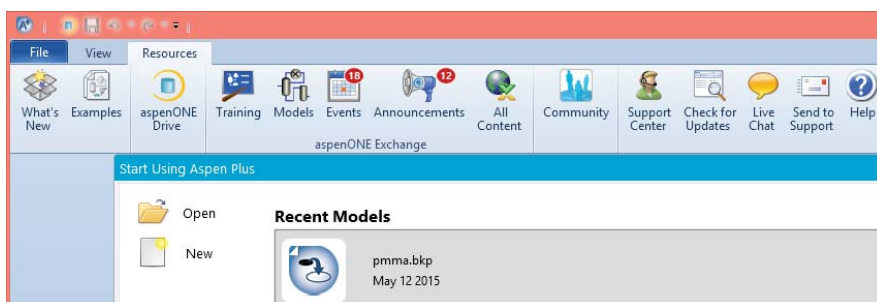
Alternatively, on the first tiled interface for tablets, key in the keyword “aspen” in Windows Search text box and Windows 8.x will furnish the menu with applications that are related to “aspen”; and finally click on “**Aspen Plus V8.8**” icon, as shown in Figure 1.2. On the other hand, for Windows 10, type the word “aspen” at the bottom-left corner of the main desktop, just right to the Windows icon, and Windows Cortana will populate the user with a list of potential aspen-based applications or files.



**Figure 1.2** On the first tiled interface for tablets, key in the keyword “aspen” in Windows Search text box and Windows 8.x will furnish the menu with applications that are related to “aspen”. Click on “**Aspen Plus V8.8**” to open.

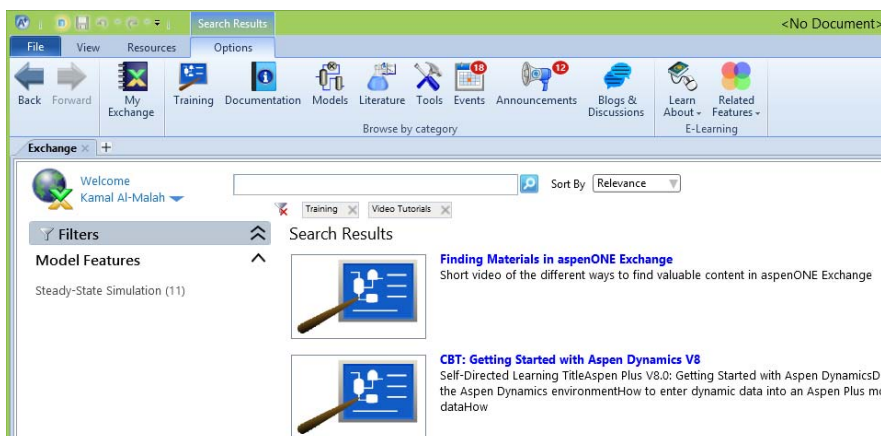
## 1.4 BEGINNING A SIMULATION

Figure 1.3 shows the first (main) window where the user may select different online (or offline) available resources, including product updates and training materials. You have to be a registered user to benefit from the online available resources. Click on “**Product Updates**” icon to see whether your software is up to date or requires installing new patches or packs. The user can select “**Open**” icon to open an existing file or select “**New**” icon to open a new file. We will discuss this issue shortly.



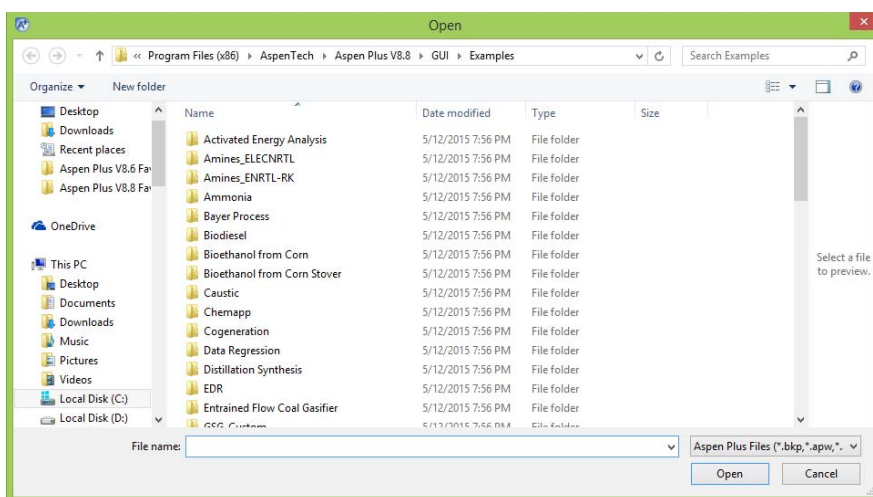
**Figure 1.3** Aspen Plus first window where the user is furnished with “**Resources**” ribbon and the choice to open either an existing or new file (i.e., simulation project).

On the other hand, clicking on “**Training**” icon and selecting “**Video Tutorials**” sub-category under the main category called “**Filters**”, which appears on the left pane, will populate your screen with different available online training resources, under “**Options**” tab, as shown in Figure 1.4.



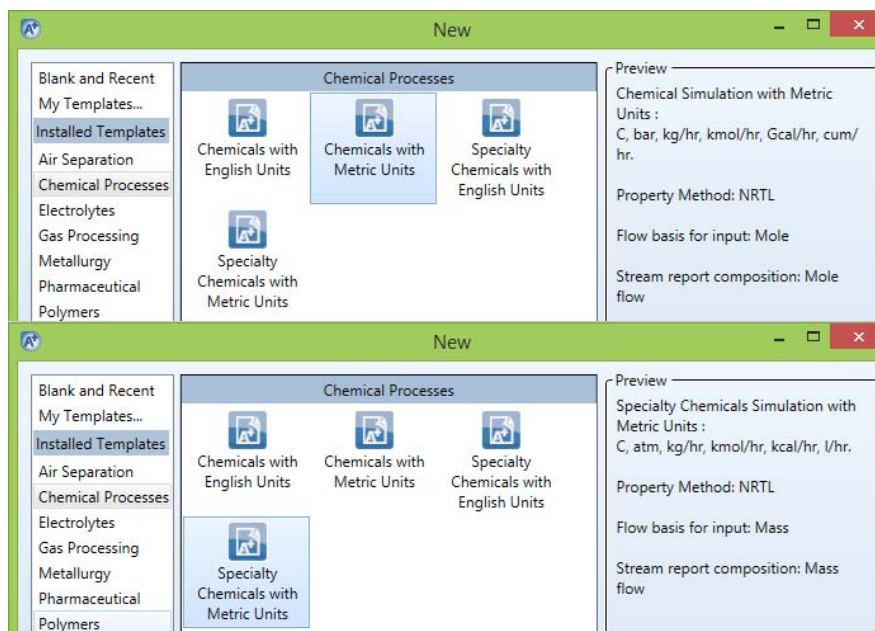
**Figure 1.4** Clicking on “**Training**” icon will populate the user’s screen with different online training media that are available to the registered user.

In addition, the user may benefit from offline available resources via clicking on “**Examples**” icon where she/he can select from different prepared case studies. Those can be found in the installation folder, for example: “**C:\Program Files (x86)\AspenTech\Aspen Plus V8.8\GUI\Examples**”. Figure 1.5 shows a portion of such offline examples that are delivered with Aspen Plus package.



**Figure 1.5** Aspen Plus provides offline examples where the user can benefit from.

As shown in Figure 1.3, we will choose opening a new file by clicking on “**New**” icon and the template window shows up where the user can select from different chemical industry–based templates. We will select “**Specialty Chemicals with Metric Units**” template, as shown in Figure 1.6 (*bottom*). Notice that the other counterpart template – “**Chemicals with Metric Units**” (*top*) – will differ in reporting the basis for stream composition and the units for pressure, volumetric flow rate, and rate of energy (power), as shown in “**Preview**” panel in Figure 1.6.



**Figure 1.6** The difference between “**Chemicals with Metric Units**” (*top*) and “**Specialty Chemicals with Metric Units**” template (*bottom*) lies in what metric units some physical properties are expressed.

Click on “**Create**” button, shown at the bottom of the template window, and the main window of Aspen Plus V8.8 shows up as in Figure 1.7.

STARTING from the top-left corner while moving row-wise to the right horizon until we finally reach the bottom-right corner, let us familiarize ourselves with what is seen, in the



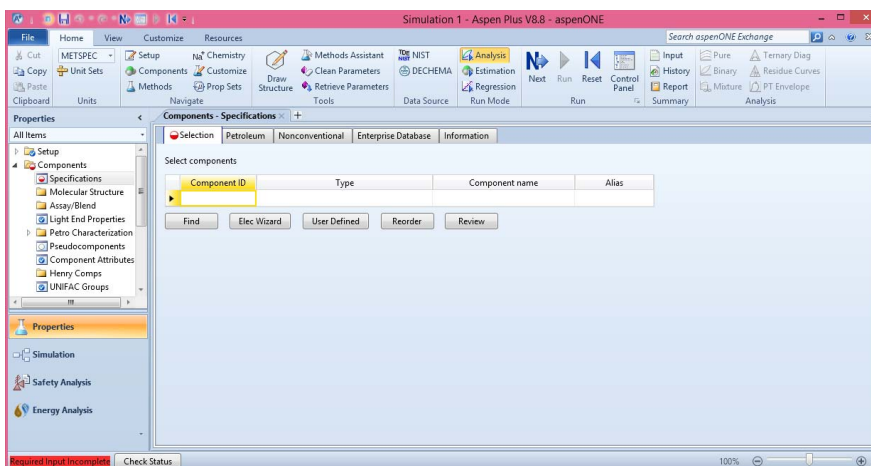


Figure 1.7 The main window of Aspen Plus flowsheet simulator.

form of a pane, ribbon, toolbar, status bar, input form, and tab, as shown in Figure 1.8. We briefly introduce each item with the understanding that, as the user keeps digging, he/she will become more comfortable because each item represents a shortcut key to one of the important features of Aspen Plus.

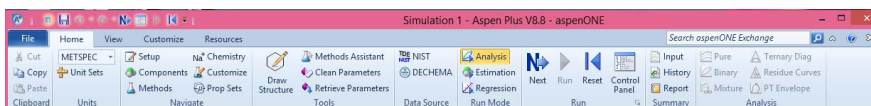


Figure 1.8 The top portion of Aspen Plus V8.8 main window contains the “Quick Access” toolbar (top bar), the “Top” toolbar, the help-related textbox and button (middle bar), and ribbon tabs associated with each “Top” toolbar menu (bottom bar).

The “**Quick Access**” toolbar contains the most commonly used functions in Aspen Plus, such as the “**Run**”, “**Restart**”, and “**Next**” buttons. Notice that other buttons can be incorporated into this toolbar simply by right-clicking on the desired function found in the “**Home**” ribbon, or in any other menu of “**Top**” toolbar, and adding it to “**Quick Access**” toolbar. The “**Top**” toolbar has “**File**”, “**Home**”, “**View**”, “**Customize**”, and “**Resources**” menus, where each menu has many submenu items that appear in the form of ribbon tabs. For example, the “**Home**” ribbon is shown in Figure 1.8 and it contains many tabs. Each “**Home**” ribbon tab will be explained shortly.

The first “**Home**” ribbon tab, called (“**Clipboard**” group), pertains to clipboard functions, such as “**Copy**”, “**Cut**”, and “**Paste**” buttons.

The second (“**Units**” group) tab deals with the unit sets. You can click on “**Unit Sets**” icon to open the form for entering a new set of your own (i.e., a customized set of units).

The third (“**Navigate**” group) tab represents the navigation pane where the user can open forms to choose components, select or modify property methods, and create or edit chemistry and property sets. Notice that this tab has the same functions as those of “**Navigation**” pane, shown later in Figure 1.10.

The fourth (“**Tools**” group) tab allows the user to draw chemical structures to better estimate property parameters for a user-defined component, to make use of the “**Methods Assistant**” wizard in defining the most suitable property method, and to retrieve/clean model parameters.

The fifth (“**Data Source**” group) tab deals with seeking additional components databanks, such as National Institute of Standards and Technology (NIST)/Thermo-Data Engine (TDE), and DECHEMA (experimental thermophysical properties of pure substances and mixtures available on the website; this is a paid service requiring an account setup directly with DECHEMA).

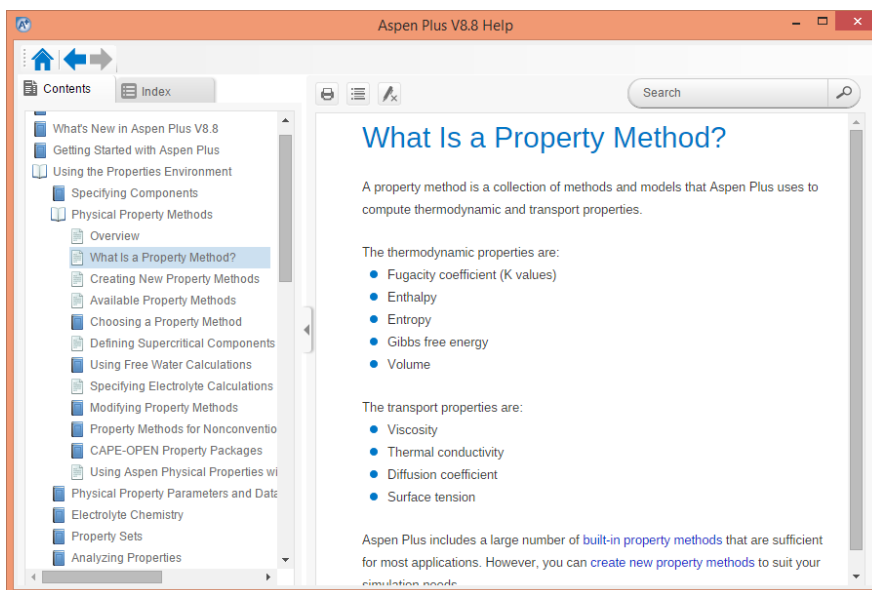
The sixth (“**Run Mode**” group) tab allows the user to select the mode of run (i.e., simulation). The run modes are analysis, estimation, and regression. In “**Analysis**” mode, the user may analyze properties of components. In “**Estimation**” mode, the user may estimate the unknown properties, such as critical properties for a known molecular structure and the model parameters for pure components and mixtures (i.e., pairwise interaction parameters). In “**Regression**” mode, the user may fit the model to data taken from Aspen Plus databanks; “NIST/TDE” databank; “DECHEMA” databank; or a user’s databank.

The seventh (“**Run**” group) tab lumps all functions related to the simulation solver, including the “**Next**”, “**Run**”, and “**Reinitialize**” (i.e., purge simulation results) buttons. The calculation status (i.e., convergence vs. divergence and presence/absence of errors and warnings) can be viewed via clicking on “**Control Panel**” button.

The eighth (“**Summary**” group) tab represents the summary where the user can view, print, and save the simulation input files, history, and reports.

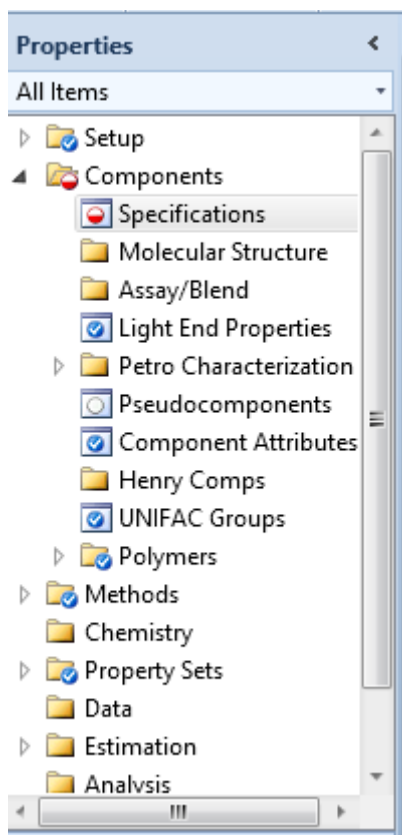
The ninth and last (“**Analysis**” group) tab will become active once the user defines the property sets and property method(s) for the selected components. This will allow the user to carry out and present both tabulated and graphical types of data analysis for a single- (i.e., pure), binary-, or multicomponent system.

The help-related search text box can be used to enter a key word and let Aspen Plus search for the relevant online resources. Clicking on “**Show Help**” icon will bring the built-in offline help database as shown in Figure 1.9.



**Figure 1.9** The offline built-in help database can be brought via clicking on the “**Show Help**” icon shown at the right top corner of the Aspen Plus v8.8 main window.

As shown in Figure 1.10, the “**Navigation**” pane is where the user can navigate to every stage of the property development process. This pane has a hierarchy (top to bottom) of input forms.

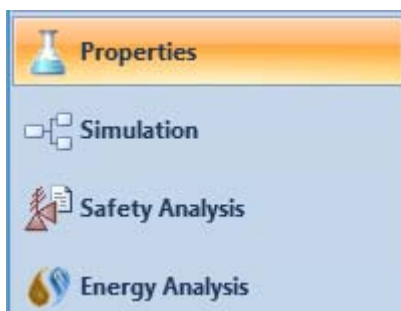


**Figure 1.10** The “Navigation” pane that acts as folder/file explorer.

Figure 1.11 shows a sample of an input form where the user types in process components.

**Figure 1.11** The input form for entering components involved in the process.

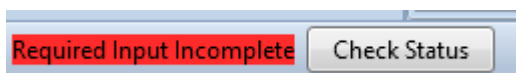
Figure 1.12 shows the “**Environments**” pane where the user is granted the luxury to switch from the “**Properties**” to “**Simulation**”, “**Safety Analysis**”, or “**Energy Analysis**” environment. Those types of environment are explained in detail in later chapters.



**Figure 1.12** The “**Environments**” pane where the user has the flexibility to switch from one to another environment.

**NOTE #0:** *Staying under “**Properties**” environment, the user does not have to specify a flowsheet; only components and the property model are needed at this stage for analysis, estimation, and regression purposes.*

Figure 1.13 shows the “**Status**” bar where the status indicator is seen, which tells the user where he/she stands in terms of the progress of process simulation, and the “**Check Status**” button, which can be used by the user to see the messages issued by Aspen Plus simulator or solver.



**Figure 1.13** The “**Status**” bar where the user is updated about the *status quo* of Aspen Plus simulator (or solver).

Finally, Figure 1.14 shows the “**Zoom**” bar with which the user can zoom in and out the input form under concern.



**Figure 1.14** The “**Zoom**” bar where the user may zoom in or out the input form under question.

After introducing the main features of Aspen Plus main window, let us pinpoint some other issues that will help the user better deal with Aspen Plus products. Notice that in “**Navigation**” pane (see Figure 1.10), there are different color codes adopted by Aspen Plus.

For example, a half-filled red circle indicates that input data are required for the simulator to proceed. In general, Figure 1.15 shows different color-coded symbols used by Aspen Plus.

This Symbol	On a(n)	Means
	Input form or sheet	Required input complete, or visited and no data required *
	Input form or sheet	Required input incomplete
	Input form	No data entered
	Mixed form	Input and results
	Results form	No results present (calculations have not been run)
	Results form	Results available without Errors or Warnings (OK) **
	Results form or flowsheet	Results available with Warnings **
	Results form or flowsheet	Results available with Errors **
	Results form	Results inconsistent with current input (input changed)
	Input folder	No data entered
	Input folder	Required input incomplete
	Input folder	Required input complete, or visited and no data required *
	Results folder	No results present
	Results folder	Results available - OK **
	Results folder	Results available with Warnings **
	Results folder	Results available with Errors **
	Results folder	Results inconsistent with current input (input changed)
	Folder or form	Object deactivated

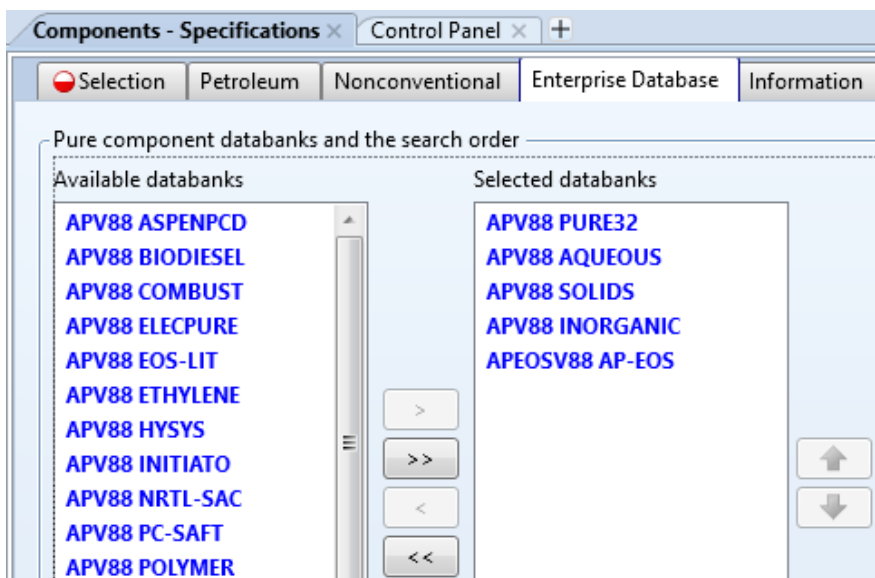
**Figure 1.15** Different color-coded symbols used by Aspen Plus to help the user better understand the status of the solver. *See Plate section for color representation of this figure.*

On the other hand, Figure 1.16 shows the field color coding for texts within input forms.

	Italic blue values are default values in input field where you have not entered a value
	Bold blue values are values you have specified
	A bright blue outline indicates the field you are currently editing
	Black values are results or non-editable values
	Gray values on a light gray background are disabled because of other specifications

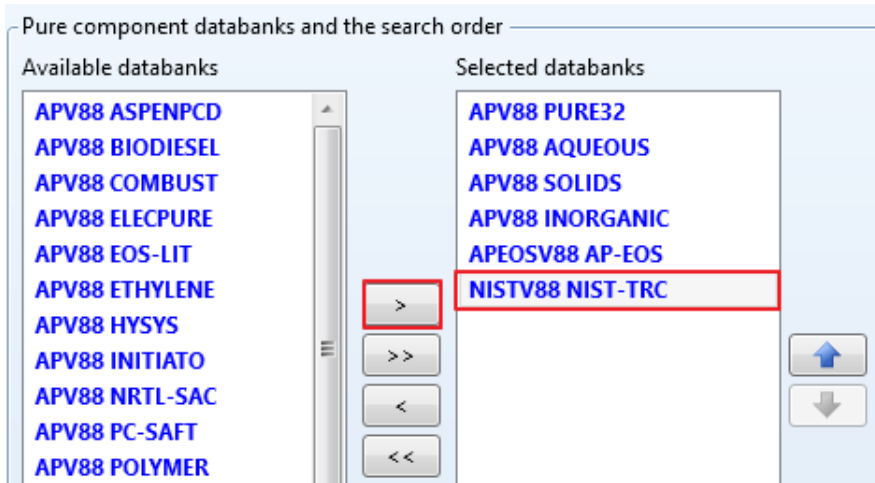
**Figure 1.16** The field color coding adopted by Aspen Plus for the text of an input form, which is either editable or noneditable by the user. *See Plate section for color representation of this figure.*

As shown in Figures 1.10 and 1.11, Aspen Plus requires us to enter the components involved in the process. A component can be either picked up from one of Aspen Plus built-in component databanks, or can be defined by the user and in the latter case it is considered as a non-databank member. Figure 1.17 shows the default (i.e., selected) databanks assigned by Aspen Plus, depending on, of course, the type of template initially chosen by the user. The user may select, however, one or more from the databanks available on the left side and add to the list of selected databanks on the right side, using the in-between arrow keys.



**Figure 1.17** The selected databanks are shown on the right side under “Enterprise Database” or “Databanks” tab.

As shown in Figure 1.18, “**NISTV88 NIST-TRC**” databank was added to the right list. The new database is provided under an agreement with the National Institute of Standards and Technology’s (NIST) Standard Reference Data Program (SRDP). The property parameters and the experimental data used were collected and evaluated by the Thermodynamics Research Center (TRC) using the NIST ThermoData Engine (TDE) and the NIST-TRC source data archival system for experimental thermophysical and thermochemical property data. The “NIST-TRC” source data is one of the world’s most comprehensive collections of such data.



**Figure 1.18** Inclusion of “NISTV88 NIST-TRC” databank that is comprehensive in resources.

**Notice** that the prefix “APV88” will be dropped from databank names if the user does not have the enterprise version of AspenOne and the “Enterprise Database” tab will be replaced by “Databanks” tab. Moreover, the capability to add “NISTV88 NIST-TRC” databank is available for the enterprise version.

Table 1.1 gives more description on such commonly used pure component databanks. Notice that PURE## databank may change from one version of Aspen Plus to another. For example, PURE26 is the primary component databank delivered with Aspen Plus V7.3.2 and is retained in the set of databanks for upward compatibility reason. In addition, when the user attempts to search for a certain name or chemical formula, then Aspen Plus search engine will look it up in the first databank appearing on the right side of Figure 1.18, followed by the second, and so on.

**TABLE 1.1 The Description and Usage of Commonly Used Pure Component Databanks.**

Databank	Contents	Uses
APV88 PURE32	Data from the Design Institute for Physical Property Data (DIPPR) and AspenTech	Primary component databank in Aspen Plus
APV88 AQUEOUS	Pure component parameters for ionic and molecular species in aqueous solution	Simulations containing electrolytes
APV88 SOLIDS	Pure component parameters for strong electrolytes, salts, and other solids	Simulations containing electrolytes and solids
APV88 INORGANIC	Thermochemical properties for inorganic components in vapor, liquid, and solid states	Solids, electrolytes, and metallurgy applications
APEOSV88	Binary and pair parameters for the Cubic-Plus-Association property model	Parameters for some compound pairs. See “Cubic-Plus-Association Parameters” offline and built-in help



## 1.5 ENTERING COMPONENTS

The user may enter the component by typing its name, such as oxygen, water, methanol, and ethanol, or its chemical formula, such as  $H_2$  and  $CH_4$ . As shown in Figure 1.19, once the user keys in the name of a compound or its chemical formula and clicks on either “tab” or “enter” key, Aspen Plus will complete the entries for the rest of columns titled: “**Type**”, “**Component name**”, and “**Alias**”. If the user, however, inadvertently keys in a word or formula that is not recognized by Aspen Plus, then it will not complete the missing information with the understanding that the user will introduce this new component to Aspen Plus environment (i.e., non-databank member).

Component ID	Type	Component name	Alias
OXYGEN	Conventional	OXYGEN	O2
WATER	Conventional	WATER	H2O
H2	Conventional	HYDROGEN	H2
CH4	Conventional	METHANE	CH4
ETHAN	Conventional		

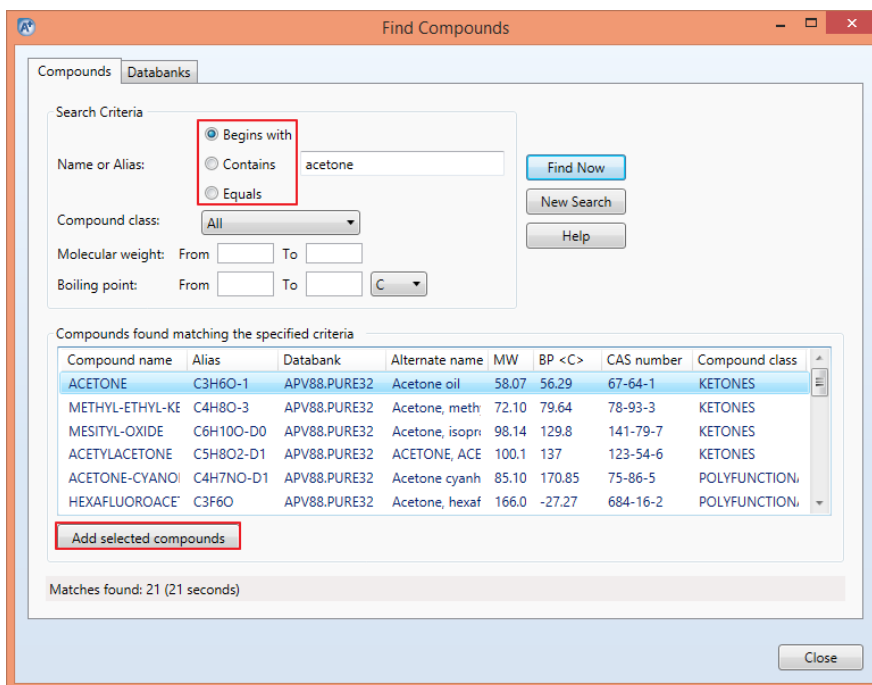
**Figure 1.19** Entering “**Component ID**” by either name or chemical formula allows Aspen Plus to recognize the component. If it is not automatically recognized, then the component name and alias will be left blank.

Regarding the component type, there are six major classes that can be dealt with in Aspen Plus:

1. Conventional: Single species fluids (vapor or liquid). Typical components that may participate in vapor–liquid-phase equilibrium.
2. Solid: Single species solids. Properties are calculated by solid-based models.
3. Non-conventional: Solids that are not pure chemical species. They are not represented as molecular components, such as coal or wood pulp. They are characterized using component attributes and do not participate in chemical or phase equilibrium.
4. Pseudocomponent, Assay, and Blend: Components representing petroleum fractions, characterized by boiling point, molecular weight, specific gravity, and other properties.
5. Polymer, Oligomer, and Segment: Components used in polymer models.
6. Hypothetical liquid: A component type that is mainly used in pyrometallurgical applications when modeling a component as a liquid when its properties should be extrapolated from solid properties, for example, modeling the carbon in molten steel.

Alternatively, the user may search for a given component via clicking on “**Find**” button (see Figure 1.11) under “**Components**” | “**Specifications**” | “**Selection**” tab form. Figure 1.20 shows “**Find Compounds**” window where the user can enter the search keyword either as a name or chemical formula within the dedicated text box. Moreover, the search criterion must be specified whether the searched phrase begins with, contains,





**Figure 1.20** The “Find Compounds” window enables the user to search using either the name or chemical formula of a compound, including the flexibility to refine search results.

or exactly equals to the entered keyword. Each criterion of search will definitely give different number of matched cases. The search criterion “**Contains**” is broader than the other two criteria. In addition, you may refine the search by

1. selecting the class of compound as being aliphatic, aromatic, polymer, inorganic salt, and so on;
2. entering the range of any of the two physical properties: molecular weight and boiling point temperature.

After you decide on the right component, highlight and click on “**Add selected compounds**” button at the bottom of “**Find Compounds**” window. Finally, the set of selected databanks can be modified using the second tab “**Databanks**” present in “**Find Compounds**” window.

## 1.6 SPECIFYING THE PROPERTY METHOD

One of the key and most important decisions is the selection of the property method. **A property method is a set of models used to calculate thermodynamic, kinetic, and transport properties.** If the components selected by the user do not work with Aspen Plus out-of-box property (i.e., default or recommended) methods, then such methods can be modified by the user. The thermodynamic method, a subset of the property method, can be broadly classified as

1. an activity coefficient-based method;
2. an equation of state method.

The activity coefficient-based method is mainly described for subcritical and non-ideal liquid systems at pressures below 10 atm. The incorporated parameters within the model are temperature dependent. Such a method becomes problematic in the critical region. The concept of ideal versus non-ideal liquid mixture can be simplified first, before entering the intricate picture of solution thermodynamics.

In general, mixing two or more similar species, to form a solution, results in an ideal liquid mixture. For example, mixing benzene with toluene forms an ideal benzene–toluene mixture and so is the case with methanol–ethanol mixture or *n*-heptane–octane mixture. The similarity among chemical species is exemplified in terms of equal number and the same type of functional groups (i.e., —OH, —OOH, —O—, —NH<sub>2</sub>, =, ≡, etc.) to a large extent and of the length of the hydrocarbon chain (or tail) of the molecule, to a small extent. The deviation from an ideal liquid mixture (or formation of non-ideal liquid mixture) arises from mixing of chemical species characterized by different chemical activities (i.e., different functional groups) and by different sizes of homologous series or both. For example, mixing ethanol with water forms a non-ideal liquid mixture, as water and ethanol are of two different categories. Mixing of ethanol with hexanol also shows some sort of deviation from ideality compared with mixing of ethanol with propanol, next to ethanol in homologous series of alcohols.

From solution thermodynamics point of view, the non-ideal liquid mixture can be described by introducing the concept of fugacity, which basically accounts for the effective “thermodynamic” presence of species *i* in a solution. This means that its thermodynamic concentration not only reflects its count (or composition) but also extends to include its “social” interaction with its neighbors, the so-called activity coefficient. Thus, the fugacity of species *i* in a mixture is given by

$$\hat{f}_i = x_i \times \gamma_i \times f_i^\circ \quad (1.1)$$

where

$\hat{f}_i$  : the fugacity of species *i* in a mixture at the given pressure, temperature, and composition;

$x_i$  : the mole fraction of species *i* in a mixture;

$\gamma_i$  : the activity coefficient of species *i* in a solution at the given pressure, temperature, and composition;

$f_i^\circ$  : the fugacity of pure liquid species *i* at the given pressure and temperature.

For an ideal liquid mixture, the activity coefficient is reduced to unity and the pure component fugacity is replaced by the vapor pressure of substance *i* at the given temperature. Thus, Equation 1.1 becomes

$$\hat{f}_i = x_i \times P_i^{\text{sat}}(T) \quad (1.2)$$

In a similar manner, the gas-phase fugacity can be expressed as

$$\hat{f}_i = \hat{\phi}_i \times y_i \times P \quad (1.3)$$

At low pressure, the fugacity coefficient of species  $i$  in a gas-phase mixture reduces to unity, and we have

$$\hat{f}_i = y_i \times P \quad (1.4)$$

The Raoult's case represents the simplest case, that is, ideal liquid mixture–ideal gas mixture under vapor–liquid phase equilibrium (VLE), where both fugacities are set equal.

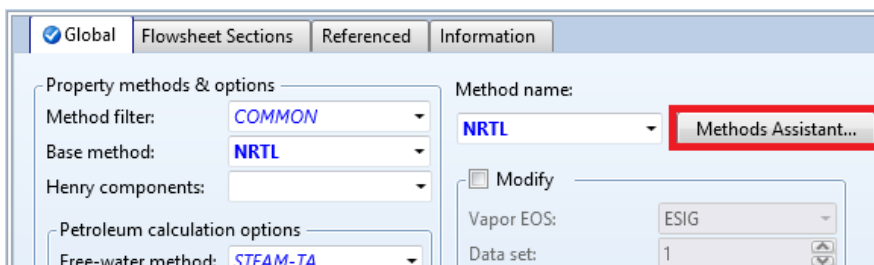
$$x_i \times P_i^{\text{sat}}(T) = y_i \times P \quad (1.5)$$

Examples of activity coefficient-based model are “**NRTL**” (Non-Random-Two-Liquid), “**UNIFAC**” (UNiversal Functional Activity Coefficient), and “**UNIQUAC**” (UNiversal QUasichemical Activity Coefficient). “**UNIFAC**” is based on group contributions rather than molecular contributions. With a limited number of group parameters and group–group interaction parameters, “**UNIFAC**” can predict activity coefficients. Because the “**UNIFAC**” model is a group-contribution model, it is very predictive. All published group parameters and group binary parameters are stored in the Aspen Plus physical property system. Activity coefficient models usually perform well for systems of polar compounds at low pressures and away from the critical region. They are the best way to represent highly nonideal liquid mixtures at low pressures (below 10 atm). They are used for the calculation of fugacity, enthalpy, entropy, and Gibbs free energy. Usually, an empirical correlation is used in parallel for the calculations of density when an activity coefficient model is used in phase equilibrium modeling.

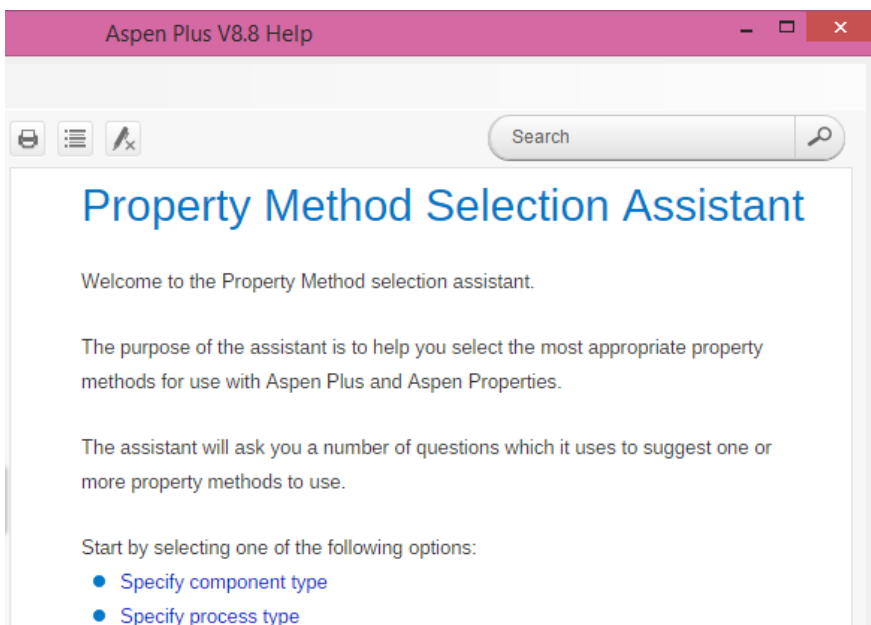
On the other hand, the equation of state model operates in the critical region and when there are no polar components. It describes the holy relationship among the three variables:  $P$ ,  $T$ , and  $\hat{V}$ . It has few binary parameters that extrapolate well with temperature. We can use equation of state model over wide ranges of temperature and pressure, including a subcritical and supercritical region. For ideal or slightly non-ideal systems, thermodynamic properties for both the vapor and liquid phases can be computed with a minimum amount of component data. An equation of state model is suitable for modeling hydrocarbon systems with light gases such as CO<sub>2</sub>, N<sub>2</sub>, and H<sub>2</sub>S. For the best representation of non-ideal systems, we must obtain binary interaction parameters from regression of experimental vapor–liquid equilibrium (VLE) data. Equation of state binary parameters for many component pairs are available in the Aspen Plus physical property system.

Examples of an equation of state model are “**PENG-ROB**” (PENG-ROBinson), “**RK-SOAVE**” (Redlich-Kwong Soave), and “**PC-SAFT**” (Perturbed-Chain Statistical Associating Fluid Theory-copolymer systems).

Since the selection of a property method, for a given chemical process/component, has the first priority, Aspen Plus provides what is called the property method selection assistant (or wizard) that can be reached via clicking on the “**Methods Assistant ...**” button found in “**Methods**” | “**Specifications**” | “**Global**” tab window, as shown in Figure 1.21 and the “**Aspen Plus V8.8 Help**” window pops up as shown in Figure 1.22.

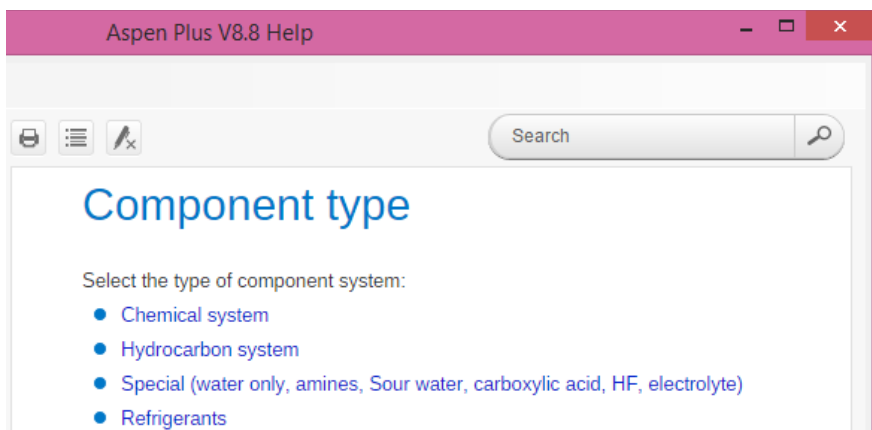


**Figure 1.21** Aspen Plus provides a wizard for helping the user select the proper property method(s) for a given chemical process or component type.



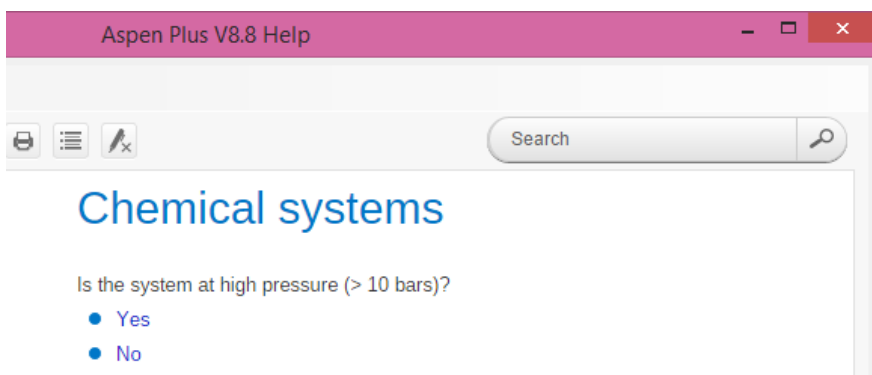
**Figure 1.22** The property method selection wizard that helps the user refine the number of suitable property methods for a given process/component.

Here, the user is to opt between component or process type. Do not panic; both choices will guide you to the city of Rome, and upon choosing “**Specify by component type**” option, the help window updates the content as shown in Figure 1.23. It shows four different component-based categories out of which the user may select. For example, if the user selects the first category, that is, “**Chemical system**” and further selects the pressure to be less than or equal to 10 bar, then the recommended property method will be activity coefficient-based method as is the case shown later in Figure 1.27. The second category better describes hydrocarbon (non-polar) systems. The third category is dedicated for some special applications, such as amines system, carboxylic acids (such as acetic acid) in the mixture, electrolyte system, hydrogen fluoride (HF) in the mixture, refrigerants, sour water system, and water only. The last category is reserved for refrigerants.



**Figure 1.23** The user has to further select the type of component system in order to refine the property method selection by Aspen Plus.

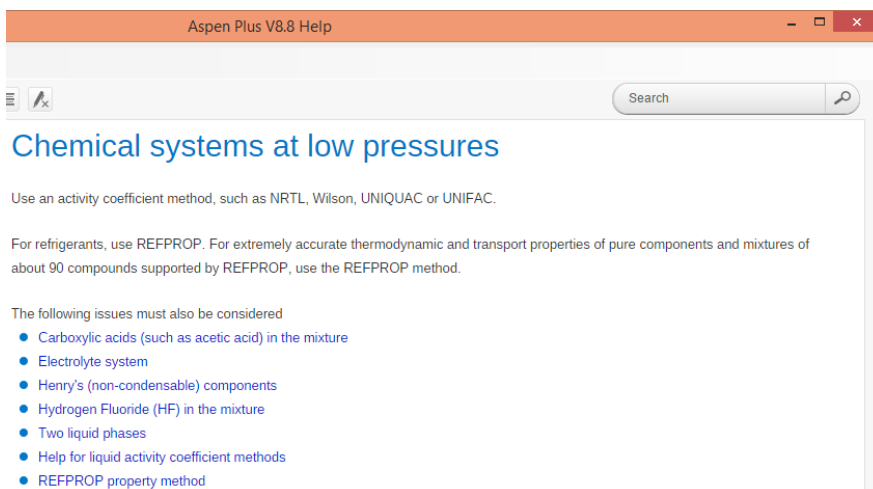
Upon selecting “**Chemical system**” option, Aspen Plus opts the user to select between a low- and a high-pressure operating condition, as shown in Figure 1.24.



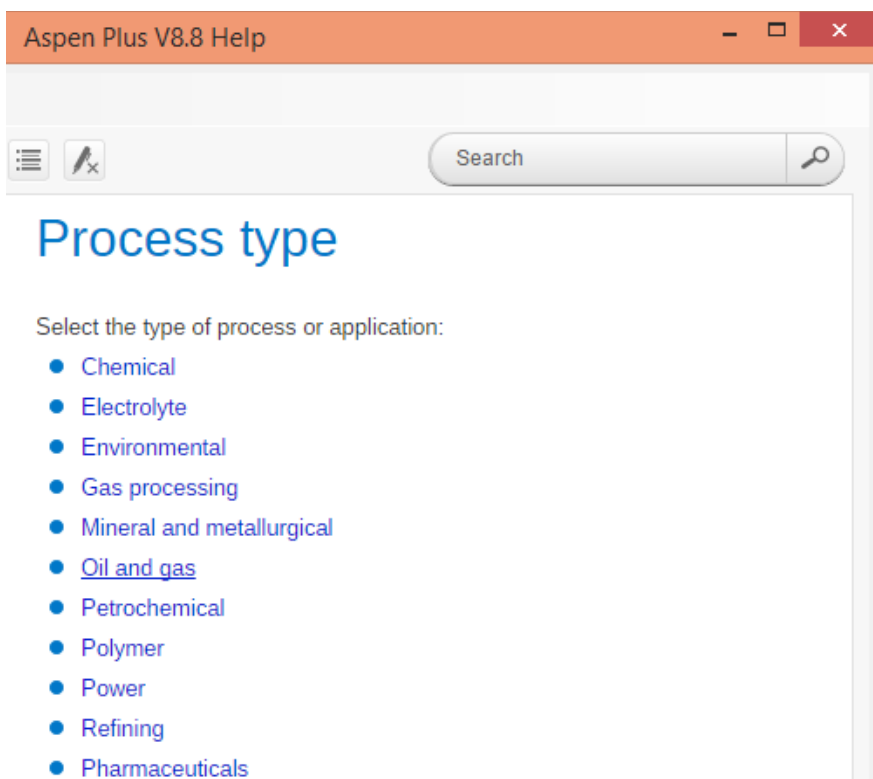
**Figure 1.24** Further zooming is carried out by choosing between a low- and a high-pressure operating condition.

Upon selecting a low-pressure condition, Aspen Plus help window finally shows up the recommended property method(s), as shown in Figure 1.25.

On the one hand, let us go by “**Specify process type**” choice and Figure 1.26 is the result of our choice. Notice that for “**Chemical**”, “**Environmental**”, “**Gas processing**”, “**Petrochemical**”, “**Power**”, and “**Refining process**” type of process, shown in Figure 1.26, the user will notice that there are additional subcategories from which the user can pick up his/her choice; this in turn will further refine the number of property methods recommended by the Aspen Plus property method wizard.

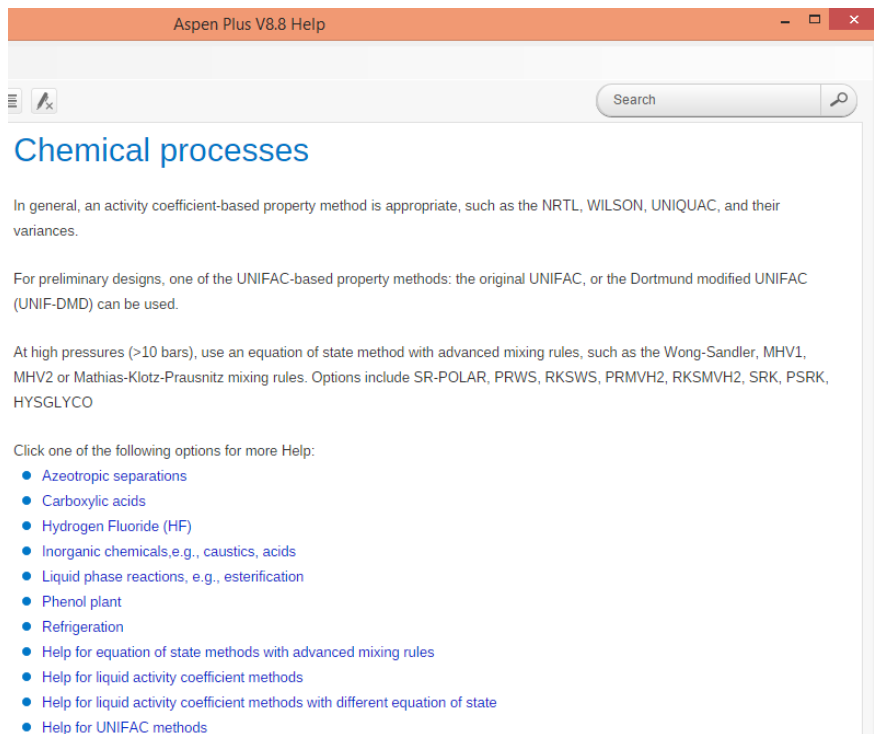


**Figure 1.25** The recommendation by Aspen Plus is to use any of the activity coefficient-based method such as NRTL, Wilson, UNIQUAC, and UNIFAC.



**Figure 1.26** The user may select one process type that best describes the process in hand.

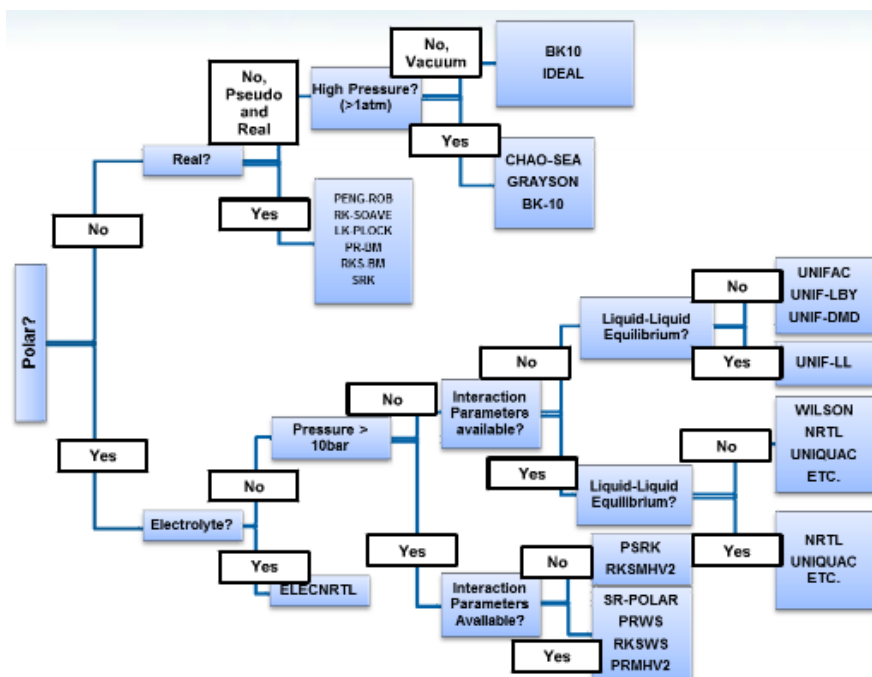
For example, if we select the type of process to be “**Chemical**”, then Figure 1.27 shows what property method(s) is (are) recommended by Aspen Plus. As one can see that Aspen Plus property method wizard recommends the activity coefficient-based method for a general chemical process for an applied pressure less than or equal to 10 bar and the equation of state method with advanced mixing rules for an applied pressure greater than 10 bar. As pointed earlier, some specialty chemical processes are also pinpointed as subcategories of chemical processes, such as azeotropic separations, and carboxylic acids.



**Figure 1.27** The property method wizard recommends the activity coefficient-based method for a general chemical process for pressure less than or equal to 10 bar and the equation of state method with advanced mixing rules for pressure greater than 10 bar. Some specialty chemical processes are also pinpointed.

Remember that the deeper you dive below the surface, as you move from the main into a subcategory of a chemical process/component, the higher the accuracy and predictability of the Aspen Plus-recommended property method will be. There are special common applications where Aspen Plus gives them extra attention in terms of model accuracy and predictability.

Finally, Figure 1.28 shows the tree for the property method selection, which is based on different categories, such as the nature of medium (i.e., polar vs. non-polar, electrolyte vs. non-electrolyte, or ideal vs. real), the operating conditions (i.e., high vs. low pressure), the presence/absence of interaction parameters, and the presence/absence of LLE.



**Figure 1.28** The “Property Method” selection tree based on different categories: The nature of medium (i.e., polar vs. nonpolar, electrolyte vs. nonelectrolyte, or ideal vs. real), the operating conditions (i.e., high vs. low pressure), the presence/absence of interaction parameters, and the presence/absence of LLE.

**NOTE #1:** The property method selection is revisited in each successive chapter as it is the heart of any simulation process. Hopefully, toward the end of the book the user will grab the essence of property method selection based on the given chemical process being handled.

**NOTE #2:** The idea behind presenting the choice of having more than one property method to try for a given process/component system is simply that one method may be superior to others in terms of getting a converging solution and realistic results. As one can see later that a given property method may fail to end up with realistic (or reasonable) results. In fact, it may not even converge to give a solution, in the first place. Thus, the built-in property method selection assistant will narrow the “search” circle for trying alternative property methods should the first suggested (or default) method fail to give reasonable results. Of course, it is intuitively assumed that the user has properly entered the flow rates, their compositions, their operating conditions (i.e.,  $P$  &  $T$ ), and any other physical, chemical, geometric, or thermodynamic constraint imposed on a given block or unit.



**NOTE #3:** Refer to Aspen Plus built-in help under the title: “Guidelines for Choosing a Property Method”; “Guidelines for Choosing a Property Method for Polar Non-Electrolyte Systems”; and “Guidelines for Choosing an Activity Coefficient Property Method”.

**NOTE #4:** The user may assign a property method for a specified section, which is different from that assigned for the rest of the process flowsheet (i.e., global section). By default, Aspen Plus assigns a section called “GLOBAL” for the entire process flowsheet; however, the user may define a new section where it may comprise existing or newly added blocks. For further information on using more than one property method in a flowsheet, see Section 18.11.

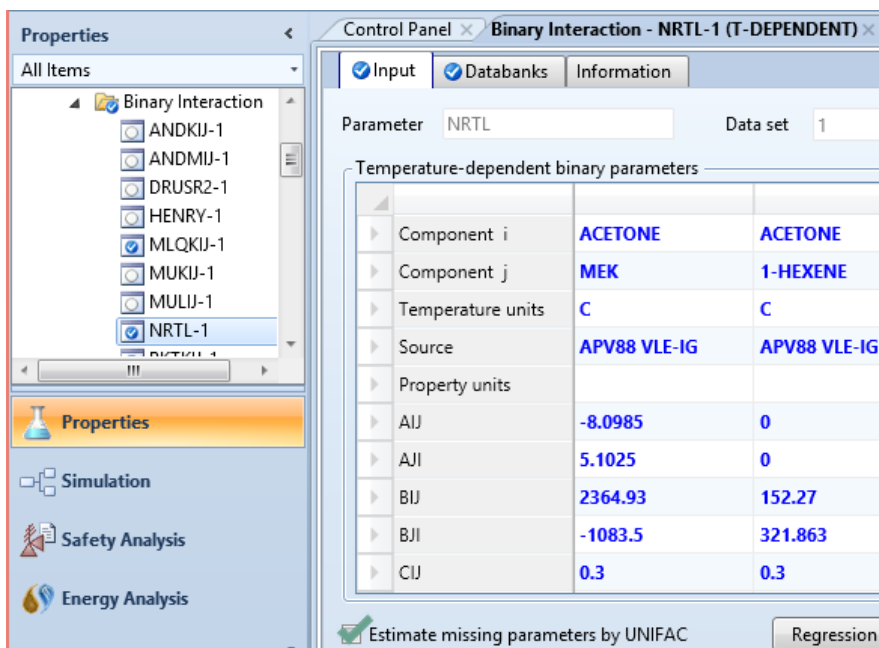
## 1.7 IMPROVEMENT OF THE PROPERTY METHOD ACCURACY

To demonstrate an example of how we can further improve the accuracy of a given model, let us look at the following set of compounds as part of a chemical process. Figure 1.29 shows three components: acetone, methyl ethyl ketone (MEK), and 1-hexene.

<div> <input checked="" type="checkbox"/> Selection         <div>PetroleumNonconventional<input checked="" type="checkbox"/> DatabanksInformation</div> </div>			
Select components:			
	Component ID	Type	Component name
▶	ACETONE	Conventional	ACETONE
▶	MEK	Conventional	METHYL-ETHYL-KETONE
▶	1-HEXENE	Conventional	1-HEXENE

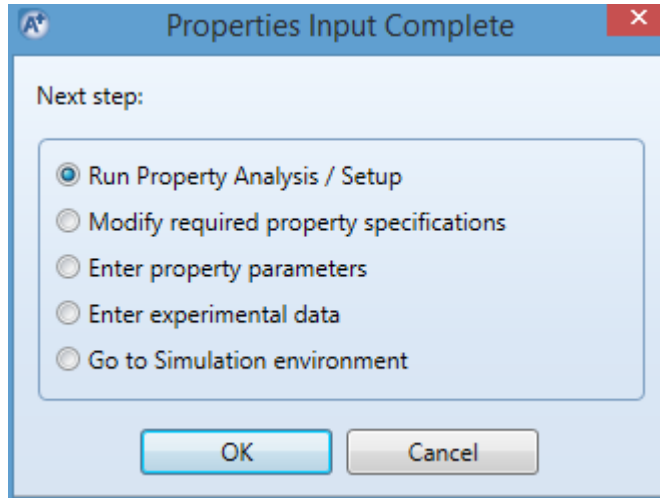
**Figure 1.29** Three components are chosen to demonstrate the improvement of the accuracy of the default property method for a chemical process, that is, “NRTL”.

Figure 1.30 shows the pairwise (i.e., binary) interaction parameters for the given three components. Notice that MEK–1-hexene interaction parameters are not given by Aspen Plus (i.e., not present in the built-in databanks). To improve the model predictability, one can select “**Estimate missing parameters by UNIFAC**”, which will let Aspen Plus complete the missing information.

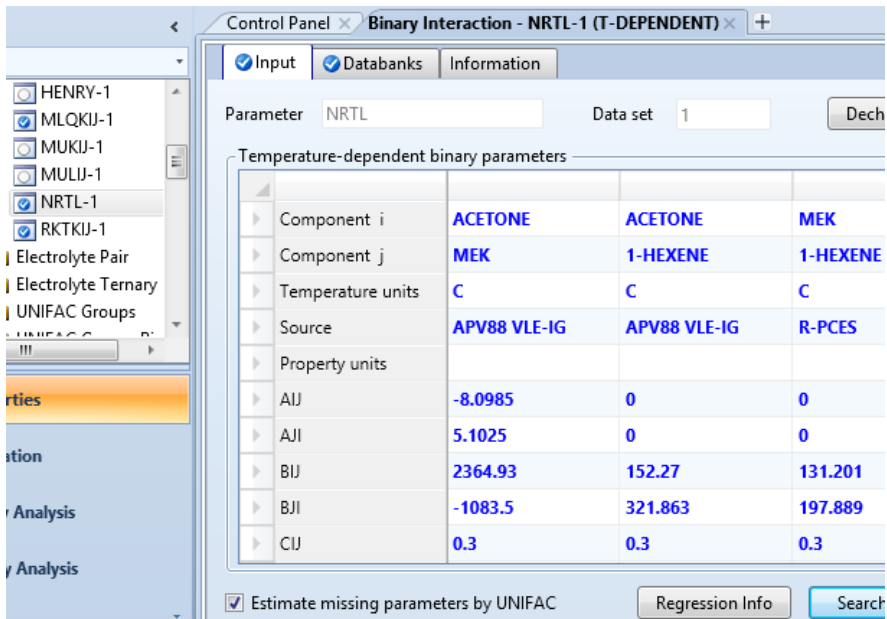


**Figure 1.30** Initially, the binary interaction parameters for MEK–1-hexene are missing. They can be calculated using “UNIFAC” method.

After selecting “**Estimate missing parameters by UNIFAC**”, while being under “**Properties**” environment | “**Analysis**” mode, click on “**Next**” button and Figure 1.31 window shows up. Select the “**Run Property Analysis/Setup**” option and click on the “**OK**” button and “**Control Panel**” tells that table generation is completed. Switch back to “**Binary Interaction - NRTL-1 (T-DEPENDENT)**” tab, you will notice that Aspen Plus has already calculated the pairwise interaction parameters for MEK–1-hexene, as shown in Figure 1.32. Notice that the source for the last column is now “**R-PCES**”, which means utilizing **Property Constant EStimation (PCES) regression**. PCES provides the Bondi method for estimating the R and Q parameters for UNIFAC functional groups. The Aspen Plus physical property system uses these parameters in the UNIFAC, Dortmund UNIFAC, and Lyngby UNIFAC model. The Bondi method requires only the molecular structure as an input.



**Figure 1.31** Select “Run Property Analysis/Setup” option to calculate the missing binary interactions parameters for MEK–1-hexene.



**Figure 1.32** The binary interaction parameters are shown for MEK–1-hexene using “UNIFAC” method.

Under some circumstances, you may have to add additional databanks (see Figure 1.18) so that Aspen Plus can calculate the missing parameters.

The user may wish to carry out data analysis at this stage to check for the property model applicability. Click on the “**Binary Analysis**” button, at the right-top corner of “**Home**” ribbon, as shown in Figure 1.33.



**Figure 1.33** The “Binary Analysis” button is shown in “Home” ribbon.

The user may select *Gibbs energy of mixing*,  $T_{xy}$ , or  $P_{xy}$  as a function of mole fraction to see whether the binary mixture of MEK–1-hexene forms an ideal mixture or deviates from ideality. For instance, Figure 1.34 shows the window for preparing the  $P_{xy}$  plot of the binary system made of 1-hexene and MEK.

**Binary Analysis** | Diagnostics | Information

Analysis type: **Pxy**

Components

Component 1: **1-HEXENE**

Component 2: **MEK**

Flash options

Valid phases: **Vapor-Liquid**

Maximum iterations: **30**

Error tolerance: **0.0001**

Flash convergence algorithm:

☒ Use flash retention

Temperature

Units: **C**

☒ List of values

**25**

☐ Overall range

Lower limit: Upper limit:

No. of points: Increments:

Property options

Property method: **NRTL**

Henry components:

Chemistry ID:

Calculation approach: **True components**

**Run Analysis**

Compositions

Basis: **Mole fraction**

Vary: **1-HEXENE**

☐ List of values

☒ Overall range

Lower limit: **0**

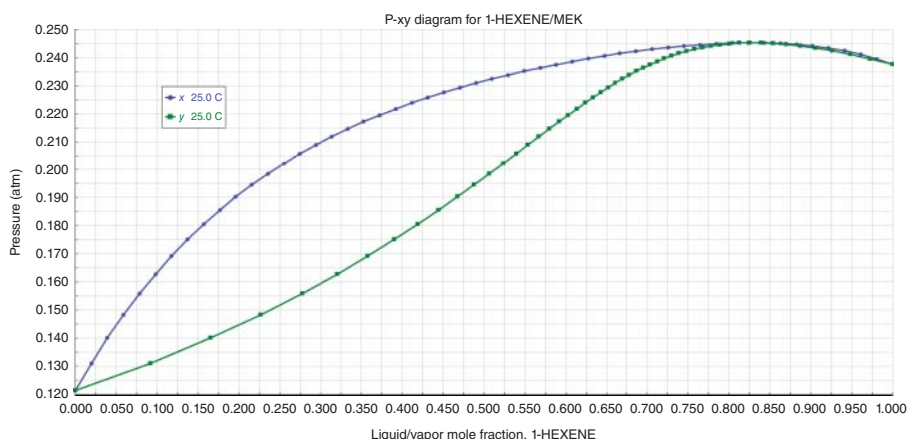
Upper limit: **1**

Number of points: **51**

Increments:

**Figure 1.34** Carrying out analysis via plotting the isothermal dew- and bubble-point pressure as a function of mole fraction of 1-hexene to see the deviation from ideality.

Click on “**Run Analysis**” button and Aspen Plus shows the  $Pxy$  plot for the selected binary mixture, as shown in Figure 1.35. The figure shows a deviation from an ideal mixture in the form of an azeotrope at a mole fraction of 1-hexene higher than 0.80. An ideal liquid mixture (i.e., Raoult’s case) gives a straight line of  $P$  versus  $x$  with no formation of an azeotrope. Notice that the top blue curve, a non-straight line, represents the bubble-point pressure as  $f(x_{\text{hexene}})$ , which also indicates that we have a non-ideal binary mixture even below 0.8 mole fraction of 1-hexene.



**Figure 1.35** The dew- and bubble-point pressure as a function of 1-hexene mole fraction. Formation of an azeotrope can be seen at 1-hexene mole fraction greater than 0.80, in the form of an azeotrope.

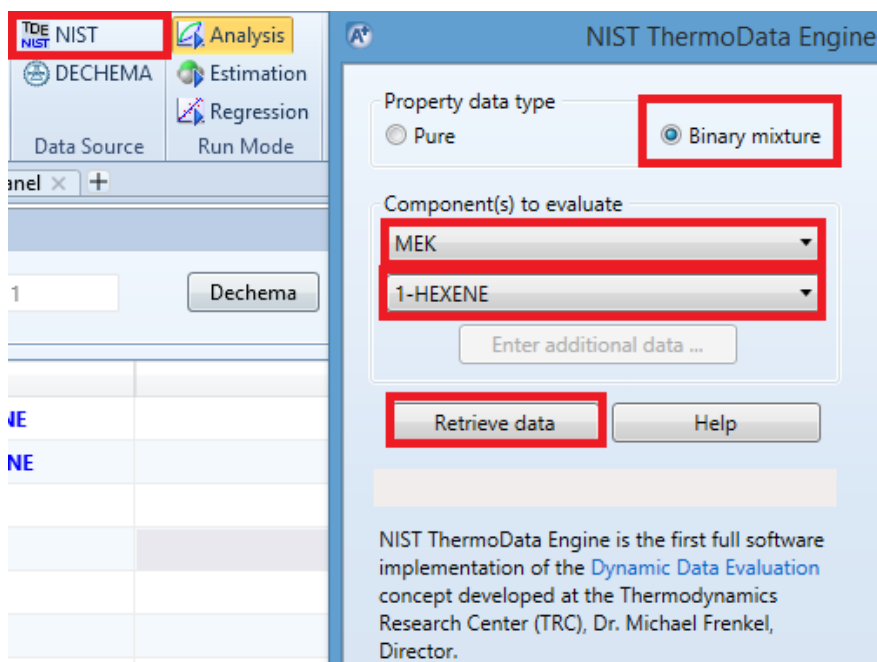
**NOTE #5:** The plot format can be accessed via “**Plot Format**” tab window found in the “**Top**” toolbar. The user may carry out cosmetic changes (i.e., font type and size) on the plot format and make it look a more plausible.

At this stage, one can say that the default property method “**NRTL**” could account for a deviation from ideality for the binary mixture of MEK–1-hexene via accounting for the azeotrope condition at higher values of 1-hexene, using UNIFAC group contribution method.

**NOTE #6:** In general, it will be sufficient, within acceptable engineering accuracy limits, to calculate the missing pairwise interaction parameters using UNIFAC method. Nevertheless, if more accuracy is required, then the experimental data can be retrieved from the **ThermoData Engine (TDE)**, which is a thermodynamic data correlation, evaluation, and prediction tool provided with Aspen Plus through a long-term collaboration agreement with the National Institute of Standards and Technology (**NIST**). The purpose of the TDE software is to provide critically evaluated thermodynamic and transport property data based on the principles of dynamic data evaluation. Critical evaluation

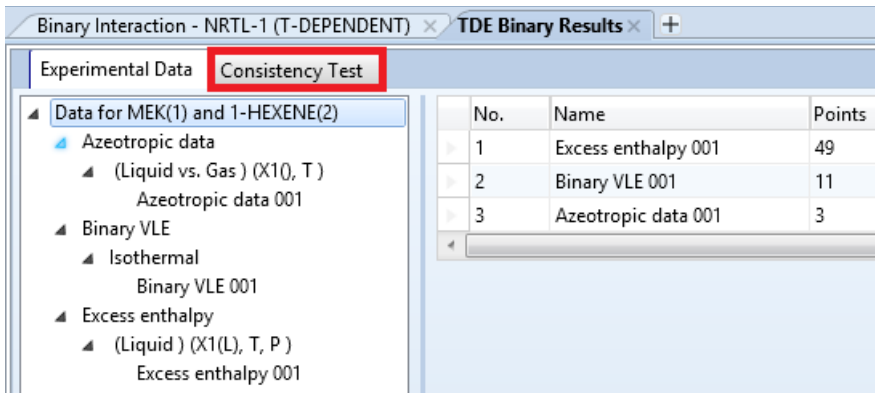
*is based on published experimental data stored in a program database, predicted values based on molecular structure and corresponding-states methods, and user supplied data, if any. The NIST source database contains more than 24,000 pure components, more than 30,000 binary pairs, and is updated quarterly.*

Here, let us show how to improve the accuracy of pairwise interactions. Either open a new simulation with the same three components or delete the third column that belongs to MEK–1-hexene binary interaction parameters. Click on the “**NIST**” button as shown in Figure 1.36 (left) and the “**NIST ThermoData Engine**” window shows up as shown in Figure 1.36 (right). Remember to de-select “**Estimate missing parameters by UNIFAC**” option in “**Parameters**” | “**Binary Interaction**” | “**NRTL-1**” | “**Input**” tab form; otherwise, the results will be different in the following figures.



**Figure 1.36** Retrieving experiment-based data for the binary mixture of MEK–1-hexene with the help of “NIST/TDE” database.

Click on the “**Retrieve data**” button and the result is shown in Figure 1.37. It shows 11 binary VLE data points for the given binary mixture. We exploit such a data set to find the parameters describing the interaction between MEK and 1-hexene.



**Figure 1.37** A set of 11 data points are obtained from “NIST/TDE” databank for the given binary mixture.

**NOTE #7:** *Not all experimental data are reliable or trustable; in other words, the consistency test must be carried out prior to hinging upon them for the sake of extracting further pure or binary data. See Chapter 2 as a demonstration for the possibility of having some NASTY, out of NIST, data.*

Click on the “**Consistency Test**” tab to test for the data goodness and run the consistency test via clicking on the “**Run Consistency Tests**” button shown at the bottom of the “**Consistency Test**” tab form. Figure 1.38 shows the consistency test results. The overall data quality is about 0.8, which is close to unity. The closer to one the value is, the better the data quality will be.

No.	Name	Points	Year	Isotherm (K)	Isobaric (N/sqm)	Overall data quality	Herington test	Van Ness test	Piont test	Infinite dilution test	EOS test	Endpoint test
1	Binary VLE 001	11	1967	333	---	0.79	Passed	Passed	Passed	Passed	---	0.79

NIST/TDE consistency test

Thermodynamic consistency test is finished for all VLE datasets.

OK

**Figure 1.38** The NIST/TDE consistency test with an overall data quality of 0.79.

Let us go back to the “**Experimental Data**” tab window (see Figure 1.37). Click on the “**Binary VLE**” | “**Isothermal**” | “**Binary VLE 001**” form and save the data set via clicking on the “**Save Data**” button at the bottom of the active form so that we can carry out some regression/estimation steps to improve the model goodness. The “**Binary experimental data to be saved**” window pops up as in Figure 1.39.

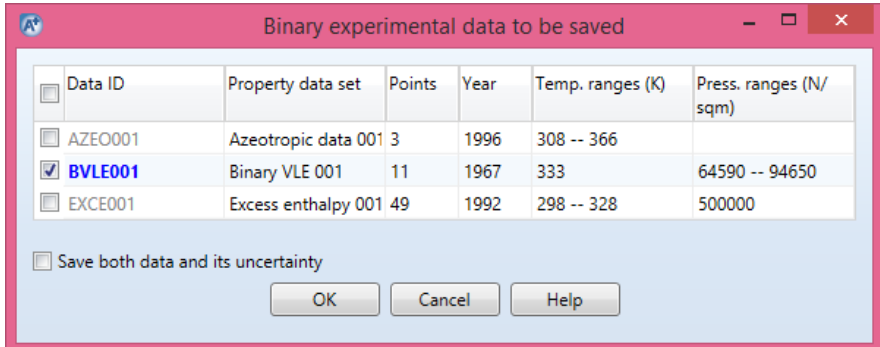


Figure 1.39 The “Binary experimental data to be saved” window for saving NIST/TDE data set.

A confirmation pop-up window will tell the user that the data are saved under “Data” folder in “Navigation” pane, as shown in Figure 1.40. Of course, you may rename the data set to a name of your choice by right-clicking on the data set shown under “Data” folder and selecting “Rename” submenu from the short pop-up context menu.

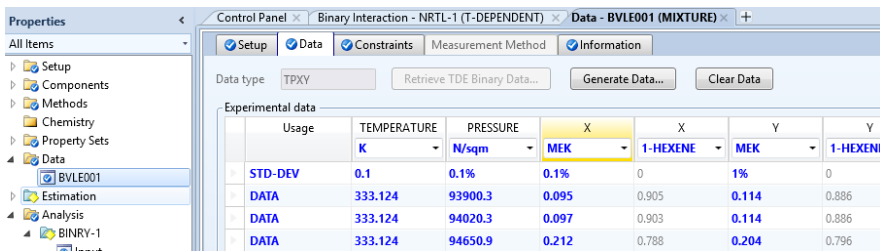
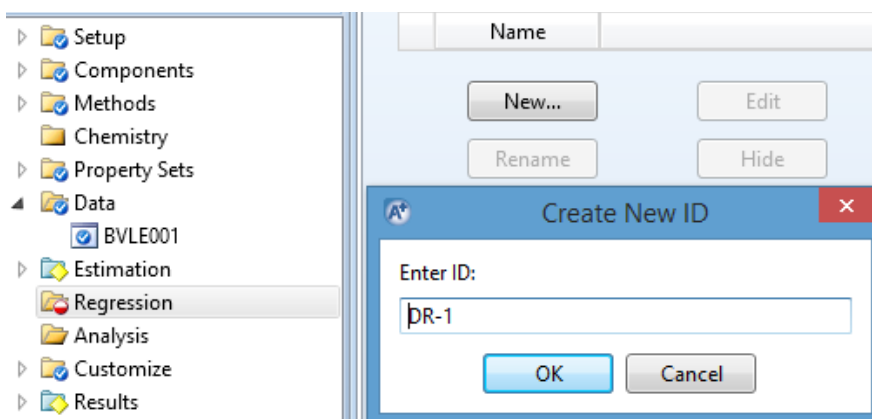


Figure 1.40 The experimental data are saved within Aspen Plus environment under “Data” folder.

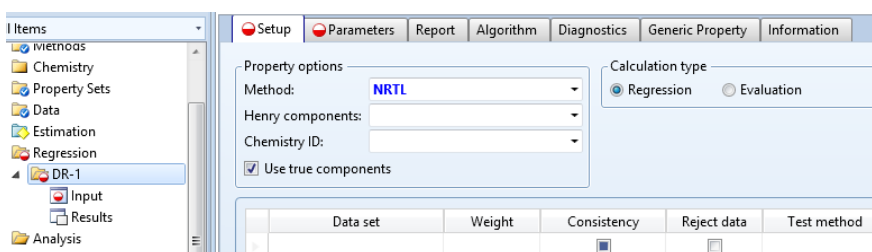
Let us switch to “Regression” mode (we are still under “Properties” environment) so that we can carry out regression or parameter evaluation step. Once the user switches to “Regression” mode, the “Regression” folder icon becomes half-filled red circle, indicating that it requires further input data to be dealt with in “Regression” mode. Under “Regression” tab form, click on “New ...” button where “Create New ID” form pops up as shown in Figure 1.41.



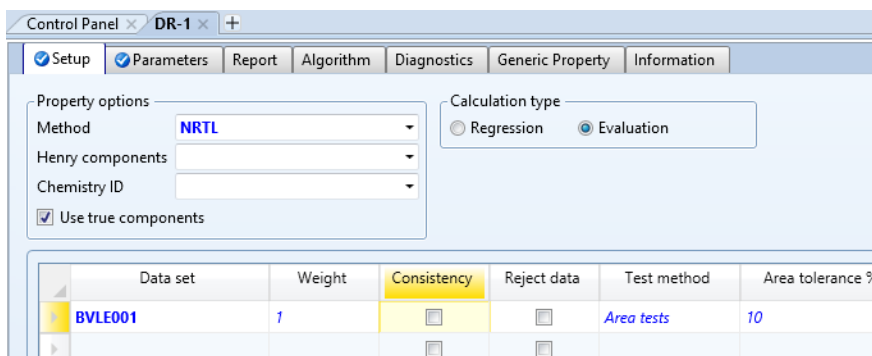


**Figure 1.41** Creation of regression data set called “DR-1”, which will be used under “Regression” mode.

Click on “OK” button, and the result is as shown in Figures 1.42 and 1.43. Here, we have the choice to either carry out regression or parameter evaluation using the given model. We will try both to see how they affect the performance of the property model being examined.



**Figure 1.42** The regression data set “DR-1” is ready to be examined using either regression or evaluation step.



**Figure 1.43** The data set “BVLE001” contains the 11 data points for VLE of MEK–1-hexene binary mixture.