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The Development of Chemical Process Simulation Software According to CAPE-OPEN

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Chemical process simulation software has a very important impact on chemical engineering manufacture design and manipulation, which can be used on process optimization and energy saving. Different software suppliers have defined different interface standards, which makes the integration of different chemical simulation software difficult. CAPE-OPEN standards were designed to solve this problem, so that various chemical simulation software can be worked together, saving time and money. According to CAPE-OPEN standards, the author has developed one chemical simulation software which has multiple functions, especially so that it can be integrated with other software. The software's accuracy and stability were tested according to practical industrial processes, and the calculation results are reliable.

1. Introduction

The Process System Engineering is one branch of Chemical Engineering, it focuses on the design, operation, control, optimization of general chemical reactions and separations, petroleum refining, agricultural production, pharmaceutical production and other aspects. And one of the most important tools for Process System Engineering is the chemical process simulation software (CPSS), especially for the design and optimization of chemicals and petroleum separation and operation. The design and optimization of chemical process needs large amounts of calculation, and at the time before digital computers, the calculation was huge and hard to be finished, and the errors will happen easily after few days. Errors in the middle of a process calculation will lead to bad results which are far from the correct one. After the bad result, the restart of calculation will be a disaster for participants. With the development of computer technology, and the energy shortage in 1970s, many chemical engineers and professors start to develop tiny programs for chemical operation calculation. Massachusetts Institute of Technology (MIT) is the first normalized organization to develop one comprehensive CPSS, with the help from US Department of Energy and many geniuses from MIT, Aspen is created and used by global researchers. After Aspen created, many other companies also make some famous products like Hysys, ProII and PetroSim and so on. Every software company has its special advantages and skills on thermodynamics and unit block calculation, but different software can't work together because their interfaces are not compatible; and all process simulation software have to achieve some same modules, the re-creation is a waste of time. With the need of software engagement and module reusing, CAPE-OPEN standards are designed and widely used by many software companies. CAPE-OPEN standards can be divided into Unit Operation, Thermodynamics Module, Petroleum Fraction and several other sub branches. The author has great passion on CPSS development and many years' experience on process simulation and CAPE-OPEN, then a CPSS according to CAPE-OPEN standards is developed.

2. The structure of process simulation software

One CPSS has several separated common modules, which makes the possibility of interface standards. Figure 1 shows the structure of one CPSS.

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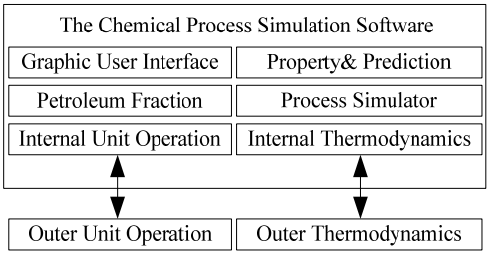

Figure 1: The structure of CPSS

2.1 The Graphic User Interface

The Graphic User Interface (GUI) is responsible for the flowsheet designing and operation units connecting, parameters' input and output, calculation control and so on. It's the direct interaction between CPSS and the user, the convenience and functions of GUI is the most important factor of CPSS.

CPSS has large amounts of parameters to be input and output, and many operation options need to be configured, which makes the software can't be very simple, every CPSS has to design rational GUI functions to deal with huge data input and output. With many years development, three popular GUI styles are formed:

(1) Aspen Plus style. Aspen Plus' GUI has one process view and several parameter views, users could build the flowsheet similar with drawing a process flow diagram, and all the data input and output windows are merged into one view. This style is very comfortable and user-friendly, and with abundant compound property databases and block modules, Aspen Plus has been the widest used CPSS in the world.

(2) Hysys style. Hysys is the original one of this style software, but Hysys company underwent some acquisition and antimonopoly problems, some technicians resigned from Hysys company then took the software design philosophy and techniques into new companies, so the following UniSim, PetroSim and VMGSim have the similar styles. Hysys style also has one process view, but can't build the flowsheet very smoothly; and the input and output views are separated into different windows, and most input and output controls are merged into one grid table, which makes the GUI not user-friendly.

(3) ProII style. ProII style represents the last century GUI style, which has standard menu bar and tool bars, simple flowsheet window, and separated parameter windows. The China's ECSS software also has similar style with ProII. This style is run-fast but outdated, so ProII and ECSS have been declined.

2.2 The Property and Prediction

One CPSS must has abundant compound properties and complete property prediction methods. The compound properties are composed of constant properties and temperature-dependent properties, they are saved into professional database management software, for example SQL Server and Access. When the user selects some compounds into the flowsheet, the properties will be loaded again from the database into the background of CPSS.

Most compound properties are achieved from lab test, but some special data are difficult and impossible to be achieved, for example some compounds will decompose when have reached the critical temperature, so the prediction methods are essential. The prediction methods can be divided into two types: the methods based on other properties, and the methods based on group contribution.

2.3 The Petroleum Fraction

Many cases have to deal with crude oil, but the crude oil is a complicated mixture, can't be described by specific compounds. The most traditional method is dividing the petroleum into pseudo compounds by distillation curve, and merging the pseudo compounds into distillation curve again after process calculation ended. This method has to deal with distillation curve interpolation, transition, cut-rules, pseudo compound property prediction, and pseudo compounds merge rules. This method is reliable and fast, has been used by most software. But the traditional method may be not accurate in some cases, so some professors have developed the molecular simulation method to make the results more accurate. But this method is very complex and time wasting, now few software use this method.

2.4 The Process Simulator

Simulator is the manager of the CPSS, it has to communicate with every modules, and must has the ability to resolve one complicated process. The simulator has the most comprehensive interfaces with Unit Operation, Thermodynamics, Petroleum Fraction, Property and Prediction, and must follows CAPE-OPEN standards. The simulator has to design one delicate multi-thread algorithm to solve the process, fast and reliable algorithm to tear recycle streams and generate initial values for torn streams.

2.5 The Unit Operation

Unit Operation represents the real block in process, it's more independent than other modules. It gets temperature, pressure, flow, compound list, composition from the inlet streams, and calculates the values by specific models, then sends the results to outlet streams.
Because of Unit Operation's independence, every Unit Operation can be packed into one isolated DLL file, and the CAPE-OPEN format Unit Operation can be used in some CAPE-OPEN-supported simulation software, for example Aspen Plus, Hysys and ProII.

2.6 The Thermodynamics

With specific compound properties and thermodynamic methods, the Thermodynamics modules can be used to calculate mixture equilibrium, enthalpy, heat duty, surface tension, density and other properties. It also has CAPE-OPEN standards, and CAPE-OPEN-supported Thermodynamics modules can be used by self simulator and third-party software.

3. The CAPE-OPEN standards

The CAPE-OPEN standards have three versions in history, and V1.1 is the latest and suggested one. Based on the structure of CPSS, the CAPE-OPEN standards are divided into several subclasses, including Unit Operation, Thermodynamics, Petroleum Fraction, Database, Simulator and so on, but the first two are most acceptable in public.

3.1 The Unit Operation CAPE-OPEN standards

Figure 2 shows the Unit Operation CAPE-OPEN interfaces. Unit Operation has to be managed by Simulator, and it also has to get mixture properties from Thermodynamics.

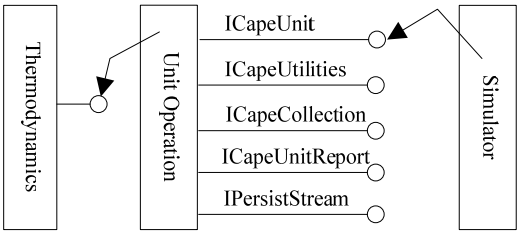

Figure 2: The interfaces of Unit Operation

(1) ICapeUnit. The Unit Operation has to expose itself to the Simulator, so ICapeUnit has three important functions including displaying stream ports, checking validation status, and running calculation.
(2) ICapeUtilities. The Unit Operation has to be edited, so ICapeUtilities allows user to set or get parameters, start or terminate this Unit Operation.
(3) IPersistStream. This interface is a public one in programming, can be used for data saving and loading.

3.2 The Thermodynamics CAPE-OPEN standards

Figure 3 shows the Thermodynamics CAPE-OPEN interfaces. Some interface's names are too long, here some names are abbreviated. Thermodynamics is used by the Unit Operation to calculate multi-phase flash and mixture properties, the accuracy of Unit Operation depends on the data and models of Thermodynamics.

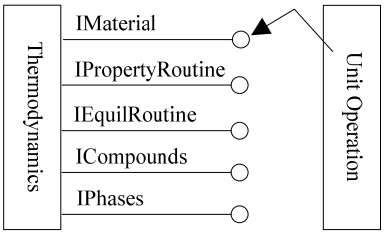

Figure 3: The interfaces of Thermodynamics

CAPE-OPEN wants to make seamless interoperability between different software, it defines one middleware named Material Object, and all the data are saved into or got from Material Object. The interfaces of Thermodynamics are used to get, set and calculate specific thermodynamic properties.

4. The development of process simulation software

CPSS is one complicated and comprehensive scientific software, it's not only depended on information technology, also depended on abundant chemical data and models. Different parts of CPSS have to comply with specific CAPE-OPEN standards, and have special development rules.

4.1 The development tools and environment

The development of CPSS needs amounts of time and money, bad initial plan will result in rebuilding and wasting of time. The developers need to take target operation system and programming language into conclusion.

Microsoft Windows, Apple Mac/iOS, Linux, Android are four popular operation systems currently, and Windows is used most widely in personal computers. CPSS is used mostly by engineers and students, and they prefer to use Windows OS computers; the mobile devices with iOS or Android are also used widely, but the screen of them is too small for operation and the internal storage of them is too low for calculation. Most CPSS just take Windows into conclusion. For other OS environments, the software supplier could design one CPSS running on the web server, and users could operate this CPSS via web browsers.

The programming tools and language are also another key point, from Aspen Plus' appearance in 1980 to now days, coding languages and tools have earth-shaking changed. Fortran is the first language in scientific area in last century, then the C++, and now days JAVA and C# are becoming more popular. A robust and everlasting language is very essential for the development. By the experience of software development, C++ and JAVA and C# are the best candidates for CPSS development.

4.2 The development team's arrangement

The development process of CPSS needs many engineers and many years, also has to cope investment and business matters, the team's arrangement is more important than individual's ability. Figure 4 shows the best team structure.

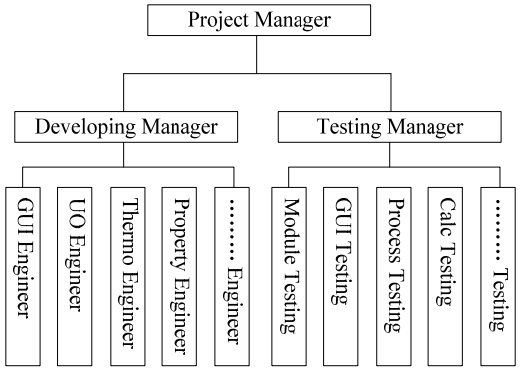

Figure 4: The arrangement of development team

The team has three layers, the Project Manager has to deal with investment, market, human resource and other troubles; and the Developing Manager must has the software architecture ability, deep mastery of computer technology and chemical knowledge, and the leading talent to keep the harmony of the development team; and the Testing Manager must has many years practical process simulation and factory experience, could find the problem quickly and decide the best property route and method for the process, and also needs a leading talent to make testing team unity.

4.3 The development of GUI

The GUI is the direct interaction between CPSS and users, the convenience and appearance of GUI will affect CPSS' popularity deeply. In history Borland C++ and Visual Basic 6.0 are the first language for GUI designing, then Visual C++ MFC becomes the tendency, and now days C# and JAVA become the main selection.

C# runs on Net platform, and JAVA runs on JAVA platform, because they are all intermediate languages, they can perform very well on different OS platforms; unlike the MFC control-button style GUI, C# could use XML style language to design the GUI; they all don't need to care pointer release and memory leak problems. The advantages of them make C# and JAVA become the best languages to develop GUI.

4.4 The development of background calculation modules

C# and JAVA have many advantages over C++ and other languages, but they also have shortages on some tasks. C# and JAVA are intermediate languages, the built software will be giant and easy to be decoded, not

suitable for huge calculation and secrecy-needed modules; and the built software of C++ is assembly language, runs fast and safely.
So C++ is the best language for background calculation modules. The thermodynamic modules are developed as dynamic link libraries (DLL files), all Unit Operations and other modules could call them and run fast and reliable. The DLL file is very safe and difficult to be decoded by hackers.

5. The test of cases

The CPSS developed by the author is temporary named PSim. Because PSim is according to CAPE-OPEN standards, so all the Unit Operations and Thermodynamics in PSim could run in other CAPE-OPEN-supported software; PSim is a CAPE-OPEN-supported software, so it also could load Unit Operations and Thermodynamics from third parties; PSim is a comprehensive and well-equipped CPSS, it can be used to simulate chemical process.

5.1 The test of single CAPE-OPEN modules

In the Aspen Plus GUI, by selecting “CAPE-OPEN” from menu “Libray/References”, the Unit Operations from PSim will appear in Aspen Plus “Model Library” window, users could insert them into the process, and the Unit Operations from PSim could run well as original ones from Aspen Plus, Figure 5 shows this case. In the Aspen Plus GUI, by selecting “Import CAPE-OPEN Package” from menu “Tools”, Aspen Plus could use the Thermodynamics from PSim for process simulation.

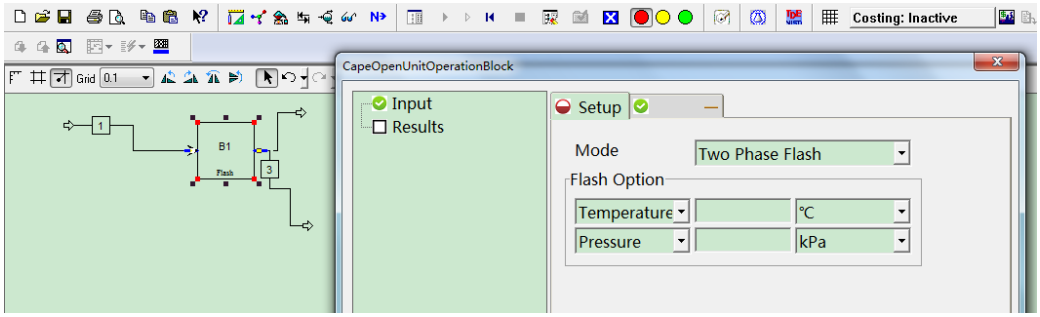

Figure 5: The Unit Operation from PSim runs in Aspen Plus

PSim has similar functions with Aspen Plus, it also could link Unit Operations and Thermodynamics from other software. Another CAPE-OPEN-supported software named COCOSimulator supplies some Unit Operations, PSim could load them and run the process, Figure 6 shows this case.

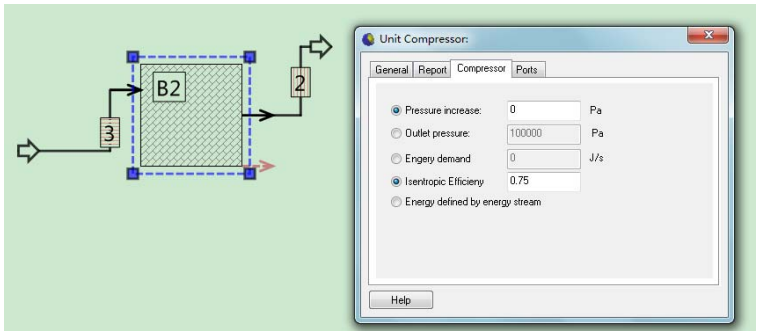

Figure 6: The Unit Operation from COCOSimulator runs in PSim

5.2 The test of process simulation ability

To check the reliability and accuracy of PSim, Figure 7 is one gas separation process, the author built the process in PSim, and Table 1 shows the results. The temperature, pressure, flow and purity data of all the product streams are too many, not listed here, they are all satisfied with Aspen Plus and reality. The results indicate that software is very reliable.

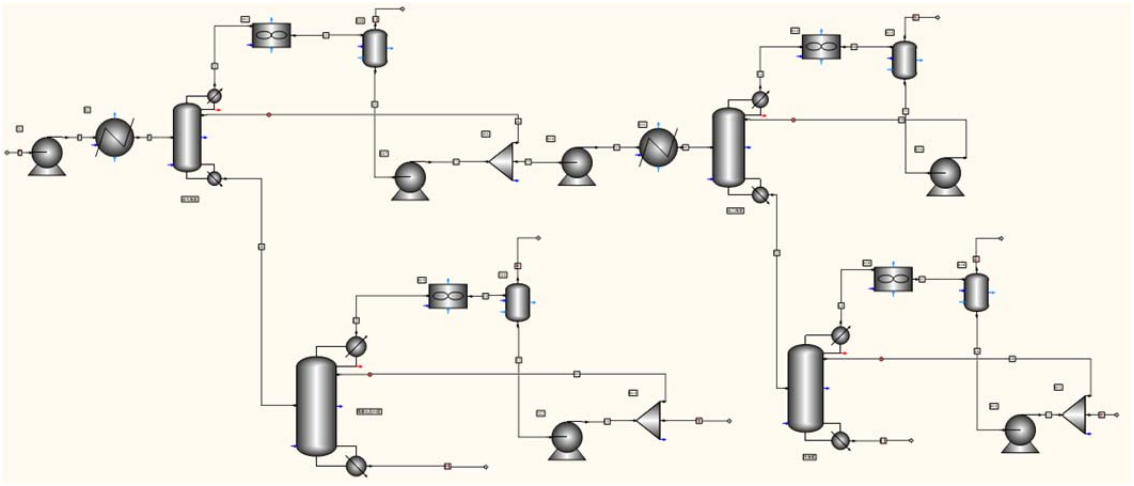

Figure 7: The gas separation process in PSim

Table 1: The simulation composition (mole basis) results of the product stream

Compound	Aspen Plus result	PSim result	Absolute error	Relative error/%
Dimethylmethane	22.68	22.61	-0.07	0.32
Propylene	74.58	74.58	0.00	0.00
Iso-butane	2.26	2.32	0.06	2.71
N-butane	0.01	0.01	0.00	1.52
Butene	0.20	0.20	0.00	0.35
Isobutene	0.25	0.27	0.01	4.59

6. Conclusion

Chemical process simulation software is very important in process design, verification, and optimization, and CAPE-OPEN standards allow multiple software work together. The author has developed one chemical process simulation software, which has petroleum fraction, property and prediction, unit operations, and thermodynamics modules. The unit operations and thermodynamics in this software could be loaded by other software, and software also could load unit operation and thermodynamics from other software. This software is demonstrated on a practical chemical process simulation.

Acknowledgments

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