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SOME EXPERIENCE IN TEACHING OF COMPUTER AIDED PROCESS SIMULATION AT PICT

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Abstract: Analysis and design of chemical technological processes is faster and more effective when using simulations. That is why knowledge of chemical process simulation is an important part of study at Prague Institute of Chemical Technology. The Computer Assisted Process Simulation course is relatively popular among students. But it does not mean that its teaching is without problems. In this contribution some experience in teaching of Computer Aided Process Simulation is introduced. Some difficulties associated with the bidirectional flow of information, with the simulation of recycle systems and with the use of subflowsheets are described and illustrated with examples.

Keywords: Process simulation, bidirectional information flow, simulation of recycles, subflowsheets.

1 INTRODUCTION

Simulations are an important tool for analysis and design of chemical technological processes. Obtained results allow to identify and to eliminate bottlenecks in production line, to decrease energy costs or to minimize pollution of the environment. Another possibility of simulation utilization is to study how system will react on changes in feed quantity and composition. The economical effect of simulations is also very important, because experiments with production facility are for the most part substituted by calculations. At Prague Institute of Chemical Technology (PICT) students acquire knowledge of chemical process simulation in the subject Computer Assisted Process Simulation (CAPS).

2 MOTIVATION OF THE PAPER

For effective process simulation knowledge of process technology (chemical plant), chemical engineering (especially models of apparatus), physical chemistry (methods for computing physical properties and databanks) and computer science (numerical methods, finding computation sequence at systems with recycle streams, problem of convergence acceleration, optimization methods etc.) is required. That is why universal simulation programs were developed. Their usage significantly facilitates user's work and enables him to concentrate his effort to creative activities and own proposals. Education of simulator‘s user needs circa 40 – 50 hours.

But it does not mean that use of simulation programs is without problems. Many users underestimate difficulties and do not obtain the correct results. In our contribution we would like to describe some experience in teaching of Computer Aided Process Simulation at PICT. We would like to show some difficulties associated with the bidirectional flow of information, with the simulation of recycle systems and with the use of subflowsheets and to illustrate them with examples.

3 HYSYS SIMULATOR

At PICT the HYSYS or rather Aspen HYSYS universal simulators are used. They represent top program products that are provided with simple and user friendly graphics interface. HYSYS differs from many of the alternative simulators in two main respects. First, it has facility for interactively interpret-

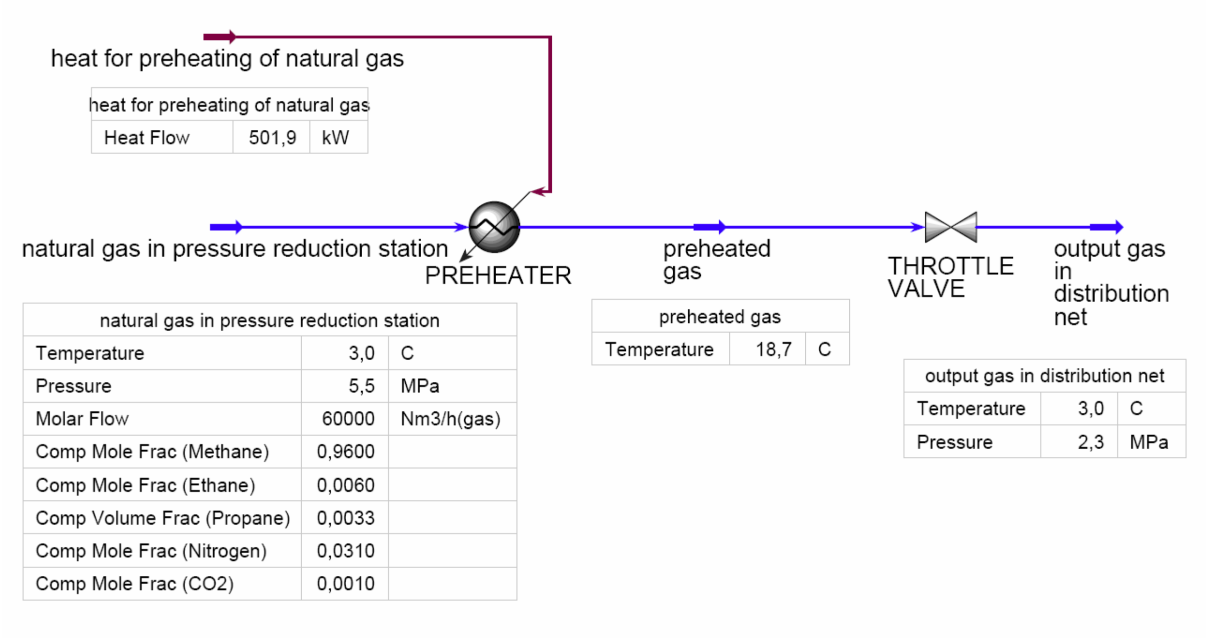

Fig. 1 Process flowsheet diagram of gas throttling at pressure reduction station

ing commands, as they are entered one at a time, whereas most of the other flowsheet simulators require that a RUN button be pressed after new entries are completed. Whenever a stream variable is altered, the adjacent process unit is resimulated. Second, it has the unique feature that information propagates in both forward and reverse direction. This bidirectionality often makes iterative calculations and the use of ADJUST operation unnecessary. The HYSYS simulator is a notable exception in that any combination of specifications is permitted for each simulation model. These two features make the program fast responding and relatively easy to use.

4 BIDIRECTIONAL INFORMATION FLOW

The sequential-modular architecture dominates the technology of steady state simulation. Computation takes place unit-by-unit following a calculation sequence. The advantages of sequential-modular architecture include modular development of capabilities, easy programming and maintenance, easy control of convergence, both at the units and flowsheet level. Rigid direction of computation, normally "outputs from inputs" belongs among disadvantages. It means that the inlet streams and the equipment parameters are specified, along with selected variables of the outlet streams (e.g. temperatures and pressures), and the unknown variables of the outlet streams (typically, the flow rates and compositions) are calculated. When it is necessary to provide specifications for variables or parameters that are not permitted by a unit subroutine, control subroutines are provided to iteratively adjust the manipulated variables so as to achieve the desired specifications. In the HYSYS, this is accomplished by the ADJUST operation, in CHEMCAD by the CONT subroutine, and in PRO/II by the CONTROLLER subroutine.

To improve the flow of information and avoid redundant computations, HYSYS implemented the bidirectional flow of information. The information propagates in both forward and reverse direction. This bidirectionality often makes iterative calculations and the use of ADJUST operation unnecessary. The HYSYS simulator is a notable exception among flowsheet simulators in that any combination of specifications is permitted for each simulation model. Specifications can be provided for the product streams and the unknown parameters of the inlet streams are computed. The concepts of bidirectional information flow are introduced in the example that follows.

4.1 Example 1 – Gas Throttling

Natural gas is transported for long distances through pipelines at high pressures. In a place of consumption the pressure must be reduced. Standardly, gas pressure reduction is accomplished in throttle-valves, where the isenthalpic expansion takes place. Most gases cool during the expansion (Joule-Thompson effect). The gas must be preheated before the expansion to ensure that no liquid or solid phase condenses at the output temperature. Students are supposed to calculate requirements for preheating of natural gas (necessary heat flow) and temperature at the input of throttle valve that is necessary for choice of the heating medium. Bidirectional information flow in HYSYS makes possible to enter parameters of output stream (temperature and pressure) and without any other disposal (e.g. use of ADJUST operation) temperature of input gas and necessary heat flow are at once calculated so as to achieve the desired output temperature that secures no liquid or solid phase condensation. It illustrates also another unique feature of the HYSYS simulator – its facility for interactively interpreting commands, as they are entered one

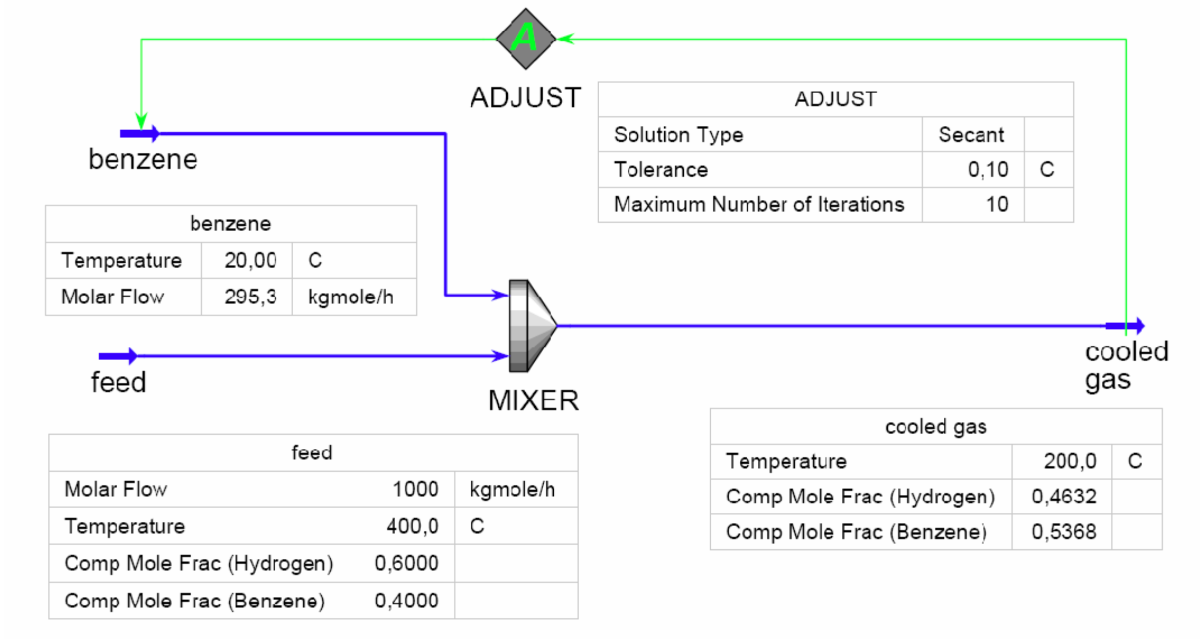

Fig. 2. Process flow diagram of the process that involves iterative control subroutine

at a time. No Run button must be depressed after new entries are completed. You can see results in Fig. 1.

4.2 Example 2 – Adiabatic Mixing

There occur other cases when using a feedback control routine is necessary. The Adjust operation varies the value of one stream variable (the independent variable) to meet a required value or specification in another stream or operation (dependent variable). This can be illustrated by an example of adiabatic mixing. Gaseous mixture of benzene and hydrogen should be cooled to 200 ^{o}C by injection of liquid benzene. The flow rate of a benzene stream should be adjusted to achieve a desired temperature of the mixer effluent. It is not possible to use bidirectional flow of information because there are more degrees of freedom – it is not uniquely given which input variable (flow or temperature of benzene or feed) should be changed. It is necessary to use the Adjust operation with benzene flow as adjusted variable and temperature of cooled gas as target variable. Adjust unit adjusts the flow rate of benzene when the specified temperature is not achieved and transfers to the MIXER to repeat the calculations. This cycle is repeated until the convergence criteria are satisfied or maximum number of iterations is exceeded. Students are supposed to calculate required molar flow of liquid benzene and composition of cooled gas. You can see results in Fig. 2.

4.3 Lesson from the Use of the Bidirectional Flow of Information

The students have often difficulties already in the first step – they must decide whether to use bidirectional information flow or Adjust block. When using bidirectional flow of information they do not enter the correct number of output specifications, they do not understand the number of degrees of freedom. The basic problem of our students at using of Adjust block lies in the right operation of the process flowsheet. That is why we recommend to test the flowsheet without Adjust block and to follow the changes of dependent (target) variable in dependence on independent variable (adjusted) variable or to perform sensitivity analysis. Only when is everything O.K. it is convenient to install Adjust block. In more complicated examples (e.g. complex network of heat exchangers) it is possible to calculate some variables with the use of bidirectional information flow and other with the use of Adjust block. The multiple Adjust blocks are then to be solved simultaneously.

5 SIMULATION OF RECYCLE SYSTEMS

Recycle streams are widely used in the chemical industry. As the industry moves towards higher yield and lower discharge, more material recycle loops will be put in place. Utilization of waste heat (heat integration) often requires energy recycle streams, as well.

Recycling is the tricky part of flowsheet modeling. At standard simulation the inlet streams and the equipment parameters are specified and the outlet streams are computed. Therefore, it is not possible to solve unit operation where one of input streams comprises recycle stream because its parameters are not known. That is why a recycle structure should be transformed in a sequential calculation sequence by means of the concept of a “tear stream” (Fig. 3). Some initial guesses for the stream “Assumed Recycle Stream” are made (temperature, pressure, flow rate, composition) so the simulation can proceed to units C and D. The resulting parameters of stream “Calculated Recycle Stream” are compared to the

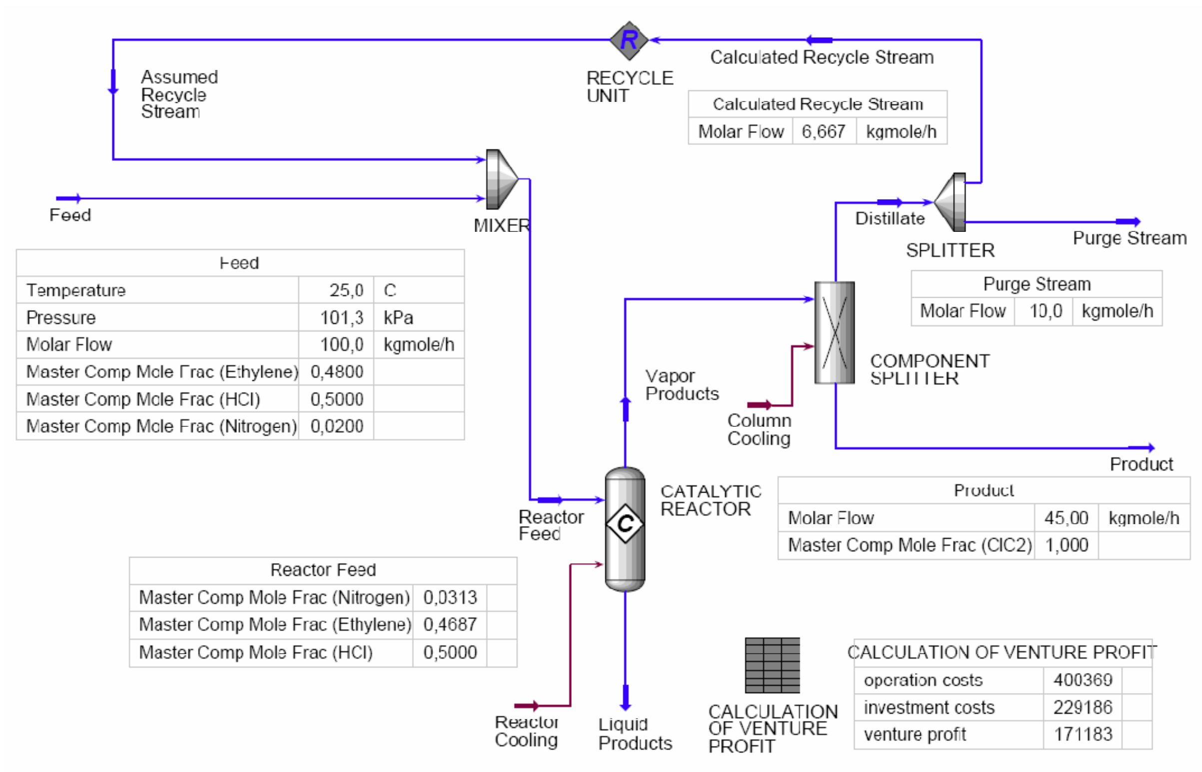

Fig. 4. Process flow diagram of the process that involves recycle

initial guesses for "Assumed Recycle Stream" and the convergence criteria are checked. The initial guesses are revised and the simulation is rerun until the values agree to within a specified tolerance.

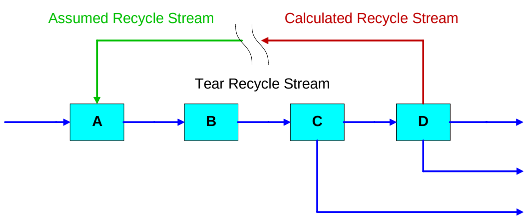

Fig. 3. The tear stream concept is used in recycle simulation

The capability of any flowsheet simulator to solve recycles reliably and efficiently is critical. For simulation of recycle streams in HYSYS it is recommended to use theoretical block RECYCLE (mathematical recycle convergence unit). We can illustrate simulation of recycles by the following example.

5.1 *Example 3 – Production of Ethyl Chloride*

One of the ways to produce ethyl chloride is by the gas-phase reaction of HCl with ethylene over a copper chloride catalyst supported on silica:

$$C_2H_4 + HCl \rightarrow C_2H_5Cl \qquad (1)$$

Since the reaction achieves only 90 mol% conversion, the ethyl chloride product is separated from the unreacted reagents, and the latter are recycled. To prevent the accumulation of inerts in the system, part of the unreacted reagents is withdrawn in a purge stream (Fig. 4).

Students should then investigate the impact of the recycle flow rate on the reactor feed composition and flow rate and on the production of ethyl chloride (product flow rate). Increasing recycle flow rate produces bigger equipment sizes (and bigger equipment costs), on the other side it causes smaller losses of raw materials (and increasing revenue for ethyl chloride). Costs are calculated in spreadsheet that is one of HYSYS units. You can see results in Fig. 5. Difference of installed cost of equipment and operation costs gives then the venture profit. It is possible to optimize the venture profit in relation to recycle flow rate.

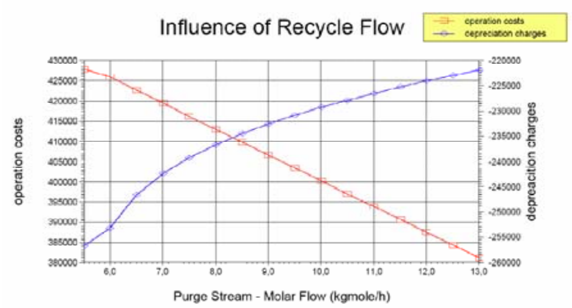

Fig. 5. Influence of Recycle Flow on Operation Costs and Depreciation Charges

5.2 *Lesson from the Simulation of Recycles*

The main problem of our students at simulation of recycles lies in the right sequence of setting up process flowsheet. Usually, sequence of setting up process flow diagram in HYSYS is not important. It is facilitated by ability of bidirectional information flow and by interactively interpreting commands in HYSYS. But at standard practice students get in case of recycles wrong results. It is necessary strictly respect this step-by-step procedure:

1. make a guess for the assumed recycle streams
2. build the flowsheet until the calculated recycle stream can be calculated
3. install the RECYCLE block
    a. set the parameters of recycle (tolerances, maximum iterations etc.)
    b. connect inlet and outlet streams

Students are also often not conscious of the fact that it is not possible to entry any pressure drop values in the units in recycle loop. Pressure drop is taken away at each pass through iterative loop. At times, Recycle operations will not converge and troubleshooting can be very difficult. Basic troubleshooting tips include: 1) decrease the "Sensitivity" on the Variables page, 2) increase the number of iterations.

6 SUBFLOWSHEETS

The multi-flowsheet architecture provides a number of technical and functional advantages. Each installed subflowsheet can have its own fluid package within a single simulation case. The use of subflowsheets breaks large and complex simulations into smaller, more easily managed components. This helps the designer to keep his simulation better organized and concise. It is very useful at debugging and verification of simulation model and also at solving of difficulties with convergence.

6.1 Example 4 – Dehydration of Ethanol

The use of a subflowsheet can be illustrate by the example of the dehydration of an almost azeotropic ethanol water mixture of fermentative processes using benzene as an entrainer. In heterogeneous azeotropic distillations, lighter azeotrop (benzene-water-ethanol) leaves in the overhead vapor outlet of the column whereas concentrated (absolute) ethanol with purity 99.99 % represents product (bottoms liquid outlet). Mixture benzene-water-ethanol when condensed, causes the formation of a second liquid phase that can be separated in decanter and recirculated to the tower as reflux. Subsequently constituent parts are mixed so as to create reflux of required composition. Because part of benzene leaves the system it must be replaced (a make-up stream). Flowsheet is in the following figure (Fig. 6).

When simulating an azeotropic distillation column with a decanter, two property methods are often preferred. A property method optimized for liquid-liquid

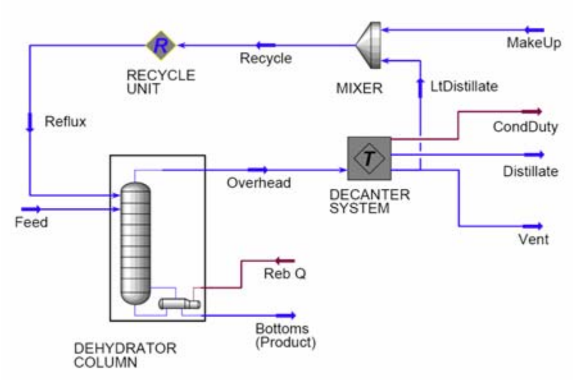

Fig. 6 Process flowsheet diagram of the dehydration of an ethanol water mixture

equilibrium is often desired for decanter, while a property method optimized for vapor-liquid equilibrium is desired for the main tower. Utilizing a subflowsheet for the decanter is the ideal way to solve these types of simulations. Subflowsheet of the decanter system is in the following figure (Fig. 7).

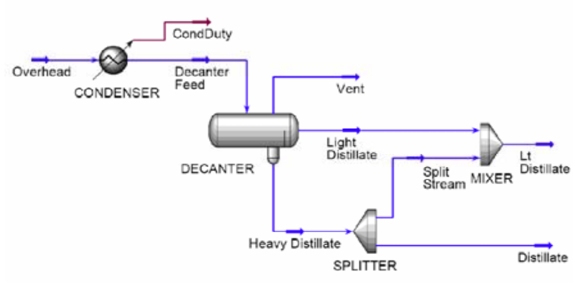

Fig. 7 Subflowsheet of the decanter system

5.2 Lesson from the Use of Subflowsheets

Students usually do not have difficulties with setting up two fluid packages or installing a subflowsheet operation. No problems are at the attaching the main flowsheet streams to the subflowsheet. But much misunderstanding occurs at specifying of proper transfer basis at bound streams. This problem is worth of detailed explanation.

The change of property method occurs at defined flowsheet boundaries. This ensures that consistent transitions between the thermodynamic bases of the different property methods are maintained and easily controlled. It is necessary to specify how stream information is exchanged as it crosses the flowsheet boundary. For example, you can specify the vapor fraction and temperature of a stream in the main simulation to be passed to the subflowsheet. Once this information is passed to the subflowsheet, the property package for the subflowsheet then calculates the remaining properties using the transferred composition. The values of remaining state variables (for example temperature) can be then different in main flowsheet and subflowsheet.

In our example the decanter's condenser should be dealing with a dew point feed and the decanter itself is producing bubble point products. Therefore, the default passing of pressure and temperature is not suitable for preserving the dew point/bubble point condition of the feed/product streams when the thermodynamic basis changes across the flowsheet boundary. It is necessary to specify that vapor fraction and pressure are passed between flowsheets and new temperature is calculated.

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