**Experiences on dynamic simulation software in chemical engineering education**

**manuscript no ECE-D-11-00041**

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**Abstract**

Commercial process simulators are increasing interest in the chemical engineer education. In this article, the use of commercial dynamic simulation software, D-SPICE® and K-Spice®, for three different chemical engineering courses is described and discussed. The courses cover the following topics: basic chemical engineering, operability and safety analysis and process control. User experiences from both teachers and students are presented. The benefits of dynamic simulation as an additional teaching tool are discussed and summarized. The experiences confirm that commercial dynamic simulators provide realistic training and can be successfully integrated into undergraduate and graduate teaching, laboratory courses and research.

**Keywords:** dynamic simulation; process model; process control; oil and gas processing; distillation; HAZOP.

**Highlights**

- Realistic training with commercial simulators
- Process operation & control
- Input to HAZOP

# 1 Introduction

Integrating dynamic simulation into the chemical engineering curriculum has aroused considerable interest due to the increasing use of simulators in industry for process design, control, training and operational support. Simple dynamic simulation models, implemented in platforms such as Matlab/Simulink, are widely used, and have been used for decades in research and teaching (Luyben 1990), (Stephanopoulos 1984). These models are often idealized and are too often focused exclusively on process control. On the other hand, simulation exercises that use realistic, commercial dynamic simulation software allows students to interact with a realistic simulation of an actual process using a user interface that resembles a plant operator interface. Such a system would prepare students better for industrial practice (Edgar et al. (2006), Wankat (2002)).

Edgar et al. (2006) report extensive use of simulation in control education, especially for graduate courses. Various process examples were given, including distillation columns, chemical reactors, pH processes, microelectronics, and as emerging simulation area, biological processes. The preferred platform for the simulation case studies was Matlab/Simulink, but other commercial simulation packages, such as Hysys, were reported. Wankat (2002) describes use of ASPEN PLUS software for a basic chemical engineering course in separation techniques. The simulator was used for the various laboratory exercises according to a modified problem based learning approach. Jimènez et al. (2002), (2004) have used Hysys.Plant® software for the simulation tasks of a chemical engineering laboratory course. The main objective of the course was to teach process dynamics and control, start up and shut down operations with examples on a continuous distillation process and a batch fermentation process. Jimènez et al. (2004) conclude that the experimentation not only improves students' understanding of theory but also promotes development of soft skills, such as team work and problem solving.

During the last decade virtual laboratories, i.e. web-accessed simulators, have become increasingly popular in chemical engineering education. The main advantage of virtual labs is that students can run the simulations independently on their location, where as many of the commercial simulators lack interactive capabilities and must be used a specific location, i.e. at the university (Martin-Villalba et al. (2008). Klein and Wozny (2006) describe a real laboratory distillation system with a web-based process control system (ABB Freelance 2000$^{TM}$). Fraser et al. (2006) have used web-accessed distillation column model in HYSYS simulation software as an example in the third year chemical engineering course. Rafael et al. (2007)describe a MATLAB-based distillation column model that is used in chemical engineering course for tutorial classes and home studies. In Rasteiro et al. (2009) the future plan of the course on integrating this simulated distillation column with laboratory demonstration column is briefly described. The online functionality is planned with Matlab, Octave and FORTRAN. Martin-Villalba et al. (2008) have combined virtual laboratory platforms Easy Java Simulations and Sysquake with Modelica/Dymola modeling and simulation software. The virtual laboratory was used for control studies on a heat exchanger, a boiler and a batch chemical reactor. Babich and Mavrommatis (2009) discuss the combination of virtual experiments and real laboratory work for an iron-making process course, where the virtual laboratory was implemented using the online Visual simulation Model (VSM) software. A large EU project called Library of Labs (2011) provides various virtual laboratories and remote experiments for physics, mathematics, chemistry, engineering and computer sciences. Chemical engineering virtual laboratories include examples on non-ideal reactors, and process dynamics and control.

The principles and features of commercial dynamic simulators are described in a review by Cameron (2002). Since then, the scale and size of facilities that can be simulated in real-time has grown and realistic simulations of large processing facilities can be run on standard office computers. The commercial simulation tools are characterized by (1) high-fidelity non-ideal models of unit operations, (2) models of the mechanical and thermal dynamics of valves, vessels and piping and (3) detailed emulations of commercial control algorithms. These features allow a modern commercial dynamic simulator to act as a credible replica of a real process. Operating companies routinely use these simulators to train operators and engineers. There is also much to be gained in allowing students to interact with these "virtual plants", especially when the virtual plant can be related to a real pilot plant.

In this article integration of a realistic dynamic simulation into three different chemical engineering courses is presented. The simulation tasks and the three different models running on the D-SPICE and K-Spice family of products are described in detail. The experiences on the commercial dynamic simulation software including both teachers and students feedback are analyzed and discussed.

## 2 Courses, simulation tasks and learning goals (theory)

### *2.1 Undergraduate Coursework: Basics in chemical engineering at Oslo University College*

The course is the first basic course in chemical engineering for BSc level students, giving 15 ECTS credit points. The topics of the course covers heat transfer, mass transfer and unit operations. Dynamic simulation is used for both binary distillation and three phase separation, in this article the details of the binary distillation module are described. The formal part of the distillation module consists of classroom lectures (7h), classroom exercises (7h), introduction to dynamic simulation (2h), simulation exercises (6 h), and laboratory experiment with prerequisites and reporting (16 h).

The learning goals of the distillation simulation exercises include (i) ability to use the software for simple case scenarios, (ii) insight into the dynamic operation of a distillation column and how the changes in the manipulated variables affects the controlled variables, and (iii) ability optimize the distillation sequence, i.e. the values of the manipulated variables that would give highest yield in the distillate.

The simulation sessions (à 2h), led by the teacher, were arranged for groups of 8 students. Every student had their own PC, but they were obliged to work in teams of two students in order to support each other and to engage into discussion about the results. A short introduction lecture to dynamic simulation with D-SPICE software was given prior the exercises. In order to ensure correct operation of the D-SPICE simulation model, the main functionalities of the simulator were demonstrated using whiteboard and projector, while the students repeated the same simulator commands on the classroom computers.

The model was ready-configured, so the students were only running the model, changing the manipulated variables and observing the simulated process behavior. Each simulation scenario was to be started from the given initial condition, and the input variables, including feed pump speed, feed temperature, reboiler heater power and reflux ratio, were to be changed one at the time.

The first task was to observe on the temperature and concentration profile trends along the distillation column, and the distillate concentration and flowrate during input variable changes, given in Table 1. Based on experiences from task 1 and the distillation theory, an optimal combination of these variables was to be chosen in order to maximize the volume flow rate times concentration in the distillate in task 2, given in Table 2. Testing of two different combinations was the formal minimum requirement. The simulation results were to be used for the design of an optimal distillation sequence for the laboratory experiment. In order to motivate the students to put a lot of effort to the simulation and to the laboratory experiment, a competition was arranged. The group achieving maximum yield in the distillate was to be granted with 10% extra points to the laboratory report.

### *2.2 Graduate Coursework: Using dynamic simulations to perform operability and safety analysis in offshore oil and gas industries (Technical University of Denmark)*

The course is a special course intended for MSc level students interested in more knowledge and practical experiences within the fields of process design, process operation, safety and risk assessment in oil & gas industry. The course learning objectives include (i) the ability to design a small part of an offshore process including valve and equipment sizing, (ii) configure a small part of offshore process in K-Spice® software and perform dynamic simulations of normal process operation, (iii) perform failure mode effect analysis, (iv) synthesize the results of failure mode and effect analysis to be used as input to the extended HAZOP analysis of the designed process part.

The workload of the course can be tailored depending on different degrees of learning objectives student's wishes to achieve and between 15 ECTS to 30 ECTS in which case the project becomes an MSc project with the added challenge of independently performing a research work as well as participating in an industrial HAZOP review study. The simulation tasks involved in this course are summarized in Table 3.

### *2.3 Undergraduate/ Graduate Coursework: Process control at Aston University*

Process control at Aston is taught within the Chemical Engineering degree course which can be taken to either Bachelor or Masters level (three or four years respectively).

The dynamic simulation forms a part of the work within modules for the teaching of process control. The use of the simulation contributes to the formal goal of understanding of the operation of a process control loop with different types of control strategies. In the second year course, the learning goals include (i) on/off and modulated feedback control, and (ii) different forms of cascade and feed-forward control. In the third year course, the learning goals include (iii) advanced control focusing on control systems design as part of wider design studies.

Dynamic simulation is used as teaching tool in two ways. It is introduced into classroom teaching where the tutor uses it to demonstrate features of controller behavior, and it is used in tutorials where each student can run the program and explore the models. These tutorials are supported by the tutor and the students have access to printed and online versions of a comprehensive manual which introduces both the simulation software, D-SPICE, and the particular model. The two tank model has been used now for several years as a part of the teaching of process control. The principles of the two tank process will be familiar to the course participants as they have already done a project which involves construction and operation of a similar process. There is no access to vary the models other than to change parameters and open and close the valves.

Examples of the simulation tasks are given in Table 4 . The tutorial course is assessed with a class test where each student has to run the model and answer questions about the performance of a set of tasks. The assessment tasks involve running the simulation, documenting results and commenting where appropriate on the behavior of the simulation. This is done in an open book environment.

## 3 Simulator software and models (materials and methods)

The simulation software used for the courses is D-SPICE and K-Spice. These are simultaneous-modular dynamic simulation software tools provided by Kongsberg Oil and Gas Technologies (2011). D-SPICE is a legacy product, whereas K-Spice is a currently marketed tool that builds on the D-SPICE technology. Dynamic simulation models were implemented using standard D-SPICE or K-Spice modules. All the necessary modules are implemented and combined into a *pressure-flow network* according to the process flow sheet. Each module calculates either flow or pressure. Mathematically, this network consists of non-linear algebraic equations of flow pressure relations and mainly linear differential mass balance equations of node pressures. These equations are discretized implicitly to form a set of algebraic equations. These are then solved simultaneously using a multi-dimensional Newton-Raphson method that is based on the mass balance for each pressure-calculating module. D-SPICE and K-Spice both use simplified local models for all thermodynamic calculations, so that the simulator can run quickly. The regression coefficients and table data for these models are generated automatically from more rigorous thermodynamic packages. K-Spice also allows direct calls to a rigorous thermodynamic package.

K-Spice and D-SPICE both use a client-server architecture. This allows a variety of computer arrangements for teaching. For example, a training lab may be implemented where every student works on the same process model from their own computer. Alternatively, each student can run their own model as a separate server process, either on their own computer, or on a common server.

The dynamic simulator is designed to be able to connect to third-party systems, such as control systems and databases. The normal approach connecting to and from the simulator uses OPC communication protocols. Custom drivers for instrumentation and control systems can also be used. The simulator implements both OPC clients and servers. The client is used to connect the simulator to plant data, whereas the server allows data to be sent to external tools, such as Excel and Matlab.

### *3.1 Model 1: Binary distillation*

The distillation model is based on the laboratory distillation column system UOP3CC produced by Armfield Ltd. The laboratory distillation system, and the simulation model, includes isolated column with eight (8) sieve trays, a reboiler tank, condenser, automatic reflux valve, thermocouple wells, manual valves, feed and product tanks, feed pump, feed heater and other column accessories. An overview of the distillation model is presented in Figure 1. The model is described in detail in Komulainen et al. (2010).

The initial condition of the model is continuous distillation of water-ethanol mixture (25 mass%) conducted at atmospheric pressure. The D-SPICE model allows manipulation and observation of hundreds of variables. For the basic chemical engineering course, the manipulated variables were feed pump speed, feed temperature, reboiler heater power and reflux ratio. The observed variables were temperature and ethanol concentration in the vapour and liquid phase on the sieve plates, and the flow rate and the ethanol concentration in the distillate stream and the bottoms product stream. The goal of the simulation tasks in the basic course was to maximize the mass flow of ethanol into the distillate tank by changing the manipulated variables within the given limits.

### *3.2 Model 2: Offshore three-phase separation process*

Three-phase (V/L/L) separation process is commonly used in offshore oil and gas industry to separate the mixture of crude, water and gas stream. The separation system studied consists of two feed streams containing a mixture of oil, water and gas flows. Both streams had flow rate of 3600 kg/h, pressure of 56 bar and temperature of 50°C. The streams consisted of the following components: methane, ethane, propane, butane, nitrogen, carbon dioxide, isobutene, pentane, isopentane, hexane, water, MEG, methanol and four pseudo components.

The streams are mixed before entering the separator unit at which the mixture is separated into three streams: water, oil and gas respectively, due to differences in density. The separator is protected by a pressure relief valve. The gas stream passes to a compressor to increase the pressure of the export gas. At the discharge side of the compressor a heat exchanger with water as cooling fluid is installed. An anti-surge controller loop is installed to protect the compressor from surging. The mathematical model is based on the three conservation equations of momentum, energy and mass together with the Soave-Redlich-Kwong equation of state as the thermodynamic model, as described in Cameron et al. (2002). The implementation of the three phase separation system in K-Spice® is shown in Figure 2. Sizing of the valves including calculation of the valve characteristics are based on Crane (1999).

The simulation methodology used for operability and safety analysis of this three phase separator system is referred to Enemark-Rasmussen (2011), which uses a combination of failure mode effect analysis (FMEA) and HAZOP procedure described by Skelton (1997). The methodology generates systematically failure scenarios by considering process equipment and pre-defined failure modes utilizing the build in functions of the K-Spice® software.

The results generated by the simulation of failure scenarios are recorded in a worksheet. Thereafter the failure scenarios are ranked by critical process parameters using quantitative sensitivity measure. The sensitivity measure, SA, is calculated numerically (Sin et al. (2010)) as shown in Eq 1 in which $SA_{ij}$ refers to the sensitivity measure of critical process parameter $y_j$ to the failure in jth equipment, $\theta_j$ . $\Delta\theta_i$ is the equipment deviation from the reference state, and f() is the dynamic model of the system:

$$SA_{ij} : \frac{\Delta y_i}{\Delta \theta_j} = \frac{f(\theta_j + \Delta\theta_j) - f(\theta_j)}{\Delta \theta_j} \Lambda \frac{f(\theta_j) - f(\theta_j - \Delta\theta_j)}{\Delta \theta_j} \quad (1)$$

### 3.3 Model 3: Two tank model with different control strategies

The two tank D-SPICE model consists of two tanks connected by flows of water, down by gravity through a valve and up through a pump and control valve, as presented in Figure 3. The main purpose of the two tank model is the teaching of process control, thus there are four versions with different control strategies; on/off feedback control, modulated feedback control, cascade control and feed-forward control. The two tank models with different control strategies can be run simultaneously, which enables the students to focus on one of control strategy at a time and/ or to compare them.

In the models, the downward flow is regulated by a manual valve which is used as the disturbance. The aim of the control is to maintain constant level in the upper tank and the set point can be changed. Changes in these two values can be used to test the performance of the controllers, with different values of the controller parameters, which can also be changed. This provides a way in which the students can be given a wide range of different exercises to gain understanding of good and bad controller performance.

In the feed-forward controller model the disturbance is measured and this is added to the output from the feedback controller on the measurement of the upper tank level. The addition is done in the gain-parameter of the Gain Relay-module. This signal is the input to a cascade controller sending a signal to the control valve. Using this model it is possible to turn on and off the two signals and to study a range of different problems including integral windup and feed-forward response, as shown in Figure 4.

# 4 Results of the simulation modules

## *4.1 Undergraduate Coursework: Dynamic simulation of distillation*

The simulation module was evaluated by 20 students twice, after completed simulation tasks and after completed laboratory experiment. A formal multiple-choice questionnaire including a total of 72 statements was used. Most of the students did not consider themselves very experienced with mathematical tools such as Matlab or Mathematica, although utilization of these tools is part of the mathematics course. Thus, beginning with a simulation tool was new for almost all of the students and after the simulation module half of the students considered D-SPICE easy to use and were comfortable using the tool alone. However, 90% of the students liked using D-SPICE, stated that utilization was a good idea and recommended it as a suitable tool for the chemical engineering course. There was only one teacher for the simulation course, but 82% of the students stated that availability of the resources was sufficient.

Most of the students agreed that simulation enhances understanding of theory and makes learning more interesting. "Simulation enhanced my learning" was agreed by 95% of the students. About 80% of the students intended to use the simulation results for the design of the distillation sequence, but only 60% used the results. However, 80% of the students agreed that the experiences gained by simulation were useful in the lab. Majority of the students were interested in having an online simulator in the lab to enable continuous monitoring of the concentrations.

The teacher has a few years experience with the software, which is an advantage when organizing the course without additional teaching resources. The teacher reports very positive learning environment, the students were fast to adapt to use the simulation tool and group size up to 10 students was manageable due to successful team work. The positive effect of the simulation was noticed also in the distillation laboratory: experiment was carried out by enthusiastic student and the two most successful groups were the ones that spent most time with the simulations.

The learning outcome of the simulation part was measured by a mid-term multiple choice exam and the formal final exam, measuring the understanding of process dynamics and causalities in continuous distillation, such as actions that would increase ethanol yield in the distillate. The mid-term average result on simulation was 52%. In the final exam the average result of the first simulation task was 77 %, and the average result of the second simulation task was 62%. Compared to the average of the whole exam 56%, performance with simulation tasks was better compared to the traditional calculation tasks.

### *4.2 Graduate Coursework: Dynamic simulations to perform failure mode and effect analysis of three phase separation process*

With two days of introduction to the software the student was able to configure and implement the process model in K-Spice ® using steady-state mass and energy balances as input information. The outcome of the simulation depends of the selection of watch points, which is a functionality in K-Spice® software that allows the user to follow the changes in any process variable at multiple positions in the process. A watch point is the selection of one unit of equipment in the model where one of the critical process variables is added to e.g. a pressure-time graph. This is demonstrated in Figure 5 where the pressure and flow at five different positions is monitored. The positions are at the compressor (23KA0001), the gas production pipe (pf_25ES0005), the oil production pipe (pf_23LV0002), the cooling fluid pipe outlet (pf_23TV0001) and the recycle pipe (pf_23UV0001).

Generation and dynamic simulation of failure scenarios allows the user to follow the changes in the critical process variables when a failure scenario is introduced in an equipment. The analysis was carried out following the steps described in Table 3. The list of failure scenarios generated is given in Table 5. As an example from the simulation analysis, in Figure 6 the failure scenario of the anti-surge valve with the equipment deviation fully closed is shown. At time equal to 30 minute mark, the failure is induced. As expected, in the top left graph a pressure drop can be observed immediately as well a temperature increase that is given in the bottom left graph. The equipment with a deviation attached is marked by a red square, in this case the anti-surge valve.

In Table 6 the three highest ranked failure scenarios are presented which corresponds to different types of transmitter failing either high or low. The values highlighted in the table are the most severe changes having different consequences such as compressor surging, fluid in the gas line, temperature increase at production output pipe lines by a factor five among others. The normal operation values and the failure scenario values are listed for the critical process parameters such as temperature, flow and pressure at the chosen watch points as demonstrated in Figure 5.

### *4.3 Undergraduate/ Graduate Coursework: Process control*

The students take modules which use the dynamic simulation in both year 3 and year 4 of the course. This is students' first encounter with dynamic simulation that follows on from a module on steady state chemical process simulation, where they have been using Aspen to model chemical plants. They are thus already familiar with the tutorial style and to work together to share understanding of the simulation scenarios.

No formal study has been made of their attitude to the model, but informal feedback has been good over a number of years. In both 3$^{rd}$ and 4$^{th}$ year classes the results of the test show a good understanding of the test tasks. There is good response to the manuals which contain a lot of screen shots of the simulation. Experience with the two tank D-SPICE model has been good in that students of all levels of ability can use it to gain confidence. Students take to the simulation tool very well and use of it leads to a lot of conversations with the students about their understanding of process control.

# 5 Discussion

## *5.1 Undergraduate Coursework: Dynamic simulation of distillation*

The simulation tasks were run on a ready-configured model and required no previous simulation skills. The student evaluations indicate that more time should be spent on the introduction of the dynamic simulator functionalities and interpretation of the simulation results. In future, the first simulation lectures and exercises will be given earlier in the semester, using a basic tutorial model (model 2). The introductory material will be further developed to include more examples on interpretation of the dynamic trends and a complete solutions manual.

These improvements should help also with the understanding of process dynamics, which one of the main reasons for the lower scores in the mid-term multiple choice exam. Process dynamics is not explained in the course book and learning was based on one lecture and the simulation exercises. Introducing a few classroom exercises on process dynamics of distillation before the distillation simulation exercises could improve the learning results. The exam results were better than the mid-term exam results, which could be due to further learning in the laboratory and in the second simulation module on separation (model 2).

## *5.2 Graduate Coursework: Using K-Spice® in performing dynamic simulations to support operability and safety analysis in offshore oil and gas industry*

The dynamic simulation methodology for operability and safety analysis was easily implemented in the K-Spice® as the software allows evaluation of many equipment deviations.

The result from the dynamic simulation methodology offers many features that improve the teaching of safety and operability analysis compared to traditional FMEA or conventional HAZOP methodology. The students can explore different failure scenarios and their significance. This information can also help remove failure scenarios from the analysis during HAZOP meeting (the basis for further refining the scope could be achieved by eliminating failure scenarios that have zero sensitivity measure on critical process parameters implying no impact or removing redundant failures due to same cause or consequences). Hence the dynamic simulations here can complement the traditional methods of teaching operability issues and safety analysis. Suggestion for improving safety can also be analyzed using dynamic simulations which offer a refinement and quality check on the qualitative reasoning of HAZOP and FMEA type of analysis methods.

### *5.3 Undergraduate/ Graduate Coursework: Process control*

The two tank model used is a good tool for introducing students to process control with a single feedback loop. The most advanced version of the model allows for feed-forward as well as feedback and this permits a range of interesting effects to be demonstrated. With the current license, the arrangement is limited in that there is no capacity to extend the model and it would be good to be able to demonstrate more advanced problems such as the interaction of control loops. Within the limitations of what is available, the students gain a lot of understanding of how control parameters affect the outcome of control actions. The model forms a small but valuable part of the teaching of process control to undergraduate chemical engineers.

## 6 Conclusions

This article presents successful integration of dynamic simulation into the chemical engineering curricula in both undergraduate and graduate courses. The experiences on dynamic simulation on the three undergraduate and graduate courses have been positive for both students and teachers.

The simulation tasks were designed to meet the learning goals of the courses using three different models implemented in D-SPICE and K-Spice® software. Note that these simulation exercises can be given as individual or group tasks, and they could be applied using other commercial dynamic simulation software. The simulation software has proven to be user friendly and students of all levels of ability have been able to benefit from the simulation tasks. Working with simulation has increased communication and co-operation between the students, which is an important pedagogical aspect that enhances learning.

Dynamic simulation was found to be very useful teaching tool for a wide range of chemical engineering courses. The simulation software enables demonstration and testing of different kind of processes and equipment, control algorithms and safety procedures. Test runs with the simulation model prior to laboratory experiments give insight to the selection of optimal process parameters and help understanding practical operation of complex chemical processes. The dynamic simulation studies prior to the HAZOP meetings improve the accuracy of the outcome recommendations, reduce the time needed to carry out safety analysis by better focusing the HAZOP/HAZID meetings, improve design of the process and the possibility for onsite analysis of design changes in view of process safety.

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## Figures

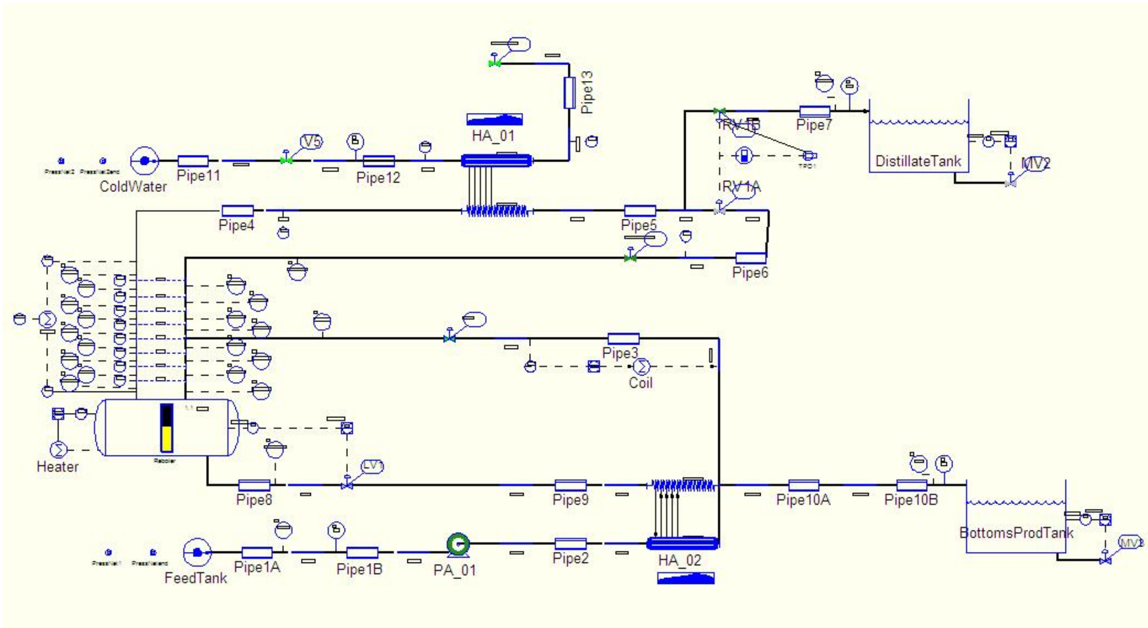


**Figure 1: D-SPICE model of the Armfield UOP3CC distillation system.**

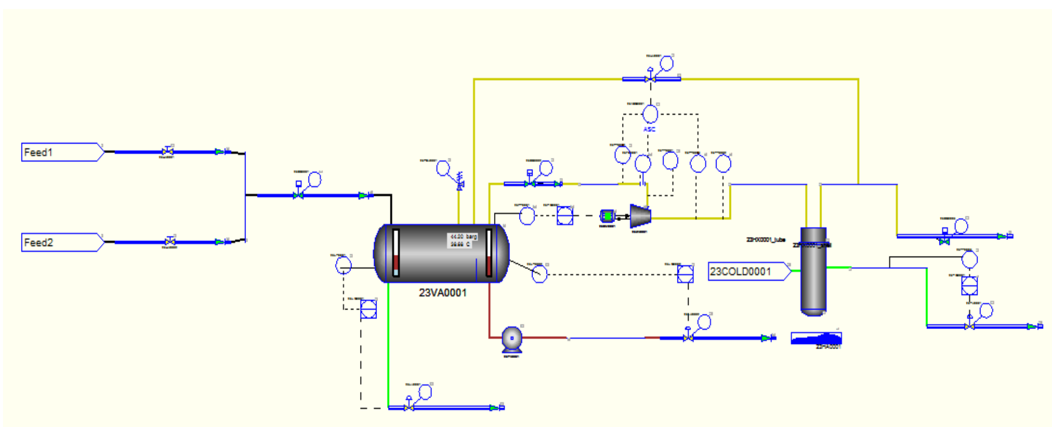


**Figure 2: Three phase separator case study implemented in K-Spice®**

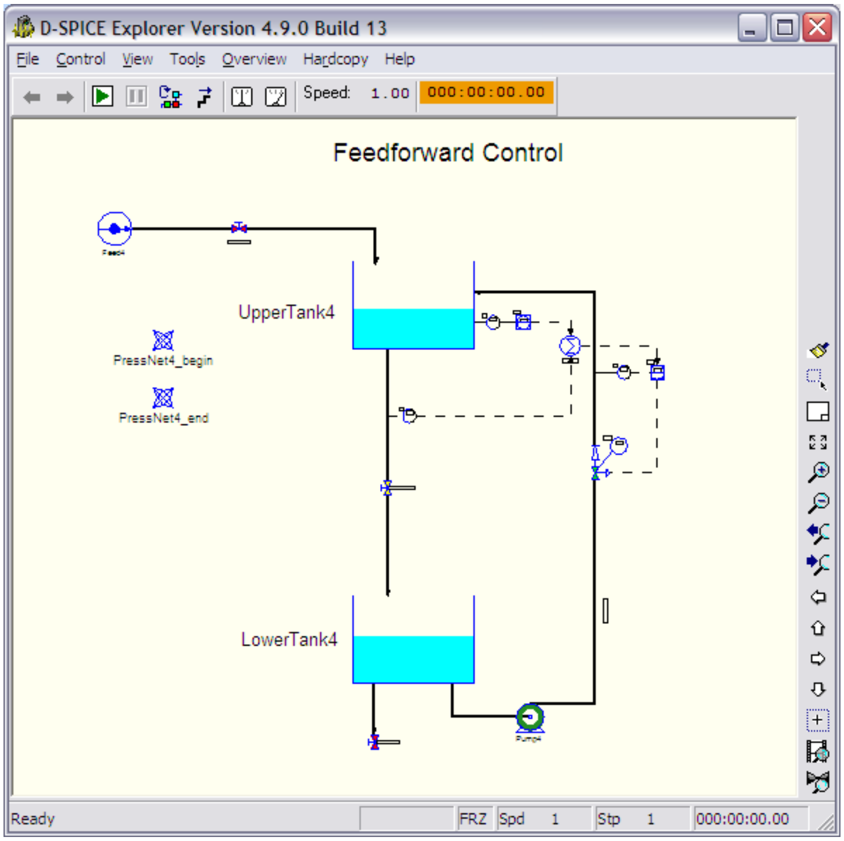


Figure 3: Example of Feed-forward control model.

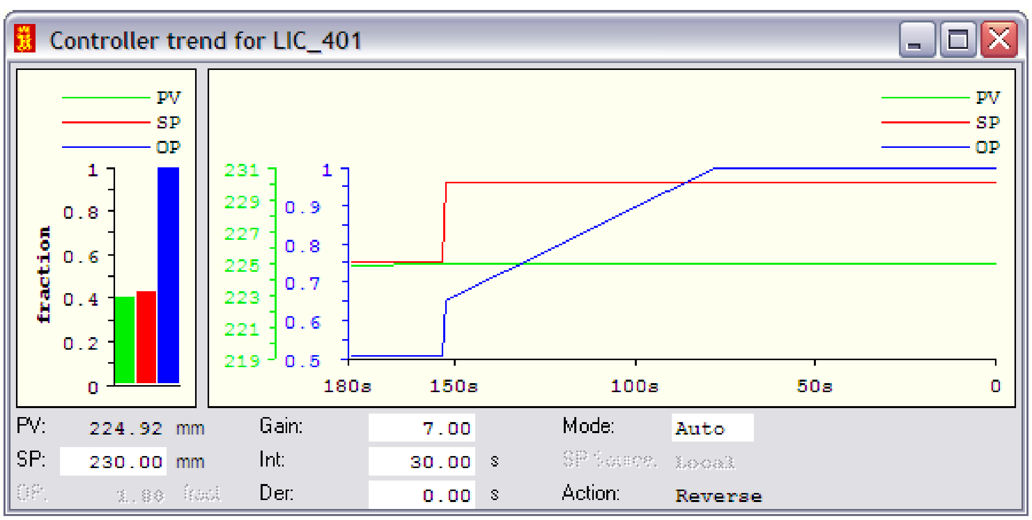


**Figure 4:** Example of integral windup response to a setpoint change – zero gain for feedback signal.

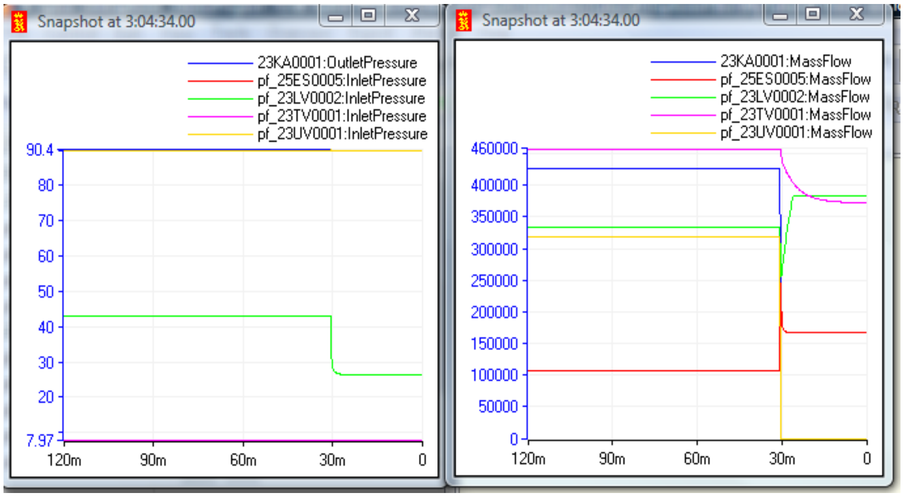


**Figure 5: Pressure and flow watch points for the three phase separator model.**

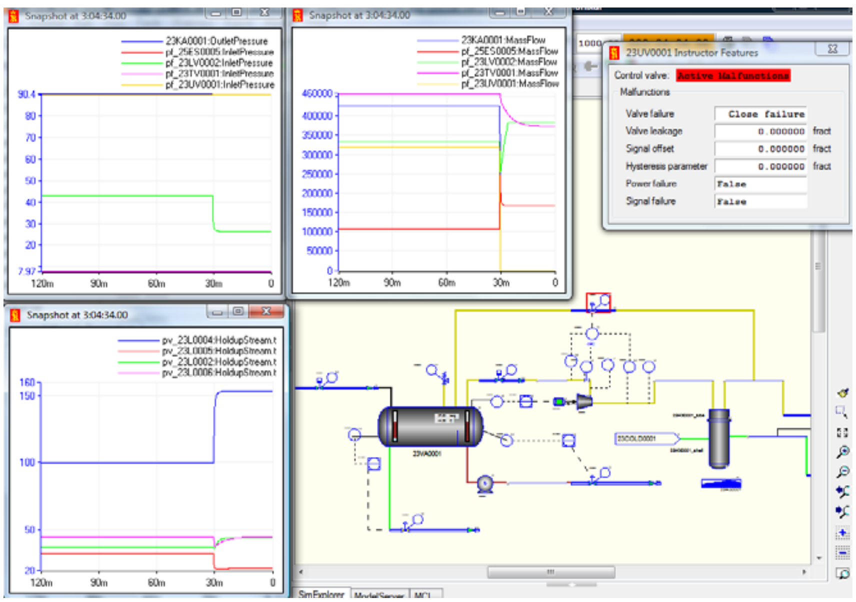


**Figure 6: Dynamic simulation of failure scenario in three phase separation process: Anti surge valve fully closed**

**Tables**

**Table 1: Simulation task 1 for the distillation column model; Make changes in the input variables and observe responses on the output variables one at the time. Start each simulation from the given initial condition.**

| No. | Change in | Temperature profile in the column | Ethanol concentration profile (vapour) in the column | Ethanol concentration profile (liquid) in the column | Distillate concentration | Distillate flow rate |
|---|---|---|---|---|---|---|
| 1 | Inlet flowrate PA_01:speed | | | | | |
| 2 | Heater power TIC09:SP | | | | | |
| 3 | Inlet temperature TIC21:SP | | | | | |
| 4 | Reflux ratio TP01:ontime TP01:offtime | | | | | |

**Table 2: Simulation task 2 for the distillation column model; Design two distillation sequences that combine the input changes, and observe responses on the output variables. Start each simulation sequence from the given initial condition.**

| Seq. | Time [min] | Action | Temperature profile in the column | Ethanol concentration profile (vapour) in the column | Ethanol concentration profile (liquid) in the column | Distillate concentration | Distillate flow rate |
|---|---|---|---|---|---|---|---|
| 1 | 0<br>5<br>15<br>120 | Start sim.<br>Change1&2<br>Change3&4<br>Stop sim. | | | | | |
| 2 | 0<br>10<br>120 | Start sim.<br>Change5&6&7<br>Stop sim. | | | | | |

**Table 3: Simulation tasks involved in three phase separator in offshore oil and gas industry: build a model for the physical system, identify the equipments, generate failure scenario, simulate, evaluate and rank the failure scenarios to provide scope for HAZOP studies**

| Task | Description |
|---|---|
| Step 1. Physical system & Model building | Understand the physical system and collect data if needed. Build the model of the system in the software in this case in K-Spice® using appropriate design data and mass balances. If design data is not delivered then these are calculated using mass and energy balances. |
| Step 2. List the equipments | Generate a list of equipment in the process model using the build-in function of the K-Spice® software. |
| Step 3. Define a failure scenario | Define a failure scenario by selecting an equipment from the list (step 2) and assigning a failure mode (see Table 3). This will generate a number of failure scenarios as input to step 4. E.g. valve x fail to close meaning plus or minus 0-100% change from the reference state of the equipment. |
| Step 4: Perform simulations | Perform dynamic simulation of the failure scenario by giving a numerical value for each failed equipment (e.g. to simulate the effect of a certain valve x failed to close, one can simulate a certain deviation from the reference state of the valve position). See Figure 7 below for an example. |
| Step 5: record results& calculate sensitivity measure | Record the results from the dynamic simulation in a worksheet and iterate from step 3 until all equipment in the generated list is covered. Calculate the sensitivity measure of the critical process parameter to equipment deviation in each failure scenario. |
| Step 6: Rank failure scenarios and provide a scope to HAZOP | Summarize and rank the failure scenarios according to the the sensitivity measure. Based on the ranking identify the important equipments and critical process parameters as input to HAZOP studies. |

**Table 4: Examples on the process control tasks.**

| Task | Description |
|---|---|
| On-off control | Become familiar with the operation of the simulation.<br><br>Vary controller setpoint, and monitor how this affects the setpoint tracking with the chosen controller parameters.<br><br>Vary the disturbance variable (output flow) and monitor controller performance including failure to control when output |
| Regulatory control | Monitor the controller behaviour in response to set point and disturbance variable changes. Change controller parameters and repeat the changes in set point and disturbance variables. |
| Cascade control | As for regulatory control, but now make changes to both sets of controller parameters. Observe the effect for set point and disturbance changes. |
| Feed-forward control | As for cascade control, plus demonstration of the effect of feed-forward of a measurement of the disturbance to reduce the effect of disturbance changes. Remove the link from feedback and demonstrate integral windup (See Figure 4). |

**Table 5: Predefined deviations or failure modes for process equipment to generate failure scenarios as input to K-Spice®**

| **Equipment** | **Failure modes** | **Failure modes for failure scenario generation** |
|---|---|---|
| Valve | closed/open | Valve fully closed/open |
| Pipe | plugging low/high | Pipe plugging low/high |
| Compressor | Motor power fail | Compressor motor power fail |
| Compressor | Deterioration | Compressor deterioration |
| Transmitter(s) | fail high/low | Transmitter fail high/low |
| Anti-surge controller | fail high/low | Anti-surge controller fail high/low |
| Heat exchanger | fouling high/low | Heat exchanger fouling high/low |
| Pipe | rupture | Pipe rupture |
| Power | failure | Power failure |
| Pump | Wear | Pump wearing |

Table 6: Summary of failure scenarios ranked by sensitivity measurement

| Scenario j = 1...N | Failure scenario: Failure mode $f_i$ | Parameter value: Normal operation | Parameter value: Failure value | $y_i$ | Process parameters: T [°C] | u [kg/h] | P [barg] | Sensitivity Measurement (SA): $\frac{\Delta T}{\Delta \theta}$ | $\frac{\Delta u}{\Delta \theta}$ | $\frac{\Delta P}{\Delta \theta}$ | Consequences |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Normal operation value / Failure value | | | | | | |
| 26 | Transmitter 23PT0002 Fail high | 0,71 | 1 | Compressor | 99,9 | 426959 | 90 | 183,10 | -894.352 | 0,00 | Compressor surging |
| | | | | | 153 | 167597 | 90 | | | | |
| | | 0,71 | 1 | Export gas | 32,6 | 107422 | 90 | -36,89 | 207500 | 0,00 | Export valve fully open. Oil builds up separator. |
| | | | | | 21,9 | 167597 | 90 | | | | |
| | | 0,71 | 1 | Cooling water outlet | 45 | 458503 | 7,97 | 0,00 | -293.217 | 0,035 | |
| | | | | | 45 | 373470 | 7,98 | | | | |
| | | 0,71 | 1 | Export oil | 37,4 | 333980 | 43,3 | 23,44 | 178.689 | -57,59 | |
| | | | | | 44,2 | 385800 | 26,6 | | | | |
| | | 0,71 | 1 | Anti-surge loop | 32,6 | 319537 | 90 | - 112,41 | - 1.101.851 | - 310,35 | After 1h22m overflow at separator. Oil entering the gas line. |
| | | | | | 0 | 0 | 0 | | | | |
| 29 | Transmitter 23TT0003fail low | 0,3 | 0 | Compressor | 99,9 | 426959 | 90 | - 180,66 | 133.530 | 0,00 | Increase in export gas temperature by a factor 5. For export oil the increase in temperature is by a factor 2. |
| | | | | | 154,1 | 386900 | 90 | | | | |
| | | 0,3 | 0 | Export gas | 32,6 | 107422 | 90 | - 404,66 | -88.466 | 0,00 | |
| | | | | | 154 | 133962 | 90 | | | | |
| | | 0,3 | 0 | Cooling water outlet | 45 | 458503 | 7,97 | 150 | 1.528.343 | 26,57 | |
| | | | | | 0 | 0 | 0 | | | | |
| | | 0,3 | 0 | Export oil | 37,4 | 333980 | 43,3 | - 101,33 | 76.730 | 0,33 | |
| | | | | | 67,8 | 310961 | 43,2 | | | | |
| | | 0,3 | 0 | Anti-surge loop | 32,6 | 319537 | 90 | - 404,66 | 222.000 | 0,00 | |
| | | | | | 154 | 252937 | 90 | | | | |
| 33 | Transmitter 23LT0002 Fail low | 0,44 | 0 | Compressor | 99,9 | 426959 | 90 | 117,04 | - 2.314.397 | -2,05 | Increase power consumption |
| | | | | | 48,4 | 1445294 | 90,9 | | | | |
| | | 0,44 | 0 | Export gas | 32,6 | 107422 | 90 | 12,95 | -879.879 | 0,00 | |
| | | | | | 26,9 | 494569 | 90 | | | | |
| | | 0,44 | 0 | Cooling water outlet | 45 | 458503 | 7,97 | -5,68 | -339.856 | 0,023 | |
| | | | | | 47,5 | 608040 | 7,96 | | | | |
| | | 0,44 | 0 | Export oil | 37,4 | 333980 | 43,3 | 85 | 759.045 | 98,40 | Overflow at separator. Oil in gas outlet |
| | | | | | 0 | 0 | 0 | | | | |
| | | 0,44 | 0 | Anti-surge loop | 32,6 | 319537 | 90 | 12,95 | - 1.434.515 | 0,00 | |
| | | | | | 26,9 | 950724 | 90 | | | | |