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The Creation of Instructional Video Tutorials for Chemical Engineering Process Simulation Software

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THE CREATION OF INSTRUCTIONAL VIDEO TUTORIALS FOR CHEMICAL ENGINEERING PROCESS SIMULATION SOFTWARE

by
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ABSTRACT

NISHAL VINOO BHIKHA: The Creation of Instructional Video Tutorials for Chemical Engineering Process Simulation Software

(Under the direction of Dr. Adam Smith)

Process simulation software is rapidly becoming a necessity in today's world. Often, learning how to use such a complex tool can be difficult and can take a significant period of time. This thesis outlines efforts to aid in the instruction of this type of software at the University of Mississippi.

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INTRODUCTION

Process simulation software allows the user to model and manipulate chemical processes in order to predict behaviors or justify changes in an extremely efficient manner. Prior to the development of process simulation software, engineers mostly completed mass and energy balances and sized equipment by hand. When designing process equipment such as distillation columns or reactors, engineers made ample use of simplifying assumptions while relying heavily on past experiences. It was common for teams of engineers to spend copious amounts of time on very meticulous calculations in order to achieve the high degree of precision and accuracy that is needed to design, build, and maintain a safe chemical process. In an effort to reduce the inefficiency of such methods, many companies began to develop flowsheeting programs specific to their needs[1]. These programs, however, were often crude and expensive to maintain. The rise of commercially-available process simulation software drastically reduced the use of these early programs because the software was much more refined and powerful in comparison. Although this software is powerful, it requires an intimate knowledge of engineering principles. The user must always analyze any results from the simulator and determine if the results are reasonable or even useful. As such, simulation software can be incredibly useful to engineers but may be rendered ineffective if engineers are not properly trained both in engineering principles and software use.

There are many process simulators that are commonly used today such as CHEMCAD, Aspen Plus, HYSYS, and PRO/II. Although they all are slightly different in terms of interface and capability, their overwhelming number of similarities make them easily interchangeable if an experienced user is given a small amount of time to adjust. The six main features that all process simulators share are a component database which houses the constants used to calculate physical properties from thermodynamic models; a thermodynamic model solver which has options for equilibria and enthalpy calculations; a flowsheet builder which serves as the main interface and keeps track of equipment, streams, etc.; a unit operation block solver which performs mass, energy, and design calculations; a data output generator which allows the user to customize the results from a simulation; and a flowsheet solver which controls the sequence of calculations and determines the precision for the overall convergence of the simulation[1].

The three main approaches simulators employ are sequential modular, simultaneous nonmodular, and simultaneous modular. In the sequential modular approach, the process is solved by moving from equipment piece to equipment piece solving the governing equations for each respectively. In the simultaneous nonmodular approach, all the governing equations for the entire process are solved simultaneously to achieve a solution. The simultaneous modular approach is a combination of the two aforementioned methods. When using this method, the process is solved by moving from equipment piece to equipment piece solving the governing equations for each respectively.

Of the three types of methods described above, the sequential modular approach is used most often. As previously mentioned, for any given piece of equipment, the input and equipment specifications will be solved and the result will become the input into the next piece of equipment until the entire process has solved and converged. Therefore for a process without recycle streams, individual pieces of equipment may require multiple iterations or algorithms to converge on a solution but the overall process is sequential and not iterative. If there are recycles streams in the process being modeled, the software usually splits the stream into two and solves multiple iterations in order to converge both streams within a set tolerance.

The widespread adoption of process simulation software in industry has created in increased demand for entry level engineers to be well versed in its use. This expectation is magnified considering that companies the software companies have made this software available for instructional purposes at a nominal cost compared industrial users. Furthermore, concepts which previously required years of experience and trial and error can now be taught with the utilization of this software which enables chemical engineering students to encounter increasingly complex problems that mimic typical entry level job assignments. Such high expectations demand a change and response from the institutions that are charged with teaching students to become engineers.

Here at the University of Mississippi, the Department of Chemical Engineering has made SimSci PRO/II an integral part of the curriculum. In the past, this software was reserved for senior level courses. This design proved problematic in several capacities. First, faculty were required to spend significant amounts of class time simply teaching the very basics of the software. This was quickly viewed as problematic because students naturally move at different paces—especially with technology. Many lectures had the tendency to have a hectic nature because instructors had to ensure all students were on the same page before continuing to subsequent steps. This can cause frustration among the faculty and students. Additionally, students learning PRO/II in the senior year were fully equipped with the tools needed for their design projects roughly four weeks into the semester. This left little time to produce a quality project that adequately represented the concepts learned throughout the curriculum. Beginning in the Fall of 2016, PRO/II will be introduced and utilized starting in sophomore chemical engineering classes. This change will allow our students to familiarize themselves with the software in preparation for their senior year.

In order to overcome the hurdle of students learning the software at different paces, it is proposed to create tutorial videos to aid students in learning PRO/II. These videos, in theory, would drastically change the dynamic of learning the simulation software. Instead of instructors spending weeks trying to teach students how to use this software in a group setting, students would be able to individually walk themselves through videos that guide them in completing a specified problem or scenario in a much more productive setting. Ideally, students would increase the use of PRO/II as they progress through the curriculum. With this model, students would still learn all the necessary concepts of chemical engineering while freeing class time to cover more complex concepts.

The nature of these videos would be appropriate to the target audience. For example, sophomores may begin with "Introduction to PRO/II's Interface" which simply familiarizes the viewer with the software's interface and very quickly explains some of the useful capabilities of said software. Subsequently, students may simulate problems or examples worked in class to check their answers. In contrast, a junior's first assignment may be to watch a series of videos covering all aspects of an example process and provide a complete, working simulation of the chemical process to the instructor. By creating numerous videos covering a variety of topics and difficulties, our department can not only increase its efficiency in teaching undergraduates but also increase the quality of the education they receive.

DESCRIPTION OF TUTORIAL VIDEOS

Introduction to PRO/II Interface

One of the earliest instructional videos the students at the University of Mississippi will be exposed to is the "Introduction to PRO/II Interface". Novice users can often be overwhelmed with the many intricacies of PRO/II or any simulation software. The purpose of this video is to gently ease students into the software. The video starts with explaining how to open and save a new flowsheet. I then systematically move from a blank flowsheet into some of the most commonly used functions of PRO/II. Instead of thoroughly explain each of these categories, I give a brief overview of what each is used for, what information can be found here, and where it is located.

Thermodynamic Package Selection

The proper selection of a thermodynamic package is of the utmost importance for accurate simulation of a chemical process. This video aims to guide students through the guidelines by using Figure 1. By creating situations and scenarios and discussing how to properly utilize the aforementioned chart, students will ideally be better equipped to discern for themselves the most appropriate thermodynamic package in future assignments.

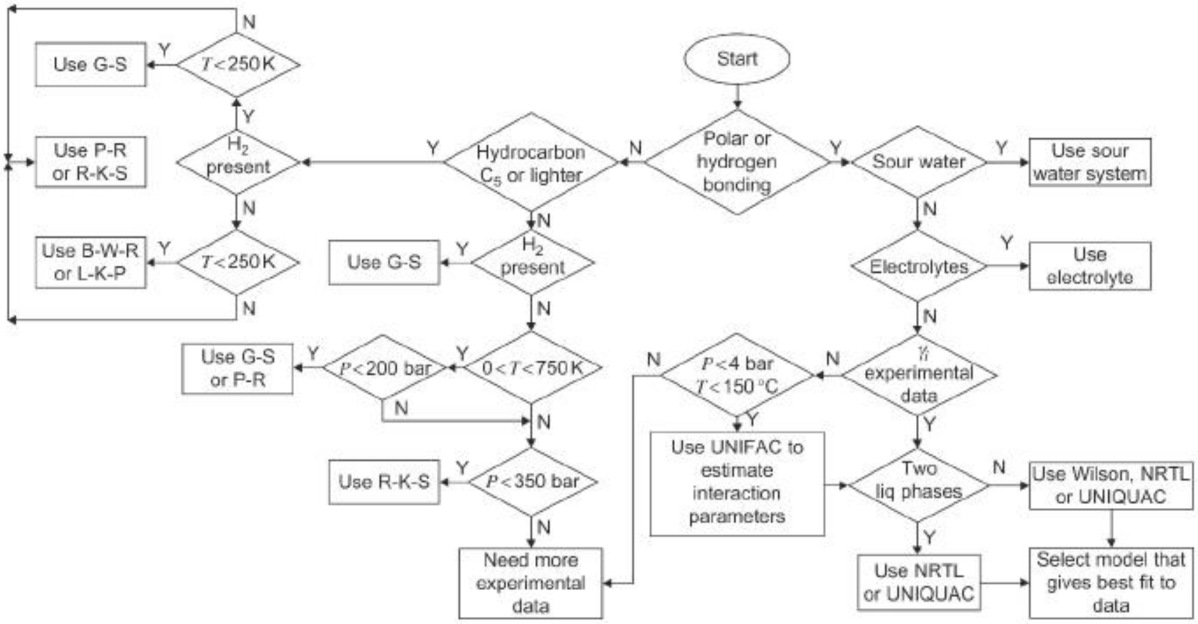

Figure 1: Therodynamic Package Selection Chart[2]

Mass and Energy Balance

The topic of this video is a simple combustion reaction of methanol. Students following the simulation covered in this video should have completed the corresponding problem, Example 9.6-2, by hand in class. To summarize the problem, liquid methanol is fed to a furnace with air and is burned to produce carbon dioxide and water. The objective is to find the maximum temperature the furnace should be able to withstand. The student must first write and balance a chemical equation for this system. Once the equation is written, the mass balance can be solved for the products. After all the masses are known, and energy balance can be written by finding the enthalpy for the product stream, the heat of combustion for the reaction, and the heat of vaporization for the water.

Solving this balance for the temperature will yield the maximum temperature the student is searching for.

Solving problems such as this by hand can prove difficult due to the natural mathematic complexity of the balances. In this particular problem, in order to find the maximum temperature the furnace would be exposed to, one is required to solve a fourth order polynomial. Modern calculators and office software can make quick work of such equations; however, finding the information for each component and simplifying the overall equation into form tools such as these can recognize can prove to be very tedious which may give rise to errors by students. This video would be of use primarily to sophomores enrolled in Ch E 307 and Ch E 308. With the earlier exposure to PRO/II, the students learning mass and energy balances can use the software to double check the calculations they have performed by hand. For example, students can easily and quickly model this basic system and check if the temperature they solved for by hand, in this case 1256°C, matches the simulator's answer. This is illustrated in the Figure 2.

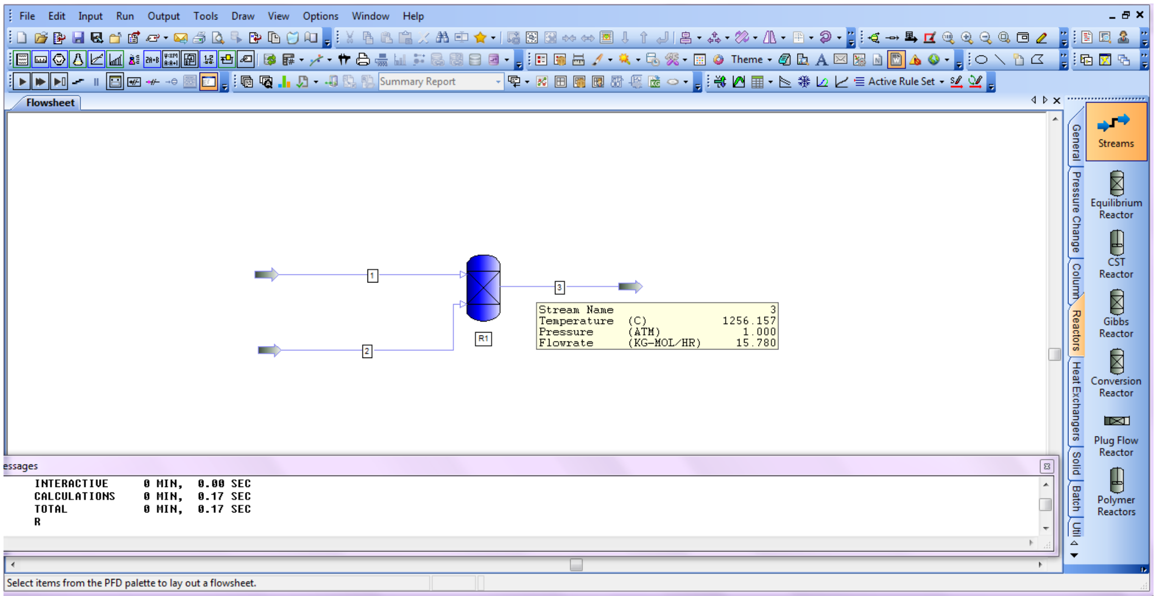

Figure 2: Verifying Maximum Furnace Temperature

Toluene Hydrodealkylation (HDA)

The Toluene HDA process has been utilized to expose seniors to PRO/II. Professors would simulate the entire process across multiple class sessions while having students follow along on their computers. This constituted the majority of the training students had in using PRO/II. As mentioned before, this method was less than ideal. Although the students should be quite familiar with PRO/II in senior classes under the new teaching model, this video will bring all of the prior videos and assignments together by allowing students to interact with a full-fledged process rather than a couple of unit ops simulated together as a homework problem . The following subsections will provide further details on each section of the process and the corresponding instructional video:

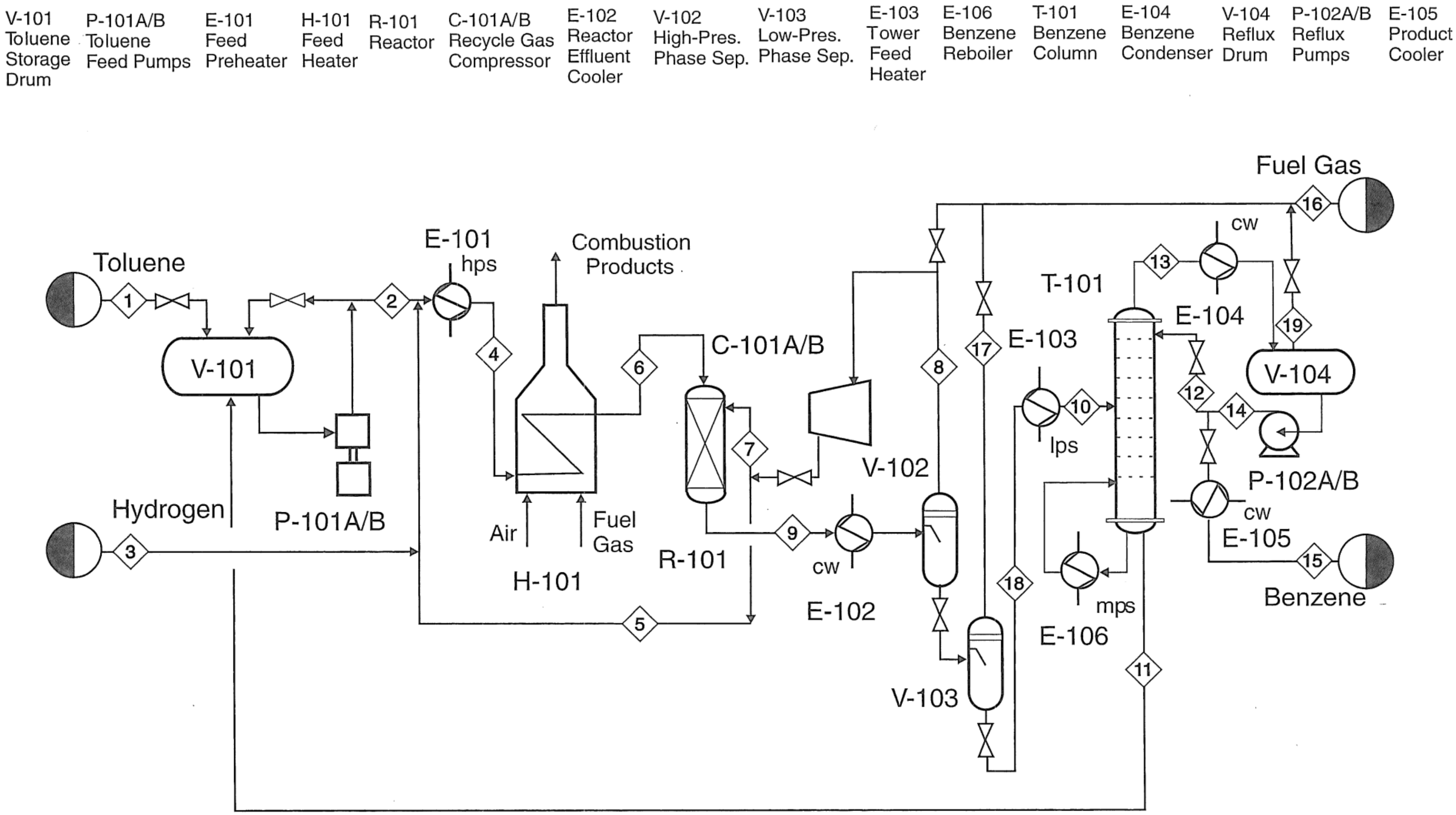

Figure 3: Toluene HDA PFD

Toluene HDA Video I

In this video, I covered how to select the chemicals used in the process, walked through the selection of the thermodynamic package, and simulated from the feed streams to the first heat exchanger, E-101, while providing the appropriate equipment specifications. Although fairly simplistic topologically, this video covers important “under the hood” settings and selections that are vital to the successful simulation of this software. Students should be able to complete most of what is covered in this particular video independently as it draws on topics covered in previous videos, topics that should be well known at this level; however, this video eases students into simulating an entire chemical process from scratch because the task may seem daunting at first. Figure 4 shows what a completed flowsheet would look like after watching this video.

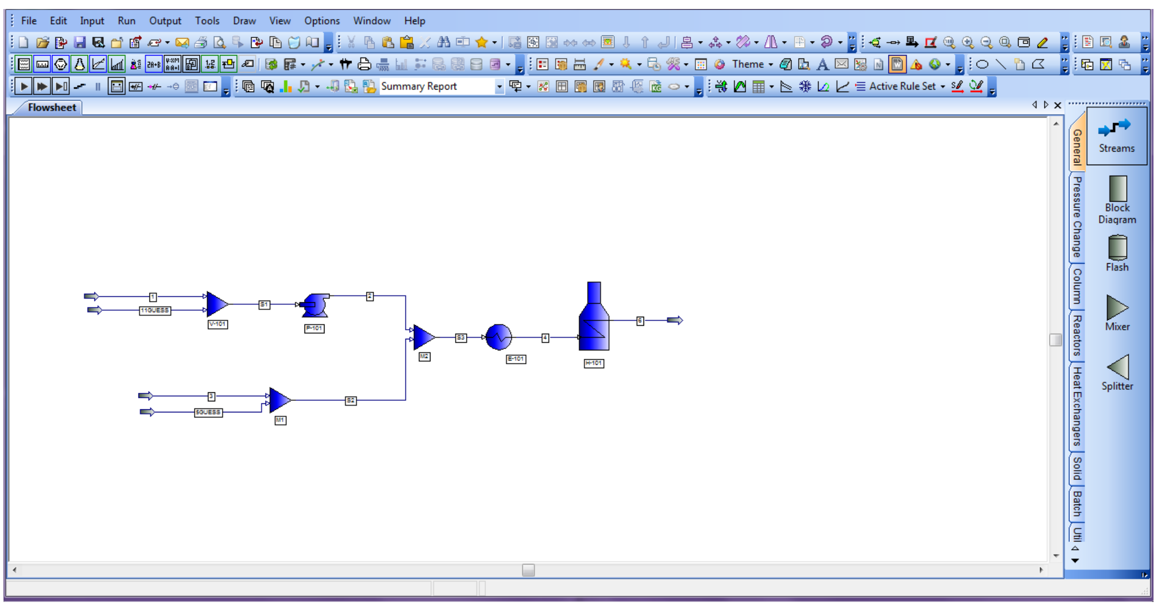

Figure 4: Completed Toluene HDA Video I Flowsheet

Toluene HDA Video II

This video spans from E-101 to the distillation column, T-101. This video covers how to properly select and utilize a reactor for this scenario. The reactor in this example is fairly simplistic; however, the method for properly setting it up can be applied to more complex reactors with marginal effort. In addition to the reactor, I also cover how to properly simulate flash drums. Care must be taking in their simulation because errors in configurations or thermodynamic package selection may yield unreasonable results such as extremely cold temperatures. Figure 5 shows how the flowsheet would progress as the student finished this video.

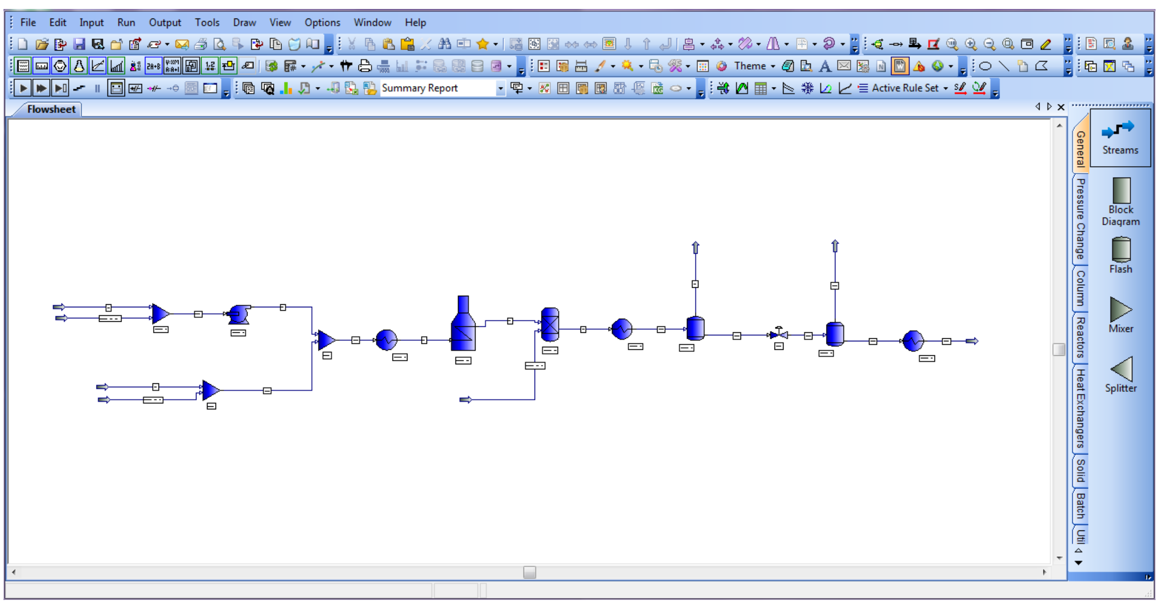

Figure 5: Completed Toluene HDA Video II Flowsheet

Toluene HDA Video III

The third video in the series is entirely dedicated to creating a shortcut column and finding the necessary information for its simulation in order to simulate a rigorous distillation column. The subject of this video alone could very well have taken an entire class period to show to a class. Figure 6 shows the specifications for a shortcut column being specified.

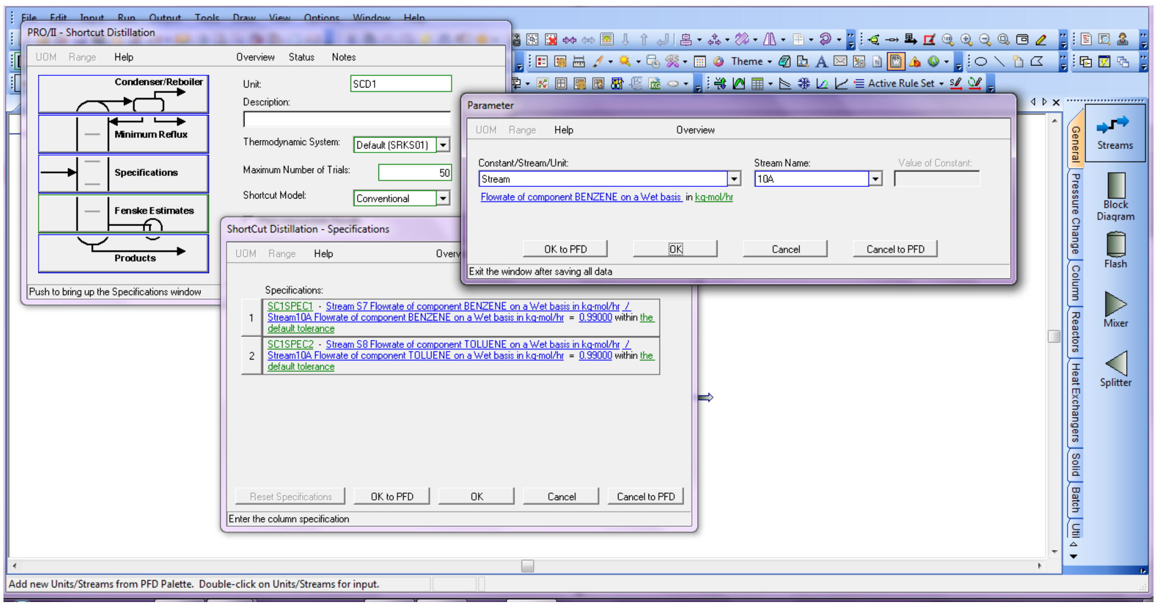

Figure 6: Shortcut Column Specifications

There are many variables that need to be specified and the process of specifying these variables often is very arduous, requiring students to be very meticulous. The creation of this video allows the user to clearly see and double check all of the specifications required to run this specific simulation thus minimizing confusion and frustration. In addition to the many specifications on just the separation requirements, the result from a simulated column must be closely reviewed. For example, one of the options when simulating a shortcut distillation column is to either have a partial or total condenser. In the first part of this video, the students are instructed to select the total condenser. After running the program and letting it converge on an answer, the students are instructed to examine the results as shown in Figure 7.

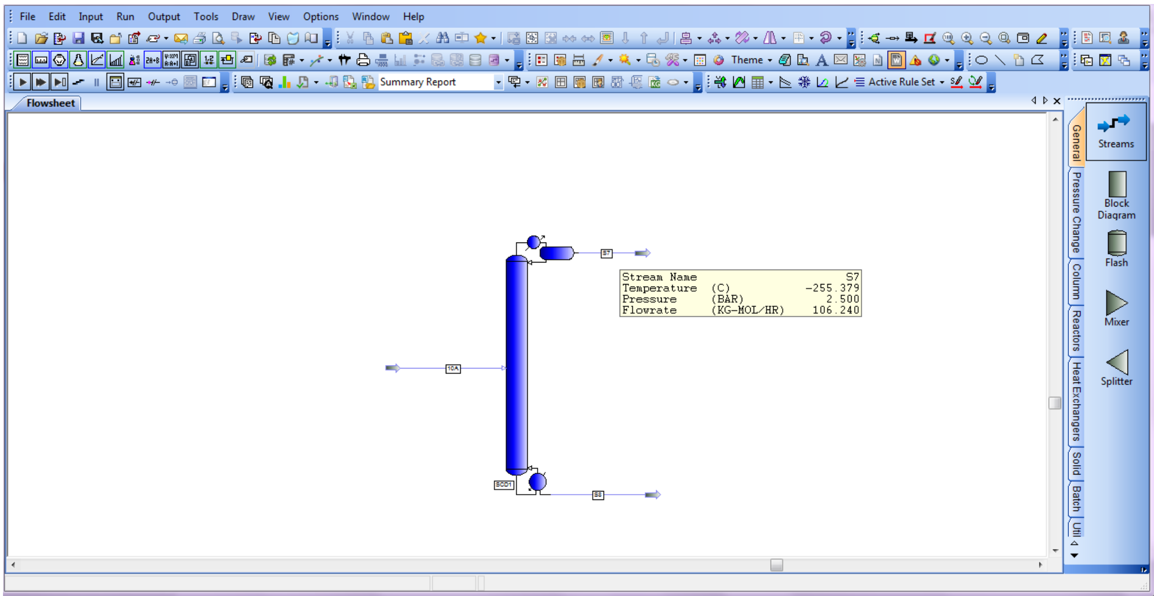

Figure 7: Shortcut Column with Extremely Low Temperature

Here they are directed to the peculiar temperature of -255°C. After discussing why the condenser selection caused this temperature, the students are told to simulate the column again with a partial condenser instead of total condenser. After making this change, the students arrive at a much more reasonable temperature for their process.

Once the specifications for the shortcut column are set, the students are to generate the results and find the information required to simulate a rigorous distillation column. This information is shown in Figure 8.

file:///C:/Users/User/AppData/Local/Temp/VWE99D.htm

FEEDS

STREAM	PHASE
10A	MIXED

PRODUCTS

STREAM + PHASE		MOLES KG-MOL/HR	WEIGHT KG/HR	LIQUID VOL M3/HR	NORM VAPOR(1) M3/HR	SECTION	NUM TRAYS
S7	V	106.24	8257.02	9.39	2381.27	1	11.82
S8	L	35.66	3269.75	3.74	799.19		
TOTALS		141.90	11526.77	13.13	3180.45		11.82

(MOLES through NORM VAPOR(1): TOTAL STREAM RATES)

SPECIFICATIONS

PARAMETER TYPE	COMP. NUM	SPECIFICATION TYPE	SPECIFIED VALUE	CALCULATED VALUE
STRM S7	3	MOL RATIO	9.900E-01	9.895E-01
STRM S8	4	MOL RATIO	9.900E-01	9.886E-01

SUMMARY OF UNDERWOOD CALCULATIONS

MINIMUM REFLUX RATIO	1.16539
FEED CONDITION Q	0.99596
FENSKE MINIMUM TRAYS	11.81823
OPERATING REFLUX RATIO	1.30 * R-MINIMUM

TOTAL TRAYS	FEED TRAY	R/R-MIN	M/M-MIN	REFLUX RATIO	DUTY, M*KJ/HR CONDENSER	DUTY, M*KJ/HR REBOILER
28	17.38	1.150	2.368	1.340	-4.132E+00	7.946E+00
26	16.27	1.225	2.212	1.428	-4.401E+00	8.216E+00
25	15.36	1.300	2.084	1.515	-4.671E+00	8.485E+00
23	14.59	1.375	1.977	1.602	-4.940E+00	8.755E+00
22	13.94	1.450	1.886	1.690	-5.210E+00	9.024E+00

Figure 8: Information from Shortcut Column

Toluene HDA Video IV

This video instructs students on how to use the information from a shortcut column to simulate a rigorous distillation column. I broke the addition of the distillation column into two separate videos (Videos III and IV) in order to more clearly communicate the process of simulating one. Once a chemical process is fully simulated, engineers often begin to make changes in order to predict results. This process of simulating a distillation column is especially important to understand because even seemly small changes in a chemical process can have a rather large impact on column design and function. Users who fully understand how to simulate columns and are comfortable with the process of doing so will have a much better experience using this type of software.

Toluene HDA Video V

This video primarily shows how to connect the recycle streams to their specified destinations. Students are taught in Video I to provide guess conditions (i.e. composition, temperature, and pressure) for the recycle streams in the initial simulation of this process. After fully simulating the process, students are told to check if the simulated values for the recycle stream match the guess values. Figure 9 shows the conditions of the initial guess stream students specified while Figure 10 shows the simulation's result.

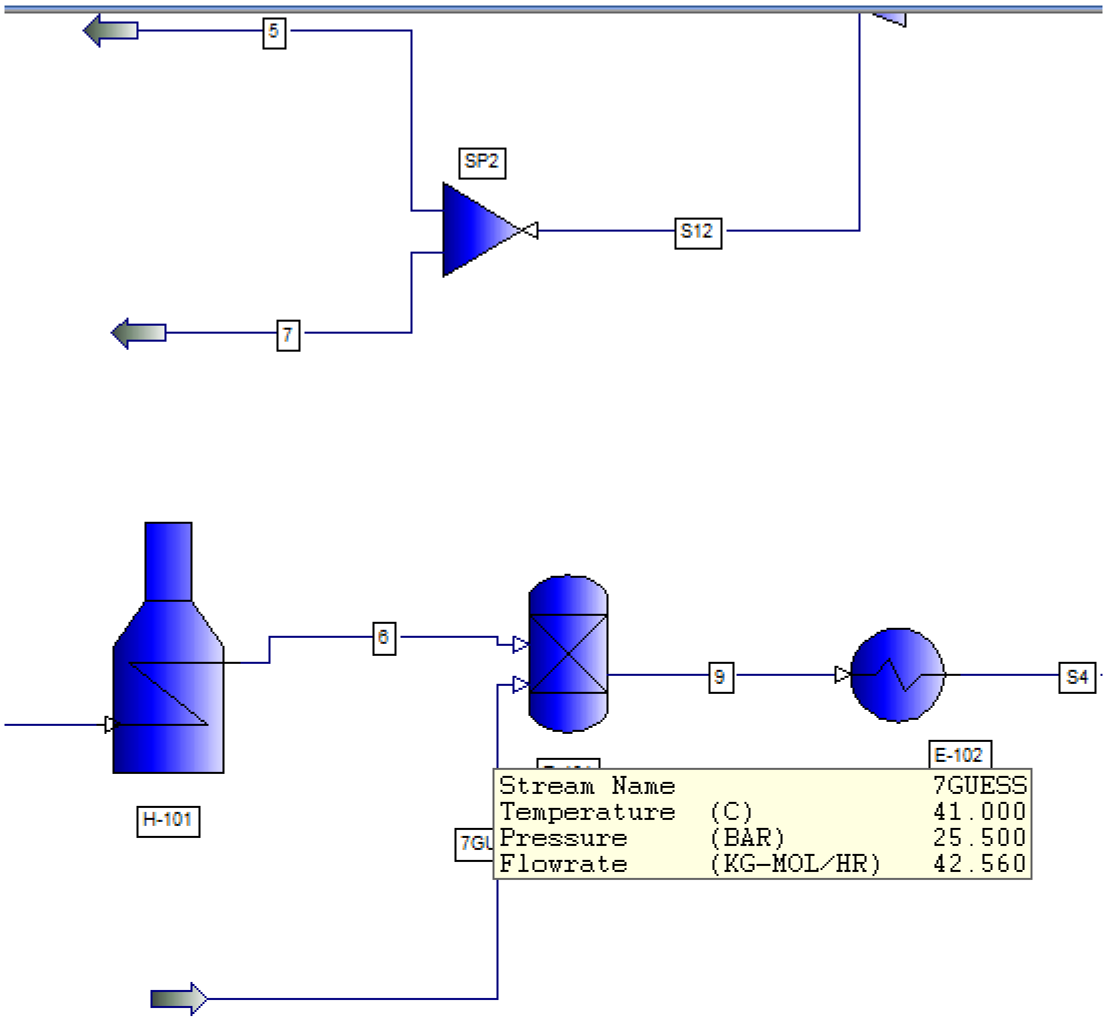

Figure 9: Guess Stream Conditions

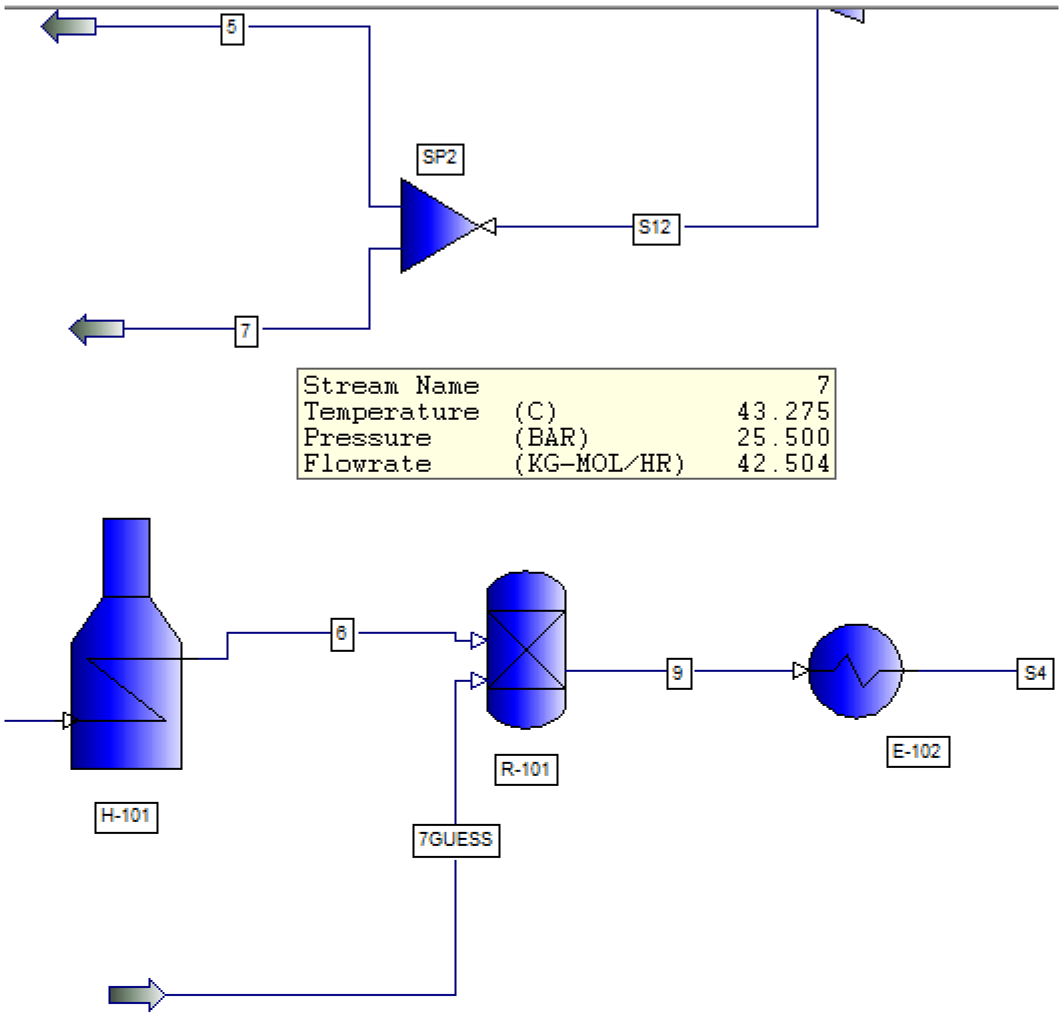

Figure 10: Simulated Stream Conditions

Because the streams are fairly similar in this particular case, students were instructed to delete the guess stream, attached the simulated stream, and run the simulation again to converge on a final answer. There were three recycle streams for the Toluene HDA process. Students verified each of these as they progressed through this video. Figure 11 shows how a completely finished flowsheet would look for this process.

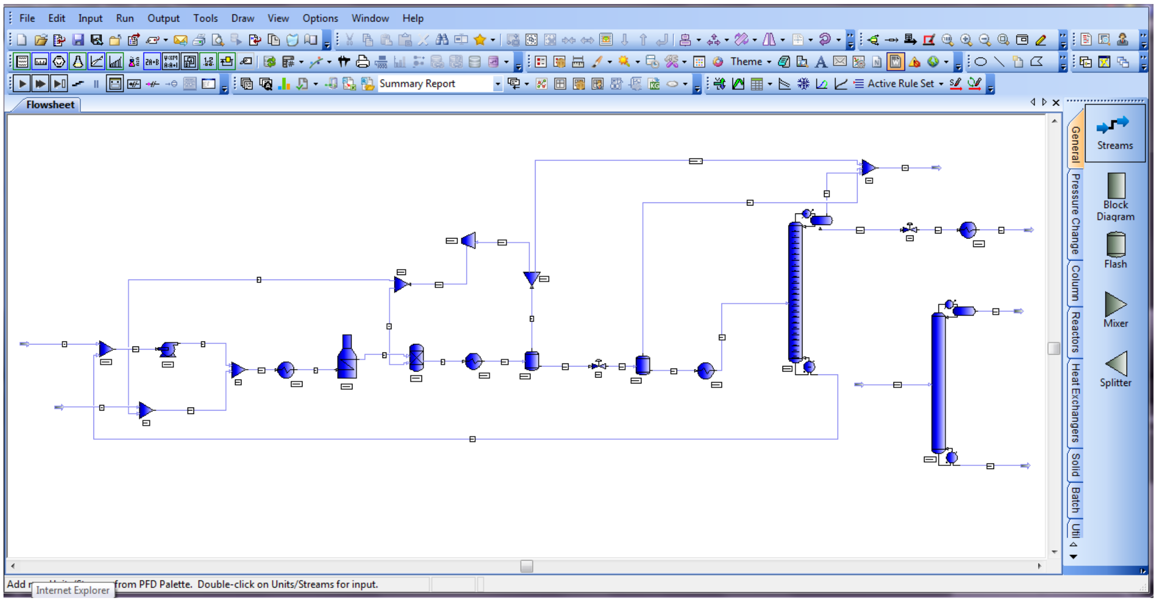

Figure 11: Finished Simultation of the Toluene HDA Process

CONCLUSION

Process simulation software definitely has a strong foothold in today's world. As time progresses, the need for engineers to be greatly familiar with this type of software will only rise. The creation and implementation of these instructional tutorial videos will greatly increase the quality of education the chemical engineering students at the University of Mississippi receive. Not only does it free more instructional time throughout the semester, it also aides in the effort to introduce the software earlier in the curriculum. The videos created as a part of this thesis are a part of a larger effort to allow students to familiarize themselves with the software outside of the classroom. There will be more instructional videos created on many more key concepts and topics.

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