Chemical and Process Engineering Research
ISSN 2224-7467 (Paper) ISSN 2225-0913 (Online)
Vol.26, 2014

Developing Aspen-Plus Procedure on Flash Separation of Methanol-Water Mixture

* Awajiogak A. Ujile[a] and Itong A Ujile[b]
[a]Department of Chemical/Petrochemical Engineering, Rivers State University of Science and Technology, P M B 5080, Port Harcourt, Nigeria. Email: ujile.awajiogak@ust.edu.ng;
Tel: +2348033398876; *Corresponding author.
[b]Department of Chemical Engineering, Texas A&M University, Kingsville, USA.
Email: itong.ujile@students.tamuk.edu; Tel: +1 (361)355-6187

Abstract
A step-by–step procedure on the separation of methanol-water mixture has been developed. Application of ASPEN PLUS Software was utilized. Aspen Plus interface with Thermodynamics Package selection and an activity coefficient model are incorporated. UNIQUAC is used. Results obtained have shown a simple method that can be easily used by all chemical engineers at all levels. The developed method can be used for separation of other mixtures in the separation process industries.
Keywords: UNIQUAC model, separation, simulation, computer package

Introduction:
Risk and uncertainty are facts of life in most business and public policy decisions. However, with the right tools one can better understand risks and identify ways to mitigate them. This is especially important when "experimenting" in the real world becomes too expensive, dangerous, or time consuming. In a short amount of time and for very little money one can run thousands of "what if" scenarios allowing us to make better decisions more quickly [Monte-Carlo Simulations, Woller, 1996]. An example is illustrating the use of Monte-Carlo Simulation to compute the value of the mathematical constant; Pi has been applied for **Computing Pi Model**. The sensitivity analysis and scenario analyses are quite useful to understand the uncertainty of the investment projects. But both approaches suffer from certain weakness. They do not consider the interactions between variables and also, they do not reflect on the profitability of the change in variables EzineArticles (2010). Simulation is one of the most widely used quantitative methods, because it is so flexible and can yield so many useful results. Here is just a sample of the applications where simulation is used, (Wharton University of Pennsylvania):

- Choosing drilling projects for oil and natural gas
- Evaluating environmental impacts of a new highway or industrial plant
- Setting stock levels to meet fluctuating demand at retail stores
- Forecasting sales and production requirements for a new drug
- Planning aircraft sorties and ship movements in the military
- Planning for retirement, given expenses and investment performance
- Deciding on reservations and overbooking policies for an airline
- Selecting projects with uncertain payoffs in capital budgeting

Chemical engineers use flow sheets/process flow diagrams to analyze unit operations. There are varieties of computer programs or packages which can be utilized. Examples of process simulation packages are: Aspen plus, Hysys, ProII, ChemCAD, Design II, to mention but a few Peters, et al (2004). The benefits of simulation package application are (Process Engineering Associates, LLC) available online:

- Accurate design information
- Software-produced mass and energy balances and process flow diagrams
- Multiple design cases at a fraction of the cost
- Process optimization, finding the process' maximum performance point
- Sensitivity analyses, determining the process' key control variables and degree of operating stability.

The availability of this powerful software is a great asset to the experienced process engineer, but such sophisticated tools can be potentially dangerous in the hands of neophyte engineer. The bottom line in doing any process simulation is that you the engineer are still responsible for analyzing the results from the computer, Turton et al (2009).

The work of Ujile and Amagbo (2013) on determination of plate efficiency of rectification column in refinery operations has shown that to gain high efficiency of separation in a distillation column requires increase in the number of trays within a given section by reducing the spacing between trays. However, optimization principle is required to obtain optimum results. They asserted this proposal to form the subject matter for further work on the plant, which might require the application of process engineering system tools.

Chemical engineers' knowledge of basic principles of one of these simulation programs is expedient to be able to carry out further work on optimization problems in industrial separation processes. However, these programs are similar; therefore basic knowledge of one of them would facilitate understanding the other programs.

This guide attempts to provide a step by step approach in modeling a flash separation of a methanol-water system using Aspen Plus such that would be easy to understand by chemical engineers at all levels, and other engineers or individuals that are involved in process design activities. The developed procedure enables the process engineer to analyze results from the computer.

Methodology

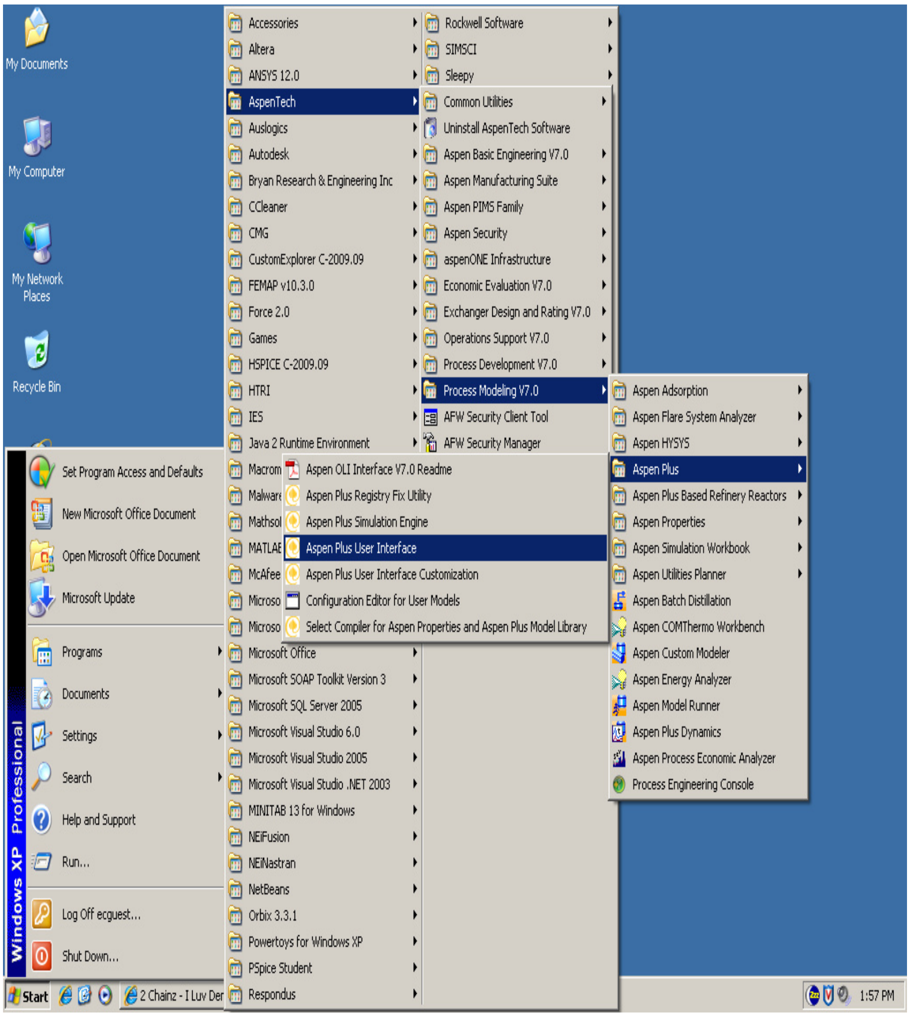
The method adopted in this work involves the process system of methanol – water mixture at different concentrations in a typical distillation (separation) unit.

Process Description

A mixture composed of methanol and water with mole fractions 0.1 and 0.9 is fed into a flash unit at 1000lbm/hr at 27 ^{o}C and atmospheric pressure. Suppose the flash unit operates at 1atm and vaporizes 30% of the mixture, determine the composition of the product streams using Aspen Plus.

START UP ASPEN PLUS: From the start menu, follow the sequence as shown in the illustration below, (Figure 1).

Fig 1: Sequence for Start-up



Select the radio button next to **Blank Simulation** and hit the **OK** button to display the GUI (Fig. 2).

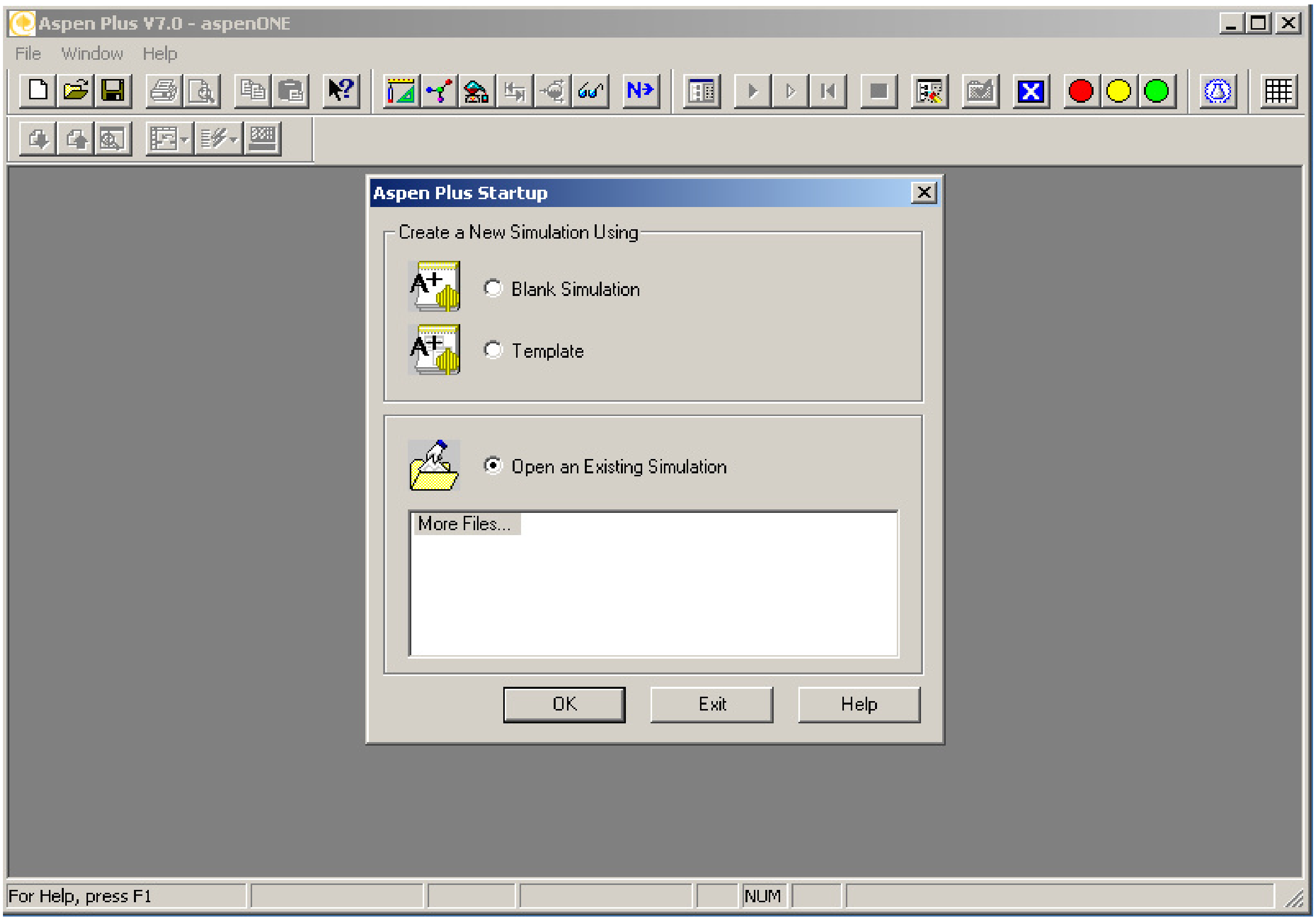


Fig.2: Selection process for Aspen-Plus

The GUI would be the environment where the process flow diagram is defined.

<u>Defining Process Flowsheet Connectivity:</u> This is the first thing to be done immediately the flow sheet is set up. The various unit operations and their connecting streams are placed on the workplace. For this tutorial, A 3-product flash separator unit is required. The unit and connecting streams can be selected as shown in Fig. 3 below.

The flash tank could be resized by regular windows operation.

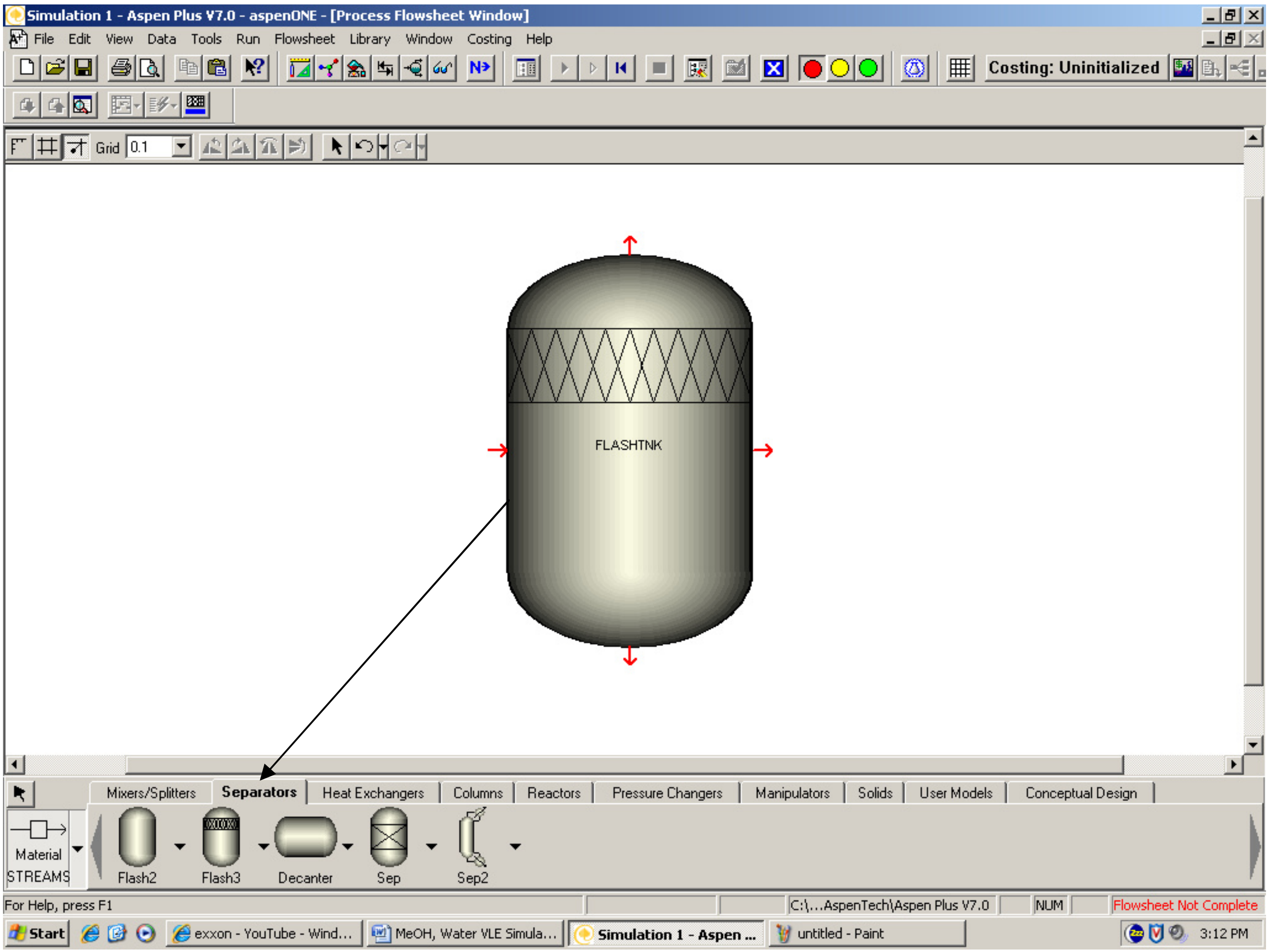


Fig. 3: Various unit operations and connecting streams

The red markers on the flash unit show where process streams can be connected.

The figure below shows the flash unit with all feed and product streams (Fig. 4). For ease of operations, the streams and flash unit can be renamed by right clicking and using the drop-down menu that appears.

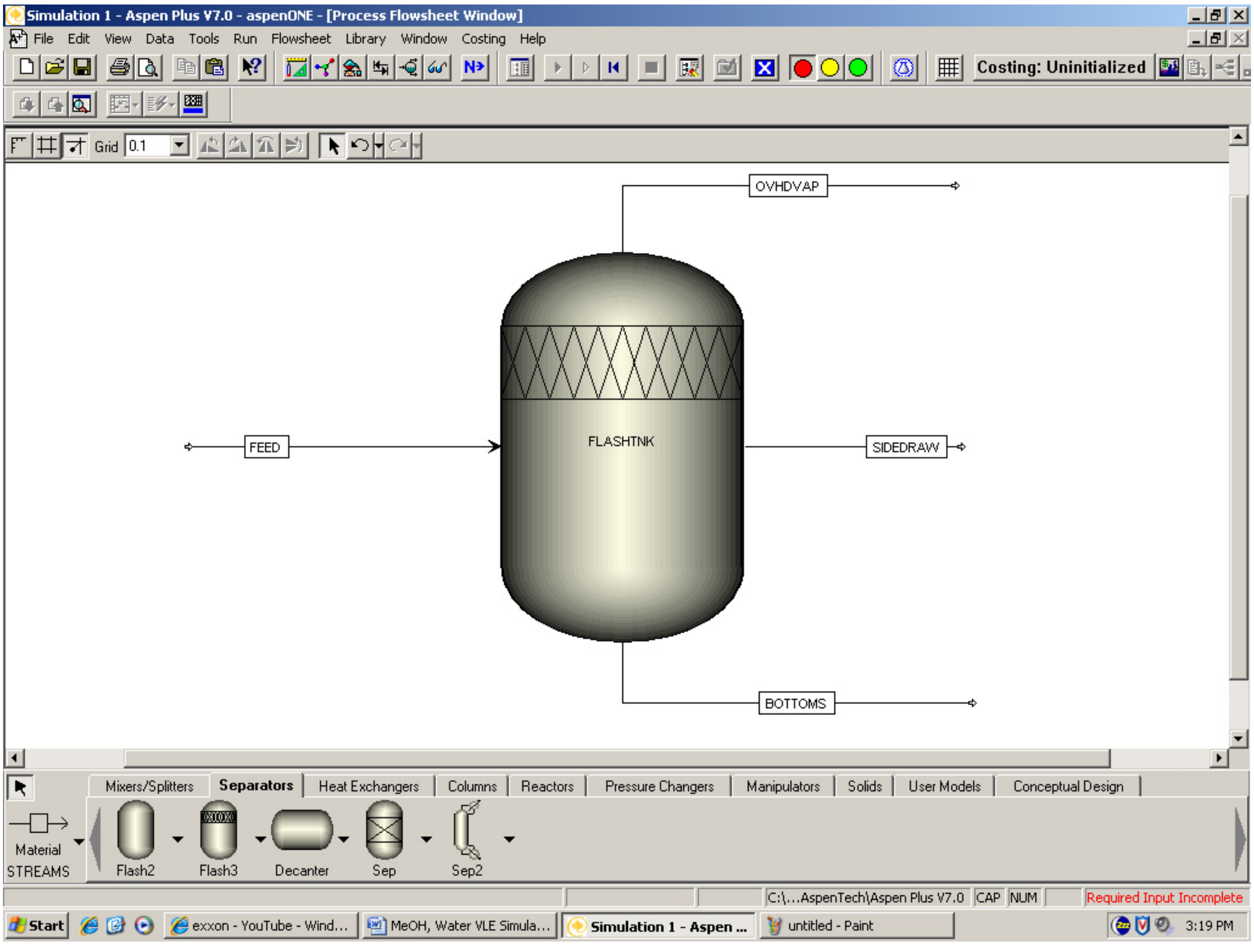
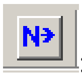


Fig. 4: Flash unit with feed and product streams

The NEXT button : The next button on the flow sheet provides an orderly procedure in preparing the flow sheet. However, it is not the only way. Aspen Plus provides a variety of approach to achieve a goal on the flow sheet.

The next button could provide a dialogue box showing the next operation required on the spreadsheet Fig. 5.

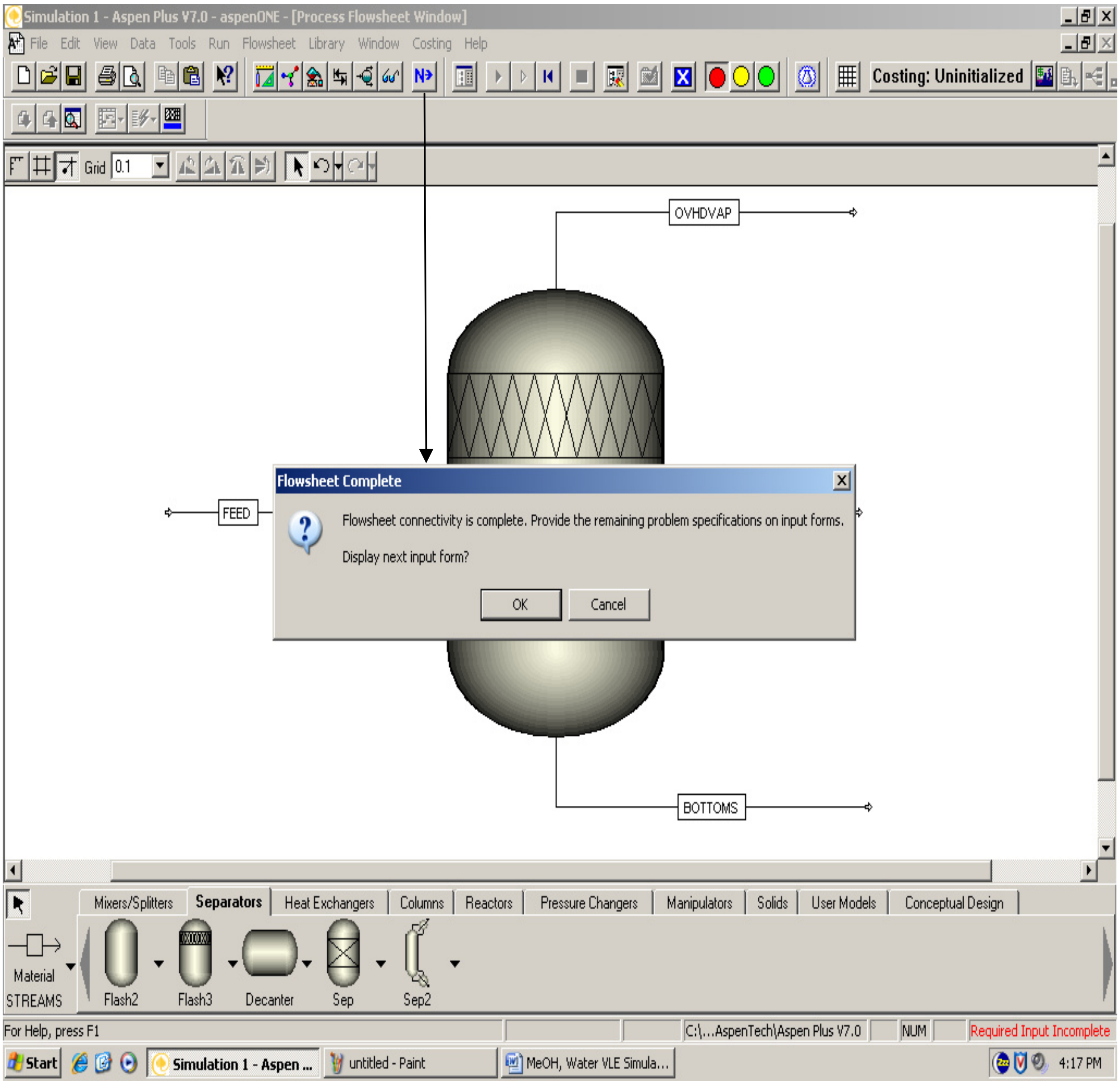


Fig. 5: Orderly procedure in preparing the flow sheet

In this case, since the process units and connecting streams have been installed on the flow sheet, the next button suggests providing problem specifications on input forms on the data browser. Clicking ok displays the SETUP SPECIFICATIONS in the DATA BROWSER

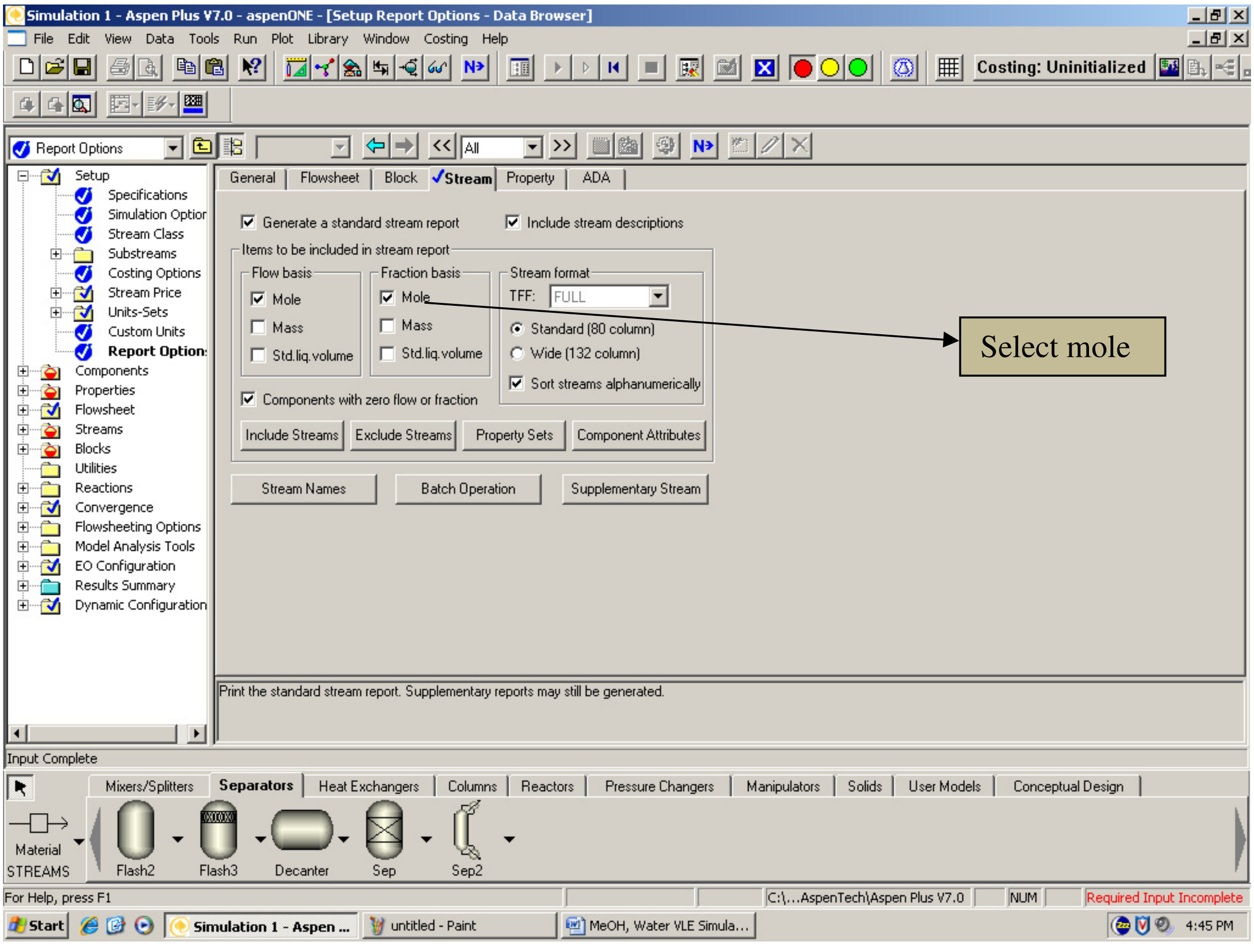


Fig. 6: Component selection display

Note that the red element shows that the required input is incomplete. The blue data shows that the required input is complete. However, the operator can modify the units, run type and other parameters to suit his or her own specifications. In this tutorial, we want our results to be displayed in mole fractions so under report options>Streams tab, select "MOLE" next to the fraction basis.

Clicking the Next button leads to the next required input which is COMPONENTS as in Fig. 6.

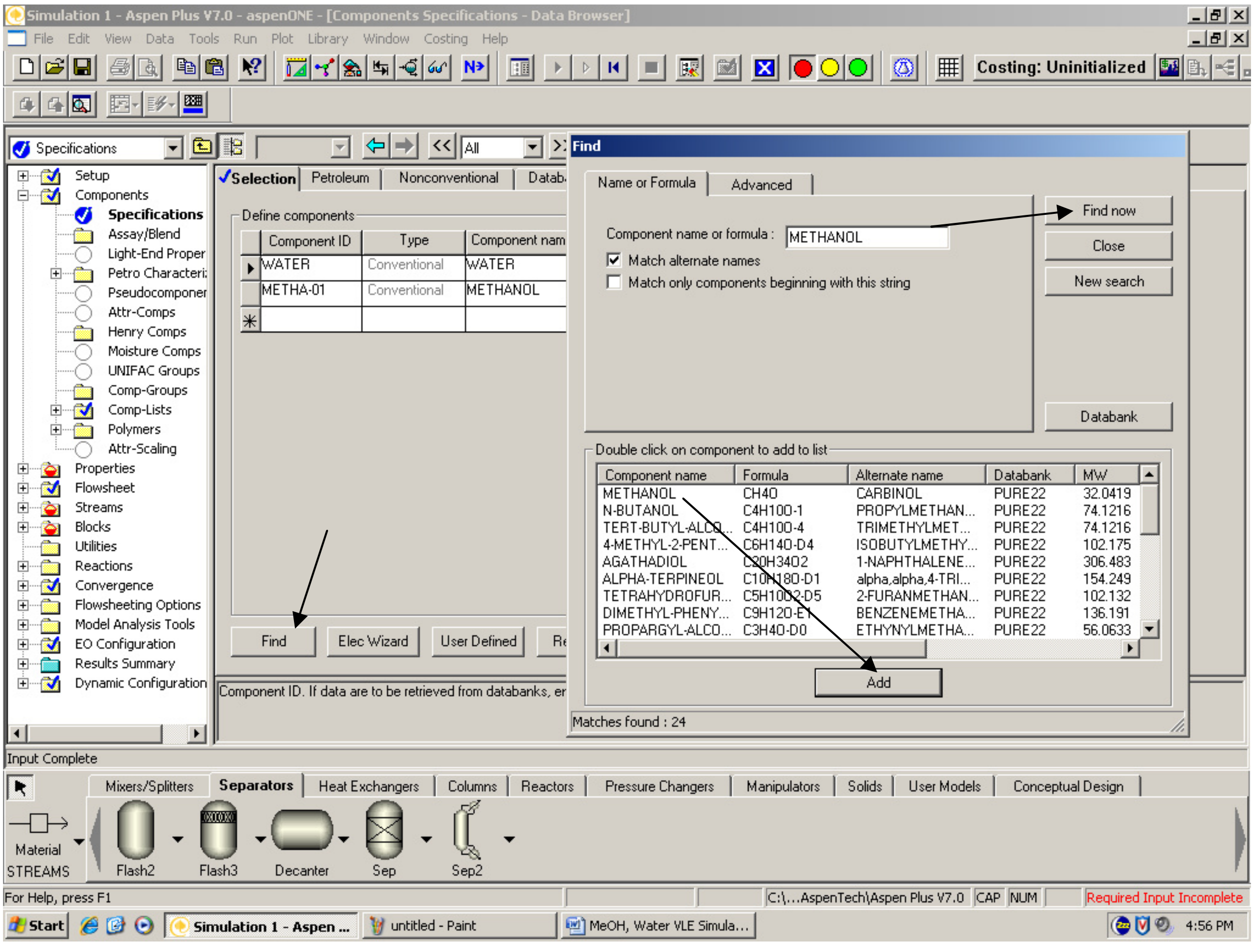


Fig. 7: Selection of component package

To add components, use the display on Fig. 7.

Click find, then type the compound name or formula and click find now. Select the name of the component and click add. (Follow arrow captions in the screenshot above).

The Next button suggests selection of Thermodynamic Package. For this example, an activity coefficient model is suitable. UNIQUAC is used and the display is shown in Fig. 8.

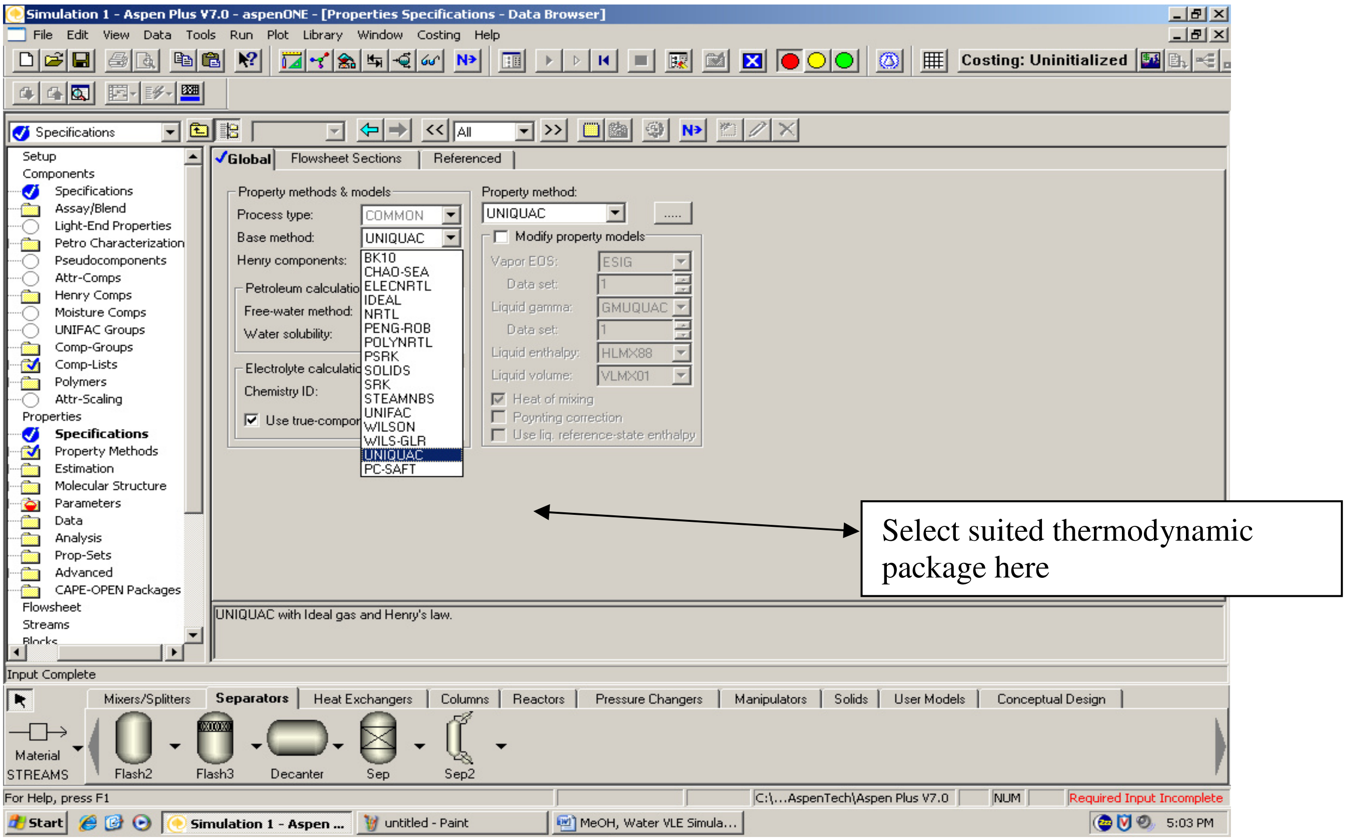


Fig. 8: Selection of thermodynamic package

Choosing the right thermodynamic package is very important and could be cumbersome.

Aspen- Plus provides a hint to choosing the right thermodynamic package as in Fig. 8.

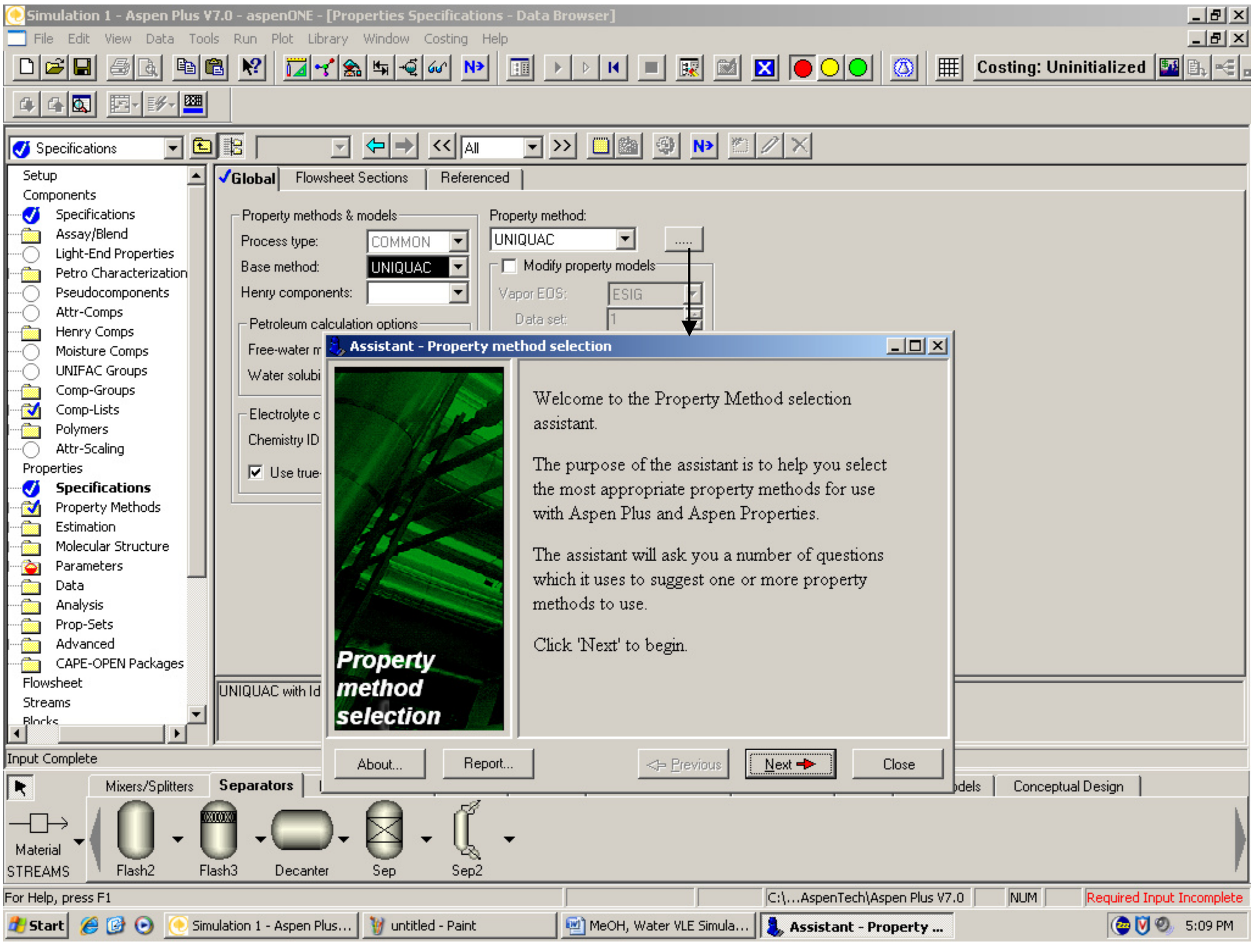


Fig. 9: Property method selection

The button  displays a wizard that aids in choosing the most suited thermodynamic package.

The next step requires a review of the binary interactions specifications for this process as shown in figure 9. The display in Fig. 10 shows the binary interaction specifications. The parameters in UNIQUAC can be obtained in Fig. 10, by searching method on the display button.

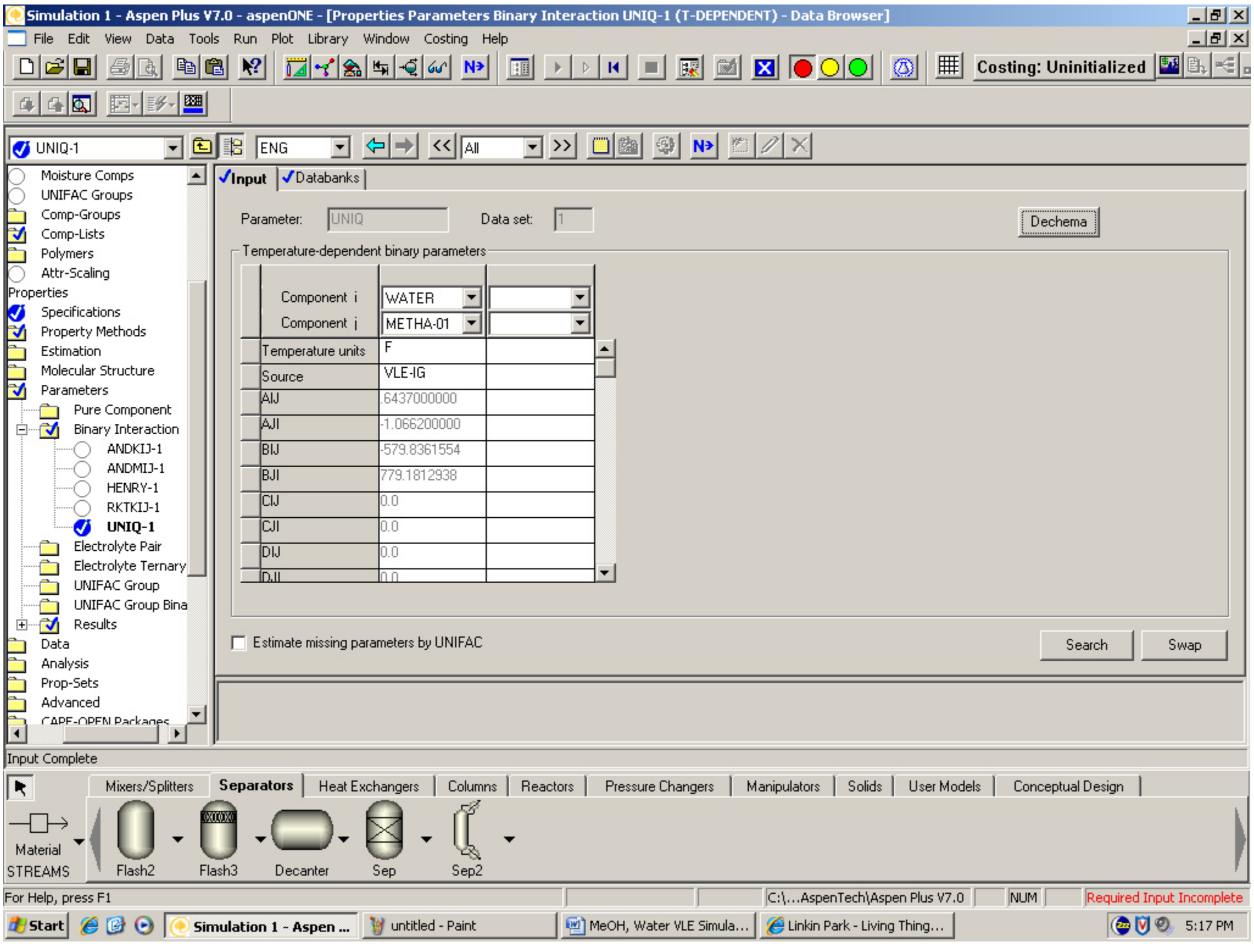


Fig. 10: Binary interactions

The next required Step is specifying the input parameters for the feed stream in Fig. 11.

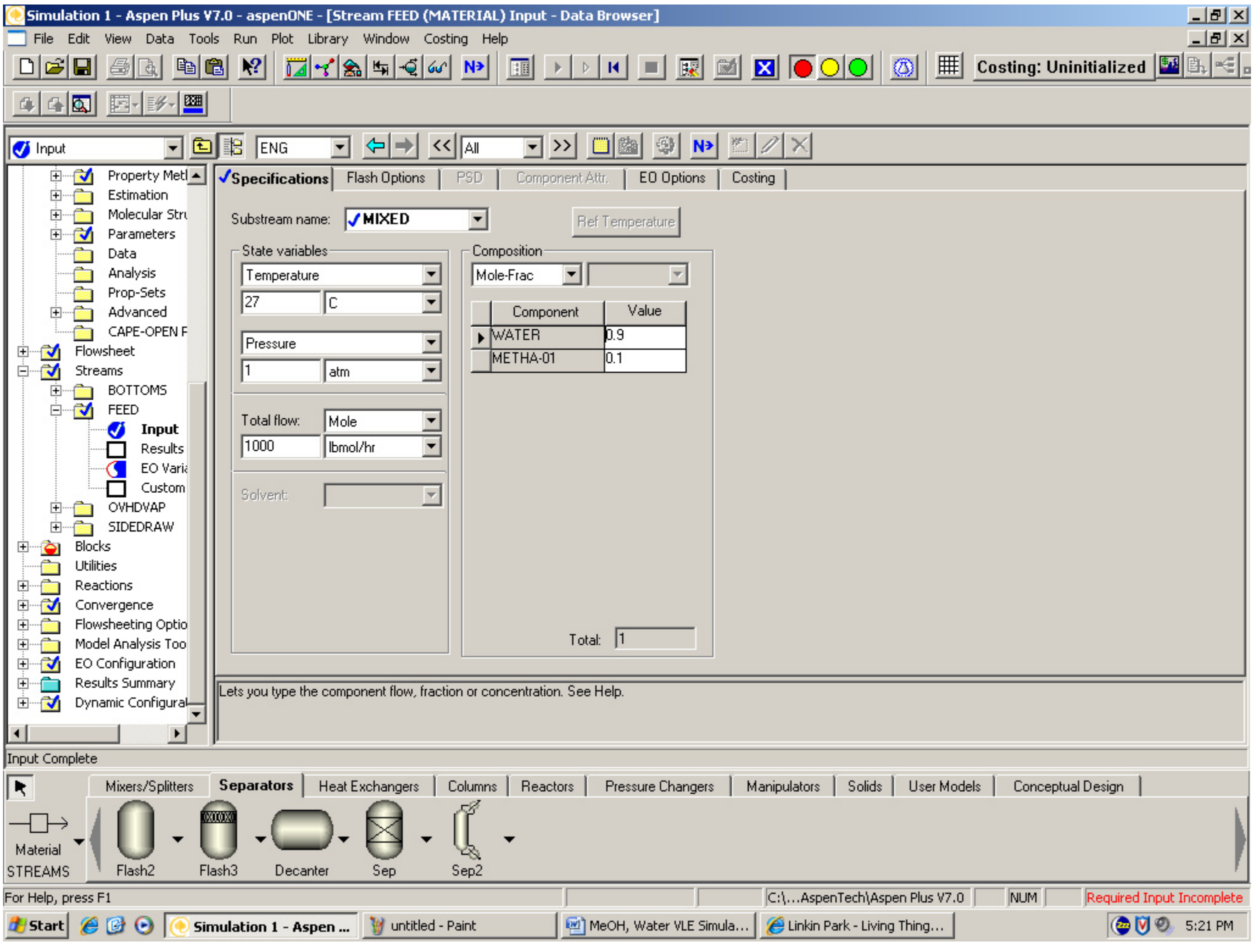


Fig. 11: Simulation for the feed stream

The Temperature, pressure, mass flow rate, composition can be specified in this section.

The Next line of action is to specify the operating conditions of the flash tank as in Fig. 12.

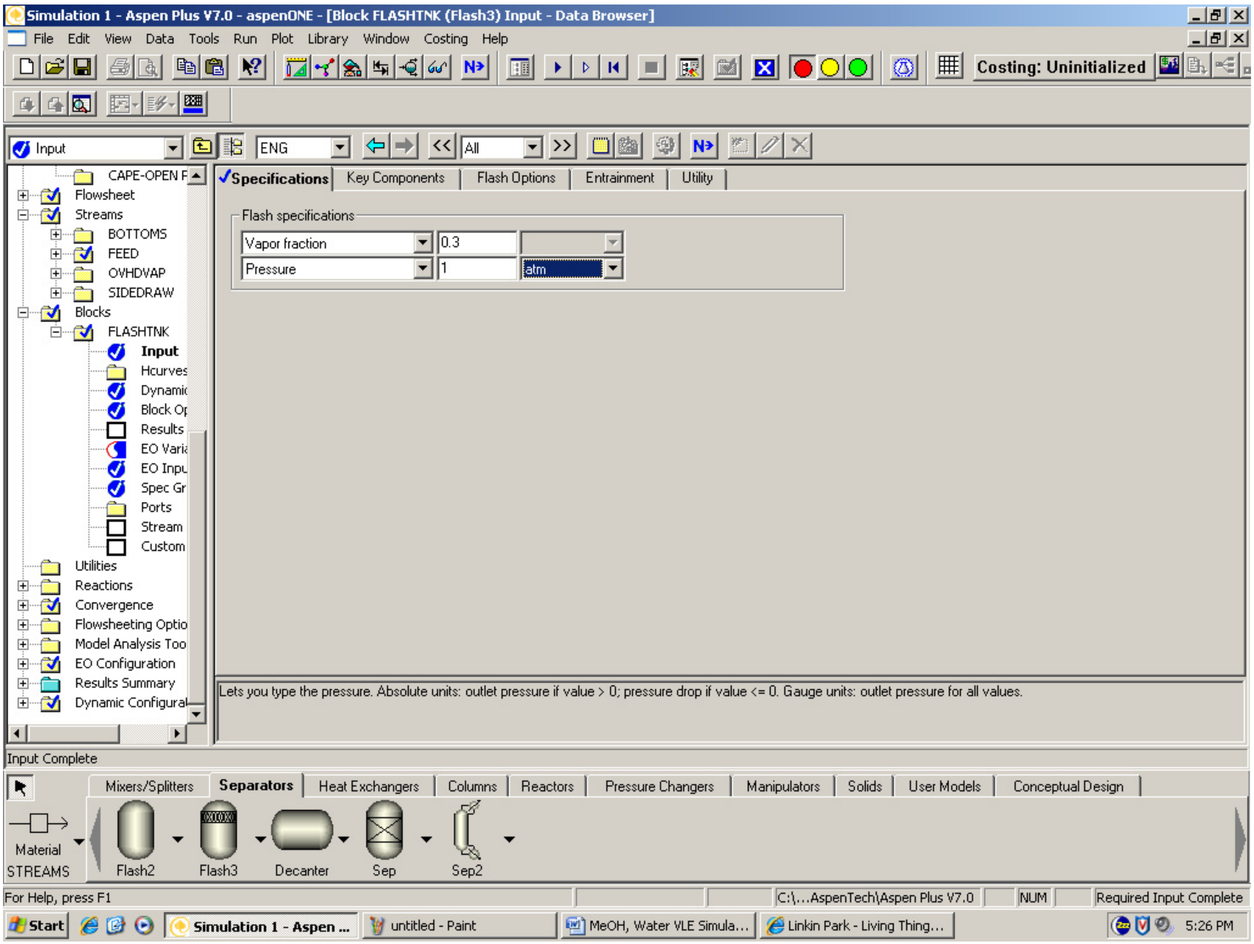


Fig. 12: Determining operating conditions for the flash tank

Note that all indicators are blue; hence all required input is specified. Either use the play or Next button to view results as in Fig. 13.

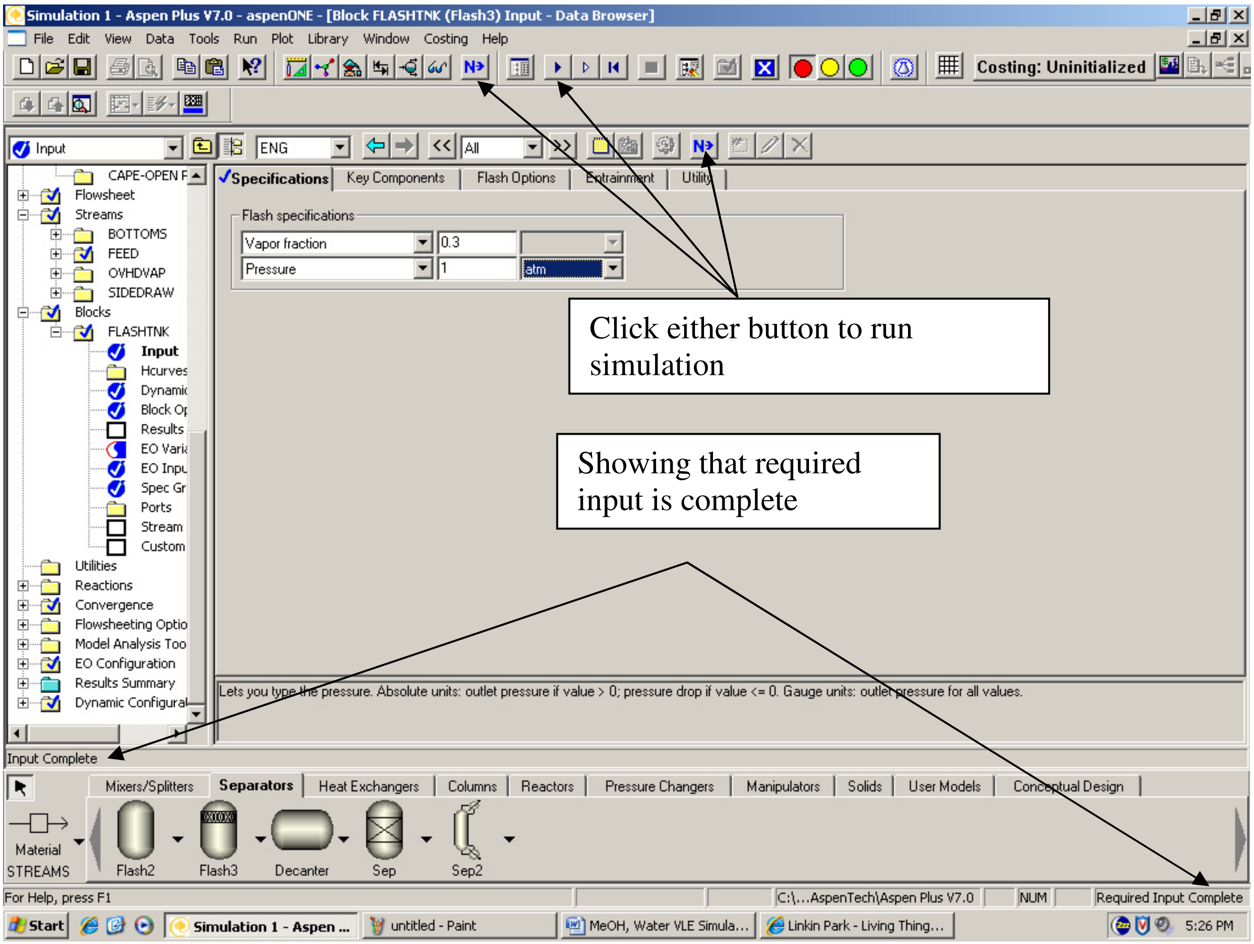


Fig.13: Viewing the results of the simulations

Clicking OK will display results as shown in figure 14.

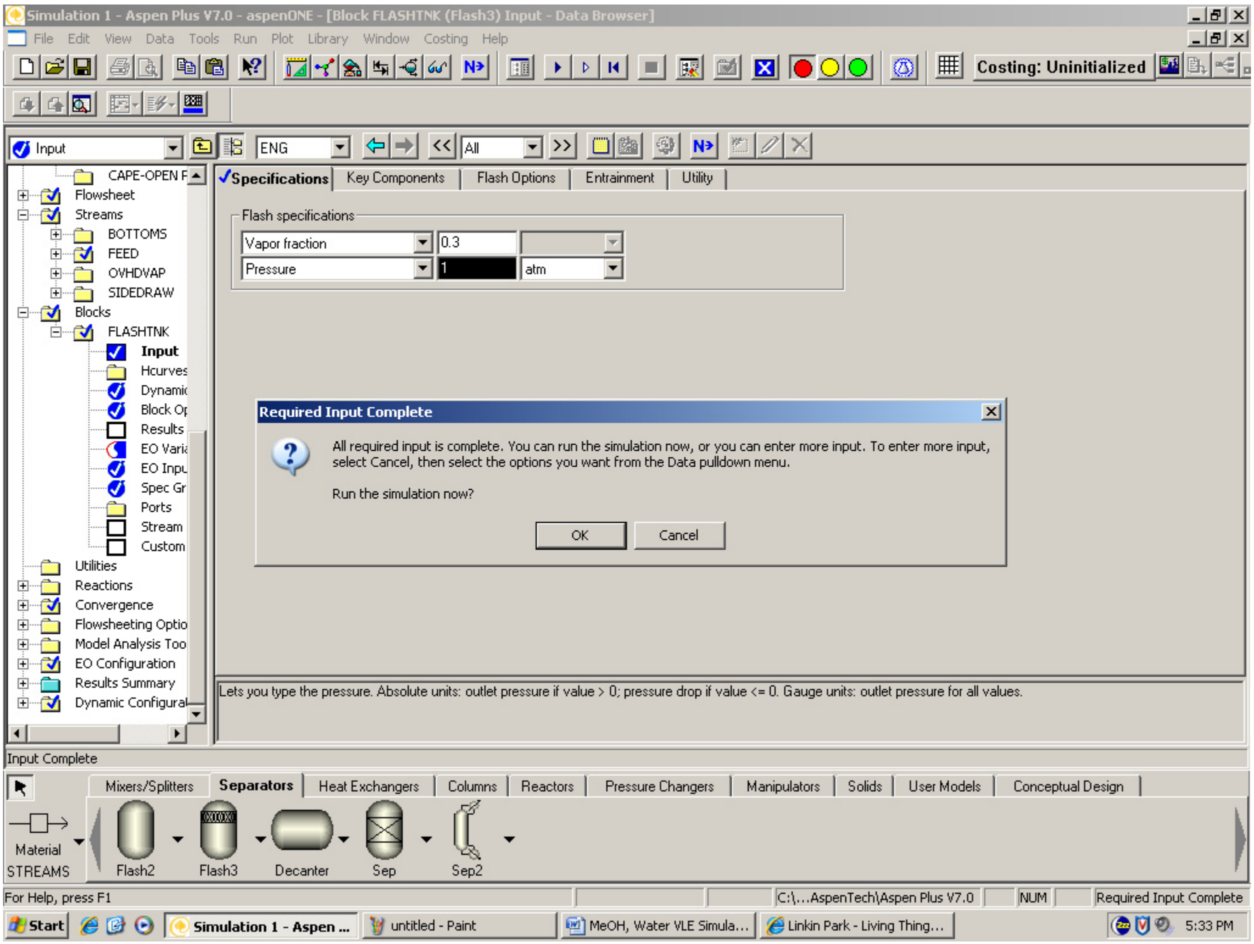


Fig. 14: Results display

The figure 15 shows the Run Control Panel.

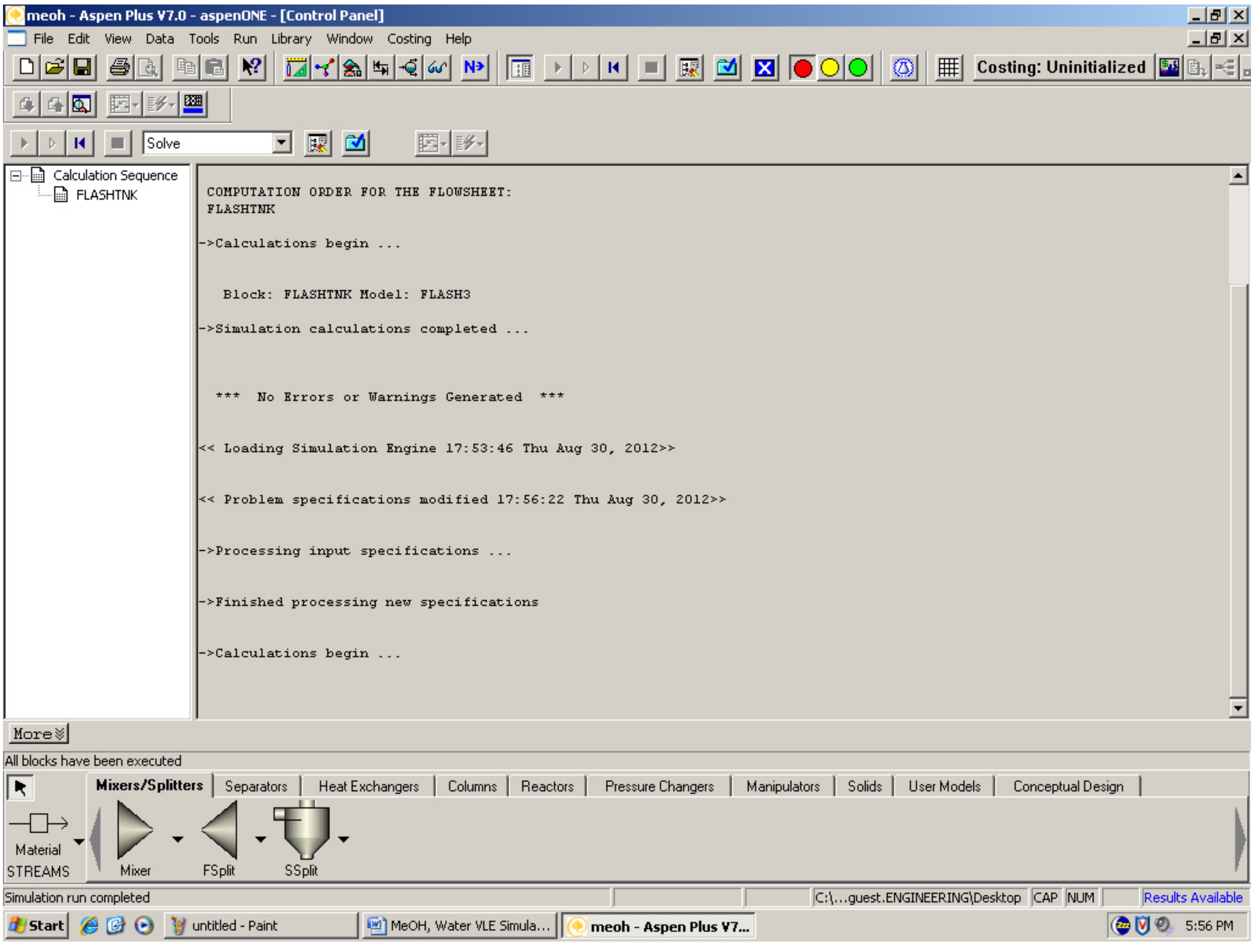


Fig. 15: Run control panel

The Stream Results can be viewed under the block menu as shown in figure 16.

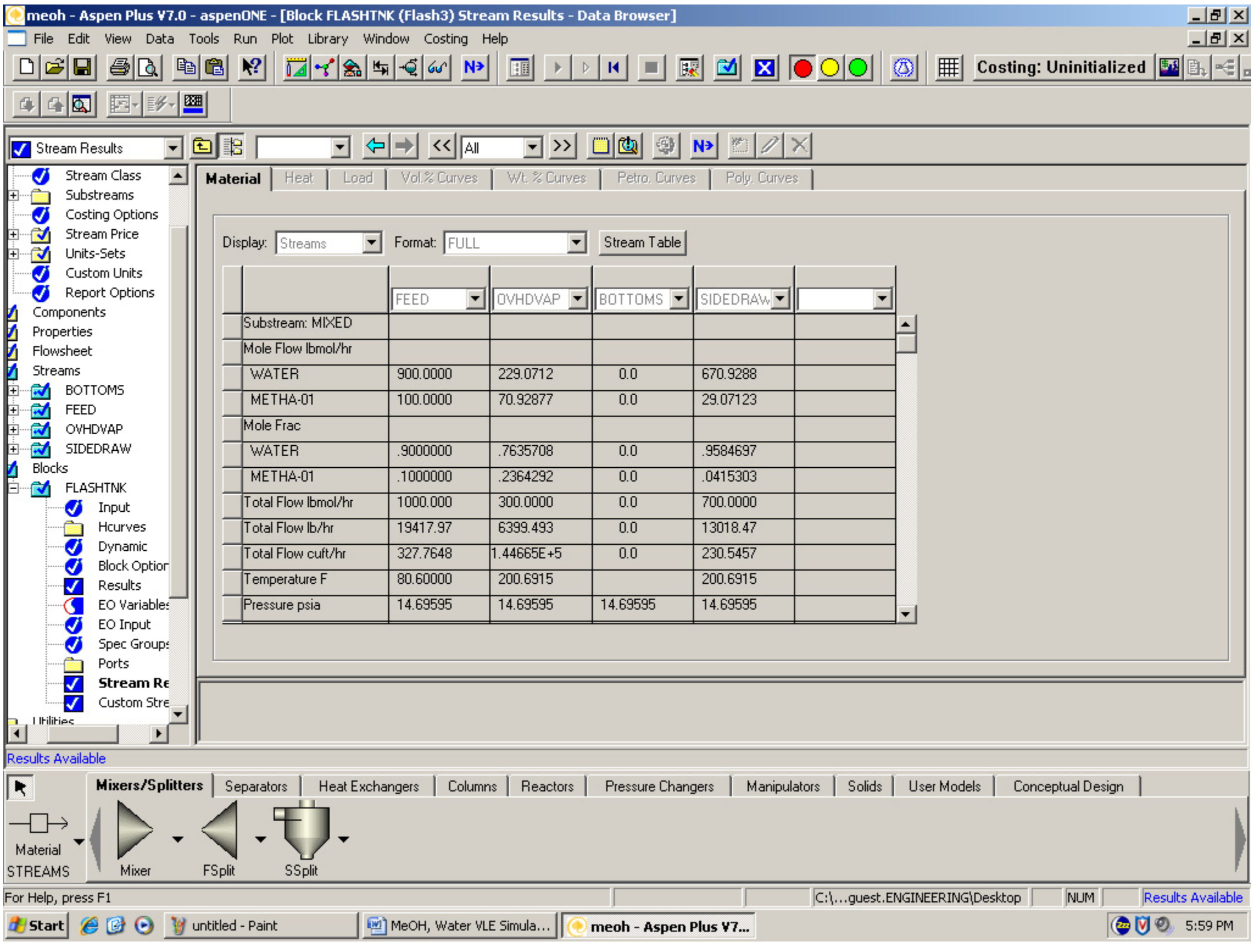
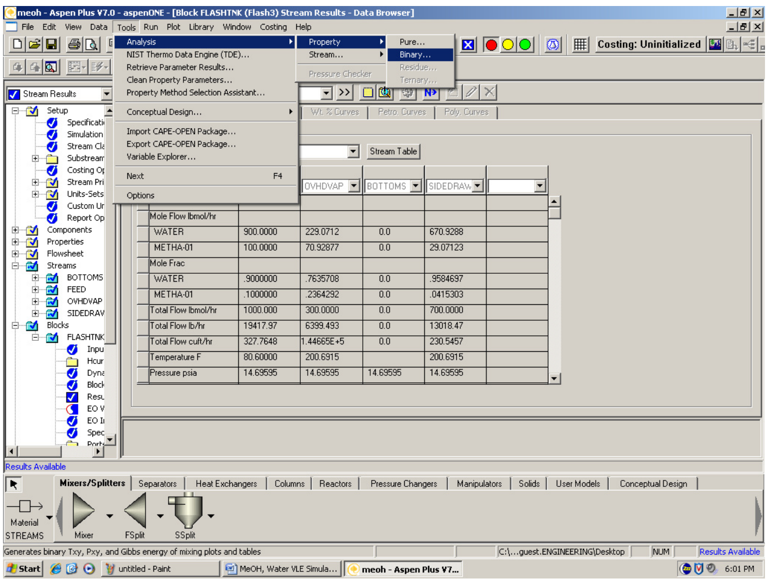


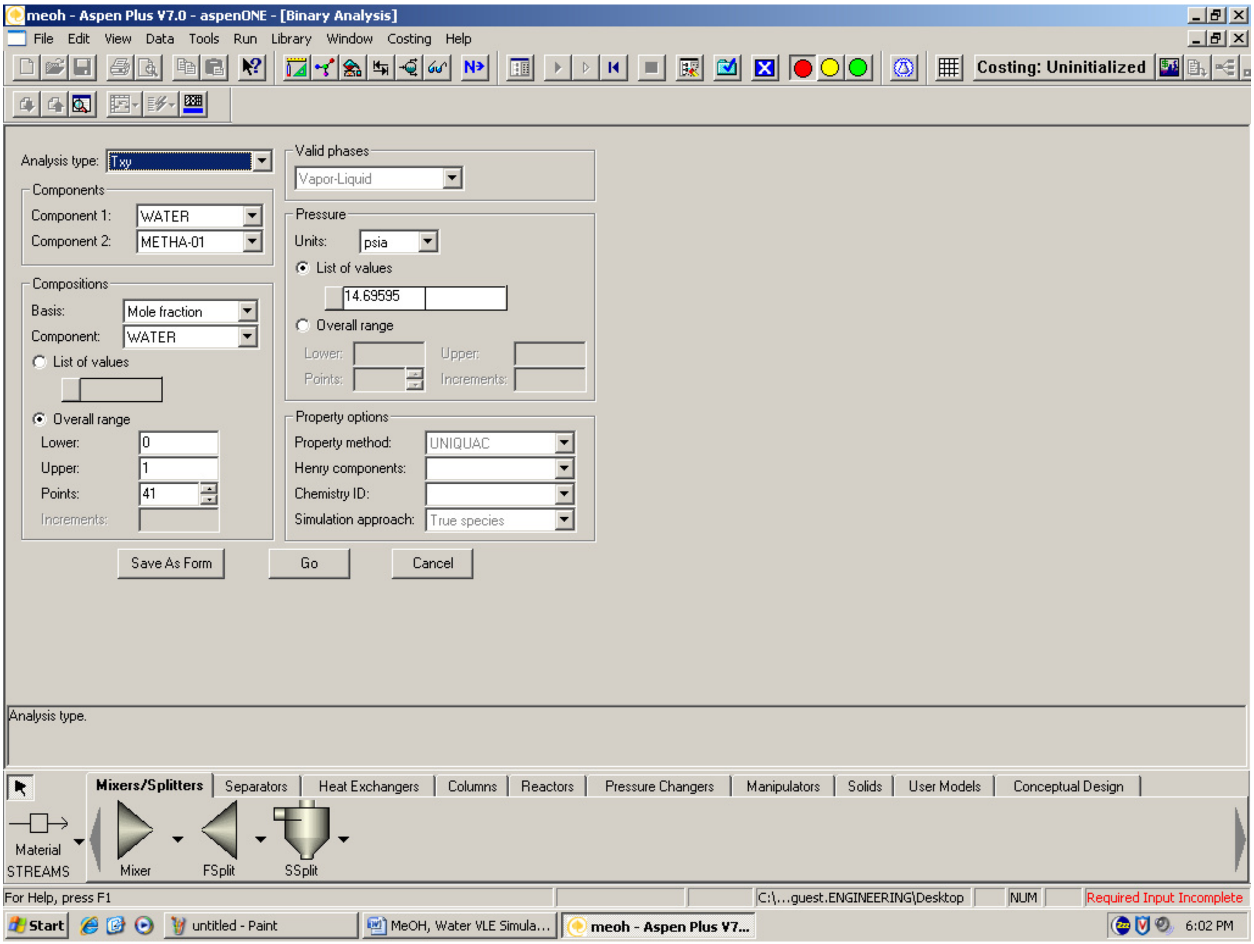
Fig. 16: Stream results

Also, VLE (vapor liquid equilibrium) Analysis can be carried out with this procedure.

Subsequent outputs show the analysis of the stream results



(a) Stream data



(b) Binary analysis

Fig. 17 (a) and (b): Binary analysis of methanol-water mixture

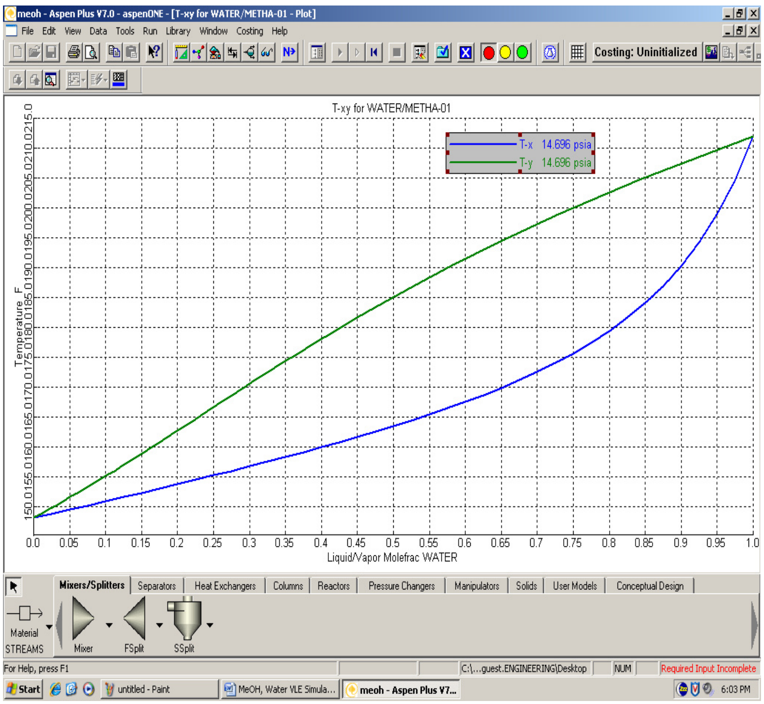
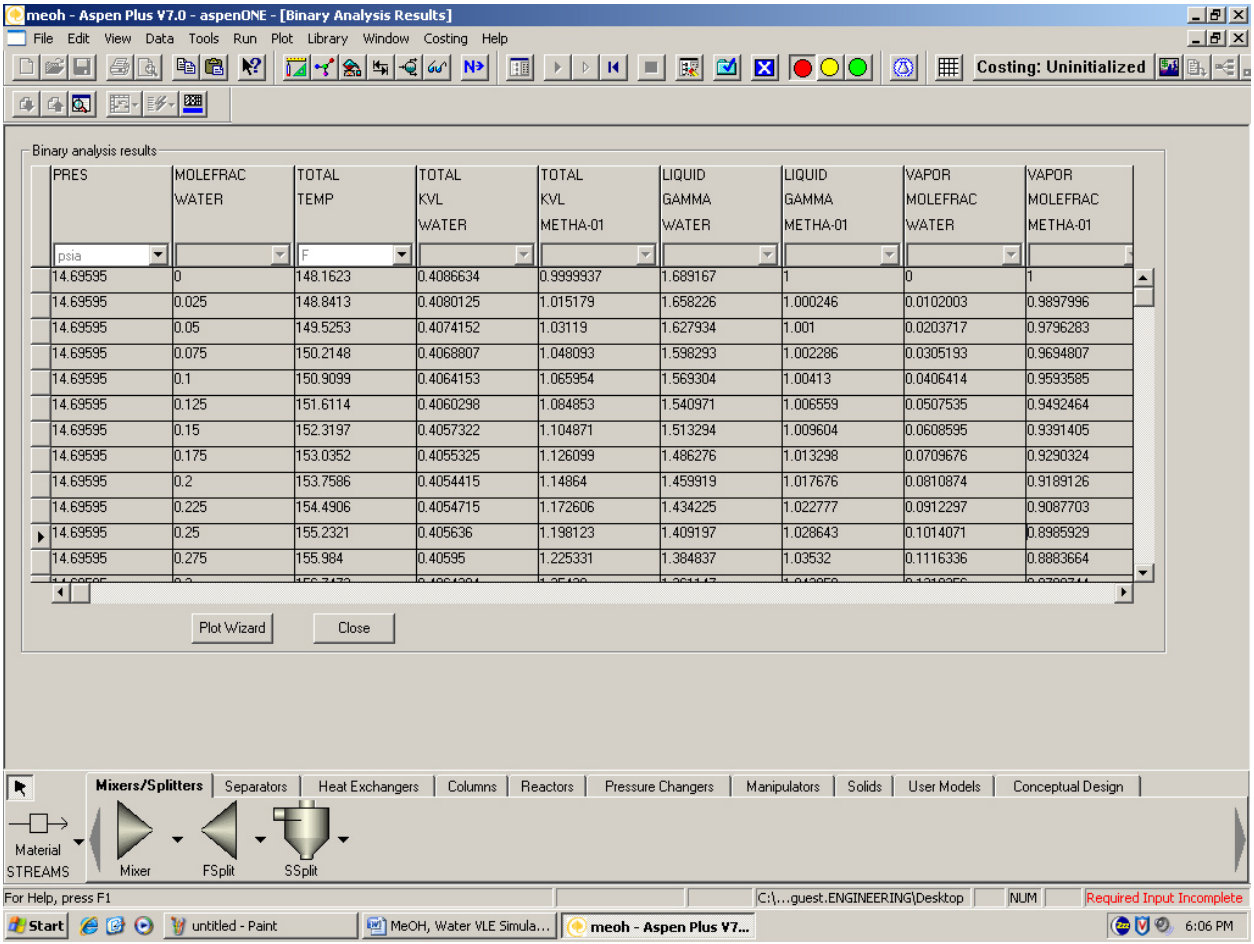


Fig. 18: Graphical results /VLE of methanol-water mixture

Exiting the screen would display data (as shown in figure 19) that can be copied to excel

spreadsheet for further

analysis.



PRES psia	MOLEFRAC WATER	TOTAL TEMP F	TOTAL KVL WATER	TOTAL KVL METHA-01	LIQUID GAMMA WATER	LIQUID GAMMA METHA-01	VAPOR MOLEFRAC WATER	VAPOR MOLEFRAC METHA-01
14.69595	0	148.1623	0.4086634	0.9999937	1.689167	1	0	1
14.69595	0.025	148.8413	0.4080125	1.015179	1.658226	1.000246	0.0102003	0.9897996
14.69595	0.05	149.5253	0.4074152	1.03119	1.627934	1.001	0.0203717	0.9796283
14.69595	0.075	150.2148	0.4068807	1.048093	1.598293	1.002286	0.0305193	0.9694807
14.69595	0.1	150.9099	0.4064153	1.065954	1.569304	1.00413	0.0406414	0.9593585
14.69595	0.125	151.6114	0.4060298	1.084853	1.540971	1.006559	0.0507535	0.9492464
14.69595	0.15	152.3197	0.4057322	1.104871	1.513294	1.009604	0.0608595	0.9391405
14.69595	0.175	153.0352	0.4055325	1.126099	1.486276	1.013298	0.0709676	0.9290324
14.69595	0.2	153.7586	0.4054415	1.14864	1.459919	1.017676	0.0810874	0.9189126
14.69595	0.225	154.4906	0.4054715	1.172606	1.434225	1.022777	0.0912297	0.9087703
14.69595	0.25	155.2321	0.405636	1.198123	1.409197	1.028643	0.1014071	0.8985929
14.69595	0.275	155.984	0.40595	1.225331	1.384837	1.03532	0.1116336	0.8883664

Fig. 19: Binary analysis results/Output data of the simulation.

Conclusion

This guide is intended as a step-by step procedure to simulate the compositions of mixture in a separation process.. However, hands-on learning is strongly recommended such that, one follows step by step running his/her own simulation because ONLY reading this would be least effective in educating the user; unless one is an expert with experience on process simulations. A procedure that could help chemical/process engineers to analyze results of process simulations from computer has been developed. The guide can be applied in various process systems. The volume liquid equilibrium (VLE) in graphical form obtained as shown in figure18 is of significant importance in separation processes. The components of various streams could be viewed with minimum difficulty.

Acknowledgements

The authors gratefully acknowledge the Aspen Technology Group for the software licenses granted Texas A & M University, Kingsville (TAMUK) which has enhanced the development of the procedure. In like manner we appreciate Invensys Systems, Inc (SimSci) for the Process Engineering Systems (PES) licenses granted Department of Chemical/Petrochemical Engineering, Rivers State University of Science and Technology, Port Harcourt, Nigeria which has supported this procedure.

References

EzineArticles (2010): http://professional-edu.blogspot.com/2010/07/216-simulation-analysis.html Article Source: http://EzineArticles.com/4763419 accessed on 15/06/2013

Peters, M. S., Timmerhaus, K. D. and West, R. E. (2004): Plant Design and Economics for Chemical Engineers, Fifth Edition, The McGraw Hill Companies

Process Engineering Associates, LLC, Available online at: http://www.processengr.com / accessed on 27/08/2014

Turton, R., Bailie, R. C., Whiting, W. B. and Shaeiwitz, J. A (2009): Analysis, Synthesis, and Design of Chemical Processes, Third Edition. Prentice Hall International Series

Ujile, A. and Amagbo, L. G. (2013): Determination of Plate Efficiency of Rectification Column in Refinery Operations; International Journal of Engineering and Technology Volume 3 No. 8, August, 2013
Wharton University of Pennsylvania, Available online at: http://opim.wharton.upenn.edu/~sok/phillydistricts/ accessed on 15/06/2013

Woller, S (1996): The Basics of Monte Carlo Simulations, Available online at: http://www.Solver.com/Monte-Carlo accessed on 14/06/2013