Izopropil-alkohol előállító üzem operátor tréning szimulátorának megalkotása

Development of operator training simulator for isopropyl alcohol producing plant

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Summary

In this study an operator training simulator was developed for isopropyl-alcohol producing plant. The product of this plant is isopropyl alcohol - water azeotrope, by-product is diisopropyl ether which are formed by direct hydrolyzation of propylene via strong acid cation exchange resins. At first the plant was designed using a stationary process simulator. Honeywell's UniSim® Design was used for it and further works. The next step was the development of the dynamic simulator and the control system. Data for this simulator was provided by the stationary simulator. The dynamic simulator contains the preheater subsystems and the reaction subsystem. Finally, an operator screen was developed and connected to the dynamic simulator via UniSim Excel Interface Tool. This operator training simulator could be used for analysis and optimization moreover it also might be used in education.

Összefoglaló

Munkánk során egy izopropil-alkohol előállító üzem operátor tréning szimulátorát alkottuk meg. A tervezett üzemben propilén közvetlen hidratálása történik erősen savas kationcserélő gyanta katalizátor jelenlétében; főterméke izopropil-alkohol – víz azeotróp, míg a kísérőterméke diizopropil-éter. Az első lépésként az üzemet terveztük meg annak stacioner szimulátorával, melyhez a Honeywell UniSim® Design szimulátorát használtuk. A következő lépésben a stacioner szimulátor által szolgáltatott adatok segítségével leképeztük a dinamikus szimulátort, mely tartalmazza az előmelegítő és a reakciós alrendszereket, valamint az irányítórendszert. Végsősoron pedig az operátori képernyőt képeztük le, és UniSim Excel Interface Tool segítségével össze tudtuk kapcsolni a képernyőt a szimulátorral. Az így kapott operátor tréning szimulátor alkalmas analízisek és optimalizálási feladatok elvégzésére, továbbá alkalmas lehet az oktatásban történő használatra.

Introduction

In the chemical industry and many other industries process simulators are increasingly used, due to their versatile application. These are such model based programs which could be used for design technologies, development, analysis and optimization. Due to the precise reproduction of the plants these simulators have to use such models which based on reliable physical phenomena including transfer processes, thermodynamics, reaction kinetics, etc. Moreover, the simulator is composed of basic operation units – valves, vessels, pumps, heat exchangers, etc. – in combination with the suitable fluid package – to determinate the state equations for calculations of the physical and thermodynamic properties [1, 2].

The control of a chemical technologies needs such professionals who have got the proper experience. It is estimated that billion dollars are lost annually in the process industry due to operator errors made during hazardous situations. The operator training simulators (OTS) can be used for training the operators, prepare them to control the technology and solve different problems via simulations. These simulators contain the dynamic simulator of the process and the distributed control system (DCS) connected to an operator screen. This screen is used as interface of these programs, which is the same as the plant's but these are linked with process simulators instead of real technologies. Operators could get enough experience training on these simulators to control the technology safely and effectively [3, 4].

The OTS are computer aided practicing and developing systems which contains the dynamic simulator of the technology and the controlling system furthermore the operator screen. Beginner operators and engineers can be trained using OTS instead of interfering the plant. Moreover, they can be used for optimization, analysis and development of the technology as engineering tasks [4].

There are two kind of OTS's: stimulation and emulation OTS. The first is plant specified, which means the operator screen of the OTS is the same as the plant's. It might be used to train beginner operators. The emulation OTS is technology specified and can be used by engineers. The advantage of this kind OTS needs fewer resources than the stimulation one. This is due to the simulator of the control system is integrated to the process simulator [3 ,4].

The isopropyl alcohol (IPA) is a widely-used solvent, detergent and disinfectant. It is also used as intermedia in pharmacology and acetone producing. The most common technology for IPA production is the hydrolyzation of propylene. At the beginning sulphuric acid was used as catalyst, but nowadays the direct hydrolyzation is preferred due to the lower environmental polluting effect. The catalysts of these reactions are acidic component which are bounded to solid support such as phosphoric acid, silico tungstic acid or strong acid cation exchange resins. Two main reactions (1-2.) can be wright down the formation of the product and the by-product which is diisopropyl ether (DIPE) [5].

$$\mathrm{CH_2 = CH - CH_3 \ + \ H_2O \overset{K_1}{\Leftrightarrow} \ (CH_3)_2CH - OH} \tag{1}$$

$$2\,\mathrm{(CH_3)_2CH - OH} \overset{K_2}{\Leftrightarrow} \ \mathrm{[(CH_3)_2CH]_2O + H_2}O \tag{2}$$

The equilibrium constants of these reactions were described with Arrhenius-type equations (3-4.) [6].

$$\mathrm{K_1} = 5.29 \cdot 10^{-6} \cdot \exp\left(-\frac{55.0}{R \cdot T}\right) \tag{3}$$

$$\mathrm{K_2} = 8.55 \cdot 10^{-2} \cdot \exp\left(-\frac{10.8}{R \cdot T}\right) \tag{4}$$

These equilibrium reactions might be shifted in the direction of the product with applying higher temperature and pressure, moreover acidic catalyst. The sample for our work was the Deutsche Texaco technology. The reason of the decision was that direct hydrolyzation is applied, furthermore the use of special construction material is not justified due to the reaction condition is not extreme (130-160 °C and 8-10 MPa). The conversion (0.75) and the selectivity (0.92-0.94) is also acceptable [5].

Development of OTS

To create an OTS, dynamic simulator of process and control system is necessary as long as the operator screen. At first, we had to get the plant data, due to lack of this we developed a stationary simulator to estimate them for the dynamic simulator. In this study an emulation OTS was developed so the control system is integrated to the process simulator. The final step is the creating the operator screen and the connection of it to the process simulator.

Stationary process simulator

The plant processes 600 kmol per hour propylene. The feed is propylene with 92% (mol percentage) purity because of the propane content and the and water (100% purity). The pressure of the hydrocarbon feed is 15 bar and its temperature is 25 °C. The pressure of the water feed is 3 bar and its temperature is 25 °C. The reactor pressure 80 bar, the temperature is 160 °C. The water-propylene mass rate in the reactor is 14:1, with 0.8 h^{-1} LHSV. A separator is applied to recover the unreacted hydrocarbons from the reaction mixture. A part of it shall be blowed-down, another part shall be recirculated. Most of the water is separated from the liquid phase of the mixture in the first distillation column. In the second distillation column, the product is separated from the by-product. The main product of this plant is IPA azeotrope, the by-product is DIPE-rich fraction. The process of the technology is shown in the block diagram below (Fig.1).

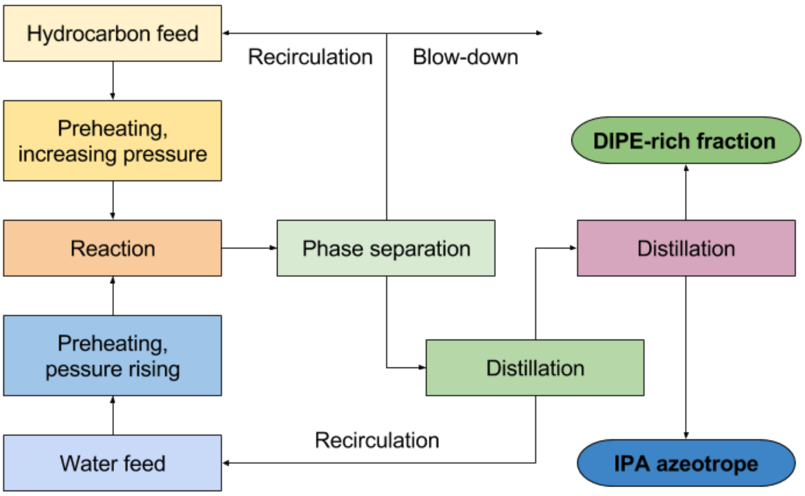

Figure 1. The block diagram of the IPA azeotrope producing process.

Honeywell's UniSim® Design was used to develop this technology to a stationary simulator. This is an intuitive process modeling software that helps engineers create steady-state and dynamic models for plant design, performance monitoring, troubleshooting, business planning, and asset management [2].

Dynamic process simulator

The dynamic simulator was developed simultaneously with the control system for the preheaters and the reaction subsystems. In every case PI controllers were applied which were tuned with the built-in Auto Tuner. However, is some cases manual tuning was necessary for the optimal working of the controllers. The process flow diagram of the dynamic simulator with the controlling system is shown below (Fig.2). In this simulator, we applied controllers for mass flow, pressure, temperature, vessel liquid level.

This dynamic simulator is also suitable for analysis and optimizing the technology. However, using a unique operator screen might be made the work more convenient. For example, Users should switch between many windows during their work, moreover the evaluation of the result could be complicated.

Operator screen

The operator screens (OS) of plant specified OTS are the same as used for plant controlling. This is for the operators to learn on the same platform as they work on. In our study the OTS was developed for engineer application, but the OS is such important. To develop the OS Microsoft Excel was used. This is a spreadsheet developed by Microsoft. It features calculation, pivot tables, graphing tools, and a macro programming language called Visual Basic for Applications (VBA). Due to these features the OS could be created without deep programming knowledge.

The main property of the streams, equipments are shown in this screen and the User can set the set point of the controllers via this OS. It has got two kind of subscreens: the actual properties are displayed, the set points, and the graph of specify energy – the energy needed to produce one kilogram IPA – could be set in the first subscreen *(Fig.3),* the graphs contained the properties of each streams or equipments change over the time are shown the second subscreens *(Fig.4).* The second subscreens might be called with the "Trend" buttons next to the actual stream or equipment.

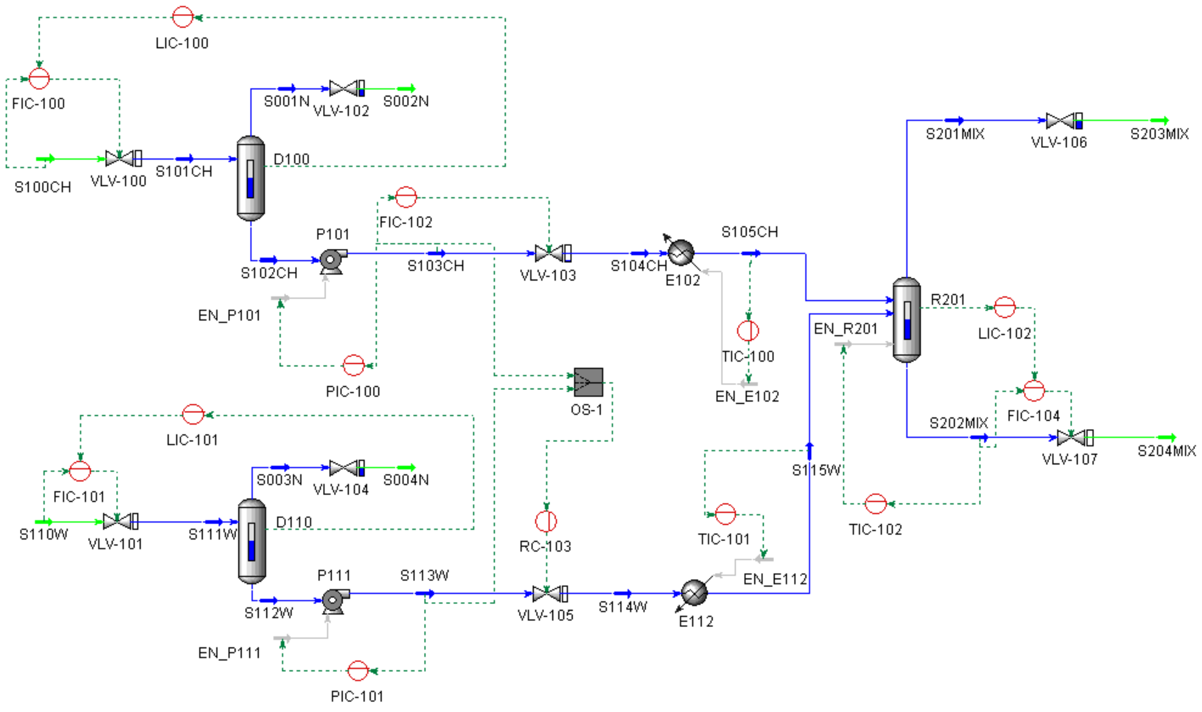

Figure 2. The dynamics process simulator with the controlling system.

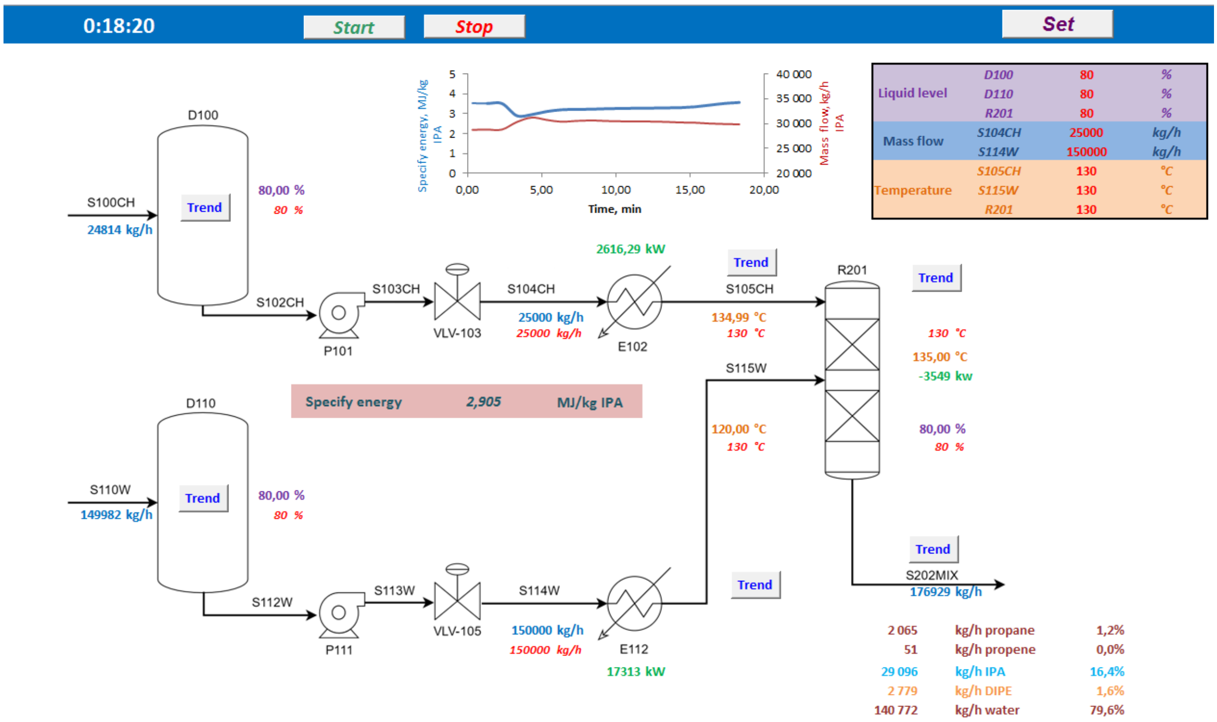

Figure 3. The first subscreen of the OTS which contains the PFD of the simulator, the main properties, the set points and the time of the simulation.

Connection between the screen and the simulator

UniSim Excel Interface Tool was used to make connection between the dynamic simulator and the operator screen. UniSim Excel Interface Tool is an Excel based tool that works with UniSim Design. It has two modes of operation: Excel based case study, and a series of in cell custom formulae that can be used to set up Automation links between UniSim Design and Excel without the user needing to write any Automation code. The tool provides a graphical front end to simplify the set-up of the case study and the writing of these functions.

The main two functions are getting property data from UniSim to Excel and giving set points from Excel to UniSim. The first function works automatically, but set points should send manually to UniSim. This is due to the values of the set points shall be confirmed via a button before they are set by UniSim.

Data to be monitored are saved every unit of time. VBA codes were used to realize that. VBA is an implementation of Microsoft's event-driven programming language Visual Basic 6, which was associated integrated development environment (IDE). Data saving is provided by a loop which engine is the time. As the result of this the time and the main properties are stored in a sheet, which are shown in the trends. Due to this connection, the two programs could work as OTS.

Operation of the OTS

After the programs (the dynamic simulator and the operator screen) were loaded with button “Start” the User can start the OTS. In a pop-up window the name of the User might be written in case of identifying the results. Then the timer starts and the investigation should be begun. In this user mode, the timer has twenty times real time factor. It is a convenient value; the changes of the simulator can be handled and it shorts the work. In the main screen the main properties can be continuously monitored. With buttons “Trend” the trends of the selected stream or equipment are shown. In case of changing the set points the User give the new value of the controller than press the button “Set”. A new window opens where values can be confirmed. When the investigation is finished the button “Stop” stops the timer, exports the property data to a csv file with the name of the user, the date and the time, and restores the simulation. This data can be analyzed after the work.

Results and analysis

Our OTS in its present form might be used as an emulation OTS for engineer application. To test it an analysis of the technology was made. Mainly the specify energy was investigated in different operating points. Before the investigation, the dynamic simulator set to stationary state. In this state the reactor works in 130 °C temperature in izoterm condition. Operating points were set in three time as follows:

1. The inlets and the reactor temperature were raised up to 135 °C
2. The water inlet temperature was decreased to 125 °C
3. The water inlet temperature was decreased to 120 °C

The trend of the inlet water stream is shown after the investigation *(Fig.4)*. Missing data can be seen in each graph at the same times. This is because of the Excel cannot run the timer when sends the values of the set point to the UniSim. The stationary values of the specify energy in each case are shown below *(Table 1.)*.

Table 1. Values of the specify energy in each case.

Case No.	**Inlet water temperature** (°C)	**Reactor temperature** (°C)	**Water preheater power** (MW)	**Reactor jacket power** (MW)	**Specify energy** (MJ/kg)
0.	130	130	19.00	- 5.640	3.340
1.	135	135	19.87	- 4.697	3.639
2.	125	135	18.13	- 4.492	3.125
3.	120	135	17.26	-3.435	2.877

The result of this analysis illustrated that direct cooling of the reactor shall be more effective instead of using jacket cooler. However, it would be an optimize task to determine the minimum of the specify energy. The primary target of the investigation was to test the working of the program and present the usage of it.

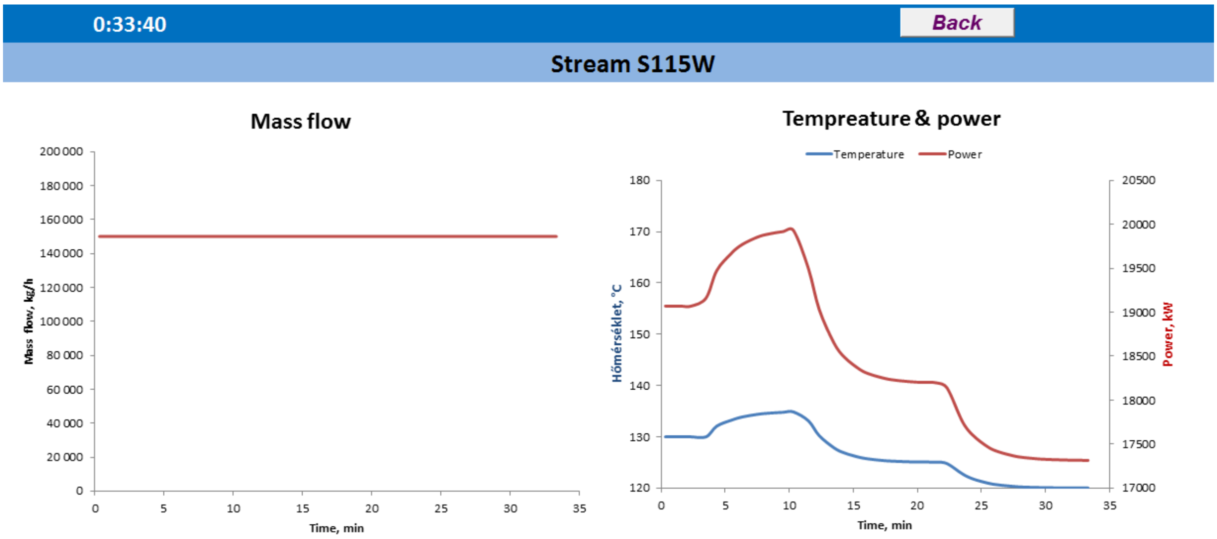

Figure 4. The subscreen with the trends on water inlet stream. The mass flow in kg/h is shown in the first graph and the temperature of the water in °C and the power of the preheater in kW are shown in the second graph.

Conclusion

After the stationary simulator was created, dynamic simulator and control system could be developed. By the time the OS was realized and connected to the simulator this system could work as OTS. Our OTS in this present form can be used for engineer application. In this present form, it is suitable to optimize and analyze the technology. It can also be used in education as a training for the students and the gained knowledge shall be exploited during their (industrial) carrier. In our further work, the dynamic process simulator will be completed with the separation subsystems, and there will be more accessories for example alarms – displayed warning and errors in the technology – and scenarios – predefined events – to the OTS could be used for training operators.

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