SIMULATION OF A BATCH REACTOR AND ITS MONOFLUID HEATING-COOLING SYSTEM

Project members

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Abstract

Long since in chemical industry creating the simulation of existing technologies has been a good practice, with the aim of process optimization, controller design and optimization, safety evaluation, transitions between operating conditions, and startup/shutdown condition testing and designing, testing, and training employees on new processes offline (OTS – Operator Training Simulation) before they are implemented. Besides it can be used for training instructors and for education, for more students in the course of laboratory practices than with the real system.

Engineering softwares like UniSim™ Design have limits in case of batch technologies, because they are designed and mostly used for continuous technologies. In UniSim™ Design no jacketed batch reactor models are provided, so approximation have to be made. We tested a couple of differently detailed models for the approximation. On this poster the differences and the deficiencies of the models and dynamic simulation results compared to measured values from the real system are presented.

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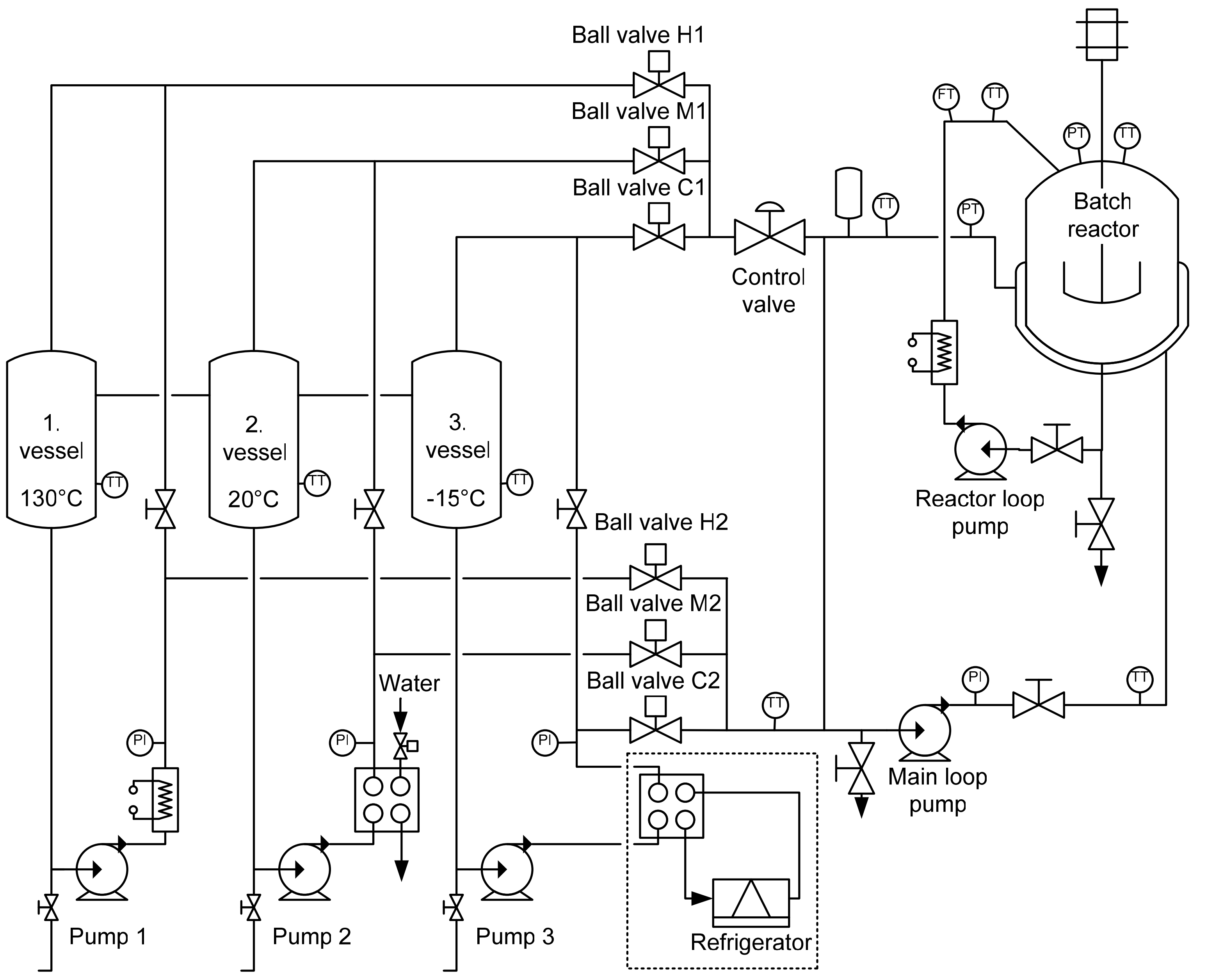
The monofluid heating-cooling system



In our laboratory a 50 litre stirred batch reactor with a monofluid jacket heating-cooling including three temperatures can be found. Besides the main economic advantage of the system with three temperatures (not only two temperatures on the boundary of the temperature range, a cheap, water controlled middle temperature can be set), it can provide the necessary (for batch reactors) homogeneous temperature distribution in the jacket, however the ball valves and control valve must be operated in accordance. With this system more economic benefit can be achieved if the recurring fluid from the jacket returns to the tank with the closest temperature. Unnecessary heating and cooling and disturbances can be avoided. It has four closed loops. Three loops represent the monofluid thermoblock, where the three different temperatures can be produced. The fourth recirculation loop is for the reactor's jacket providing homogeneous temperature distribution. The highest temperature can be adjusted with an electric heater, the middle with a heat exchanger cooled with tap water and the coolest with a refrigerator. The fluid with the required temperature can be chosen with on-off ball valves and the fluid rate can be controlled with a control valve. The batch unit is controlled with a Siemens PCS7 system.

The simulator

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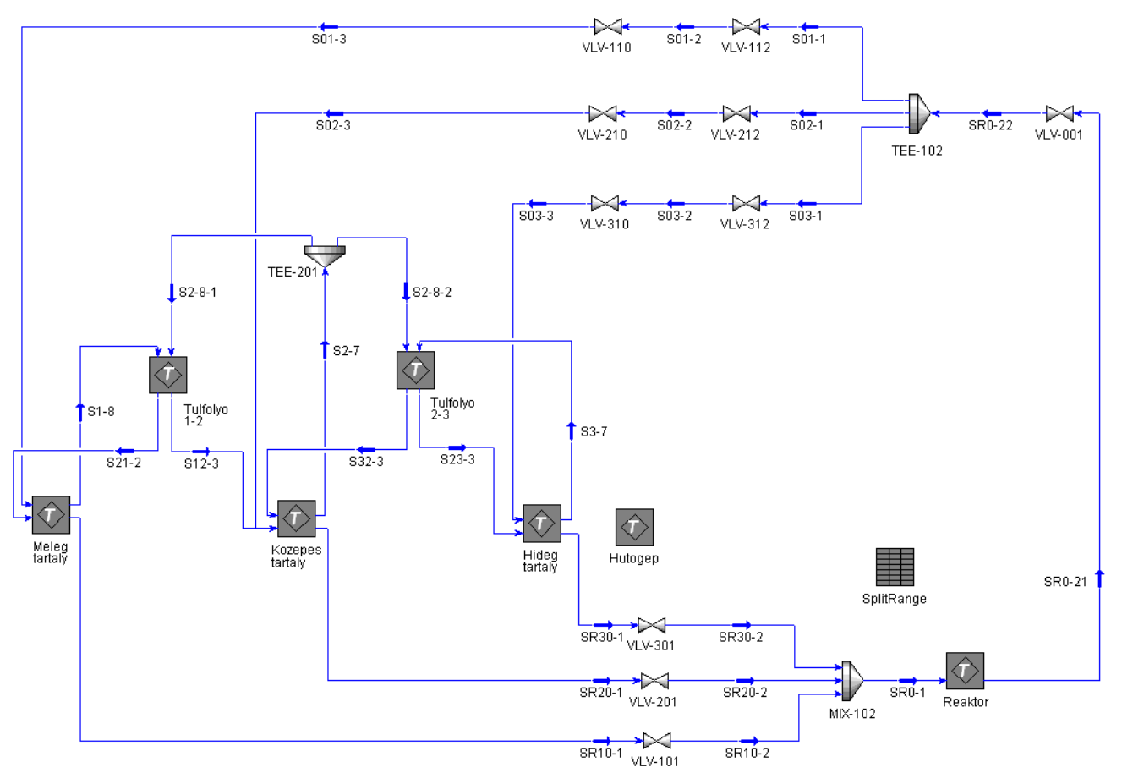
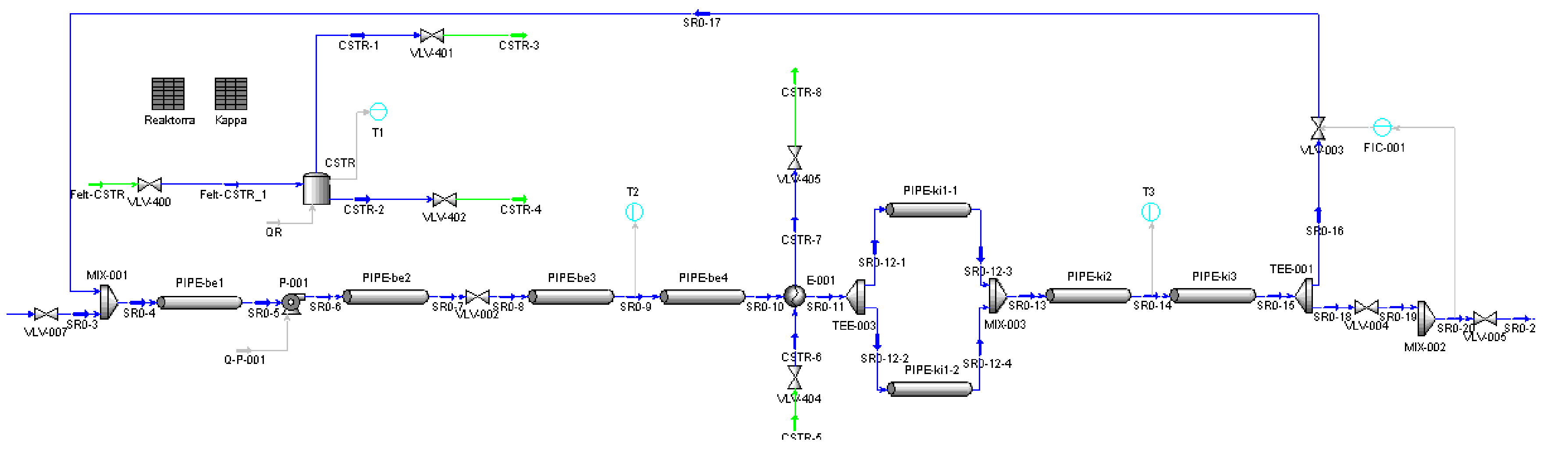
The jacketed batch reactor

According to our basic concept the jacketed batch reactor was built up from a CSTR and a 1-1 shell-tube heat exchanger. The two models were connected through heat flow. The duty of the CSTR is set equal to the heat exchanger's (which represents the jacket) duty. The heat exchanger's tube side inlet stream has the same composition and temperature as the reaction mixture, and its flow rate can be adjusted according to the stirrer's speed. The connection was achieved with UniSim™ Desgin's flexible module called "Spreadsheet". It allows accessing all the variables in the simulator, but only the user defined variables can be modified with it. It's very similar to Microsoft Excel, it has 10×4 cells as default, and the calculations can be done through cell links.

The UniSim™ Design simulation software

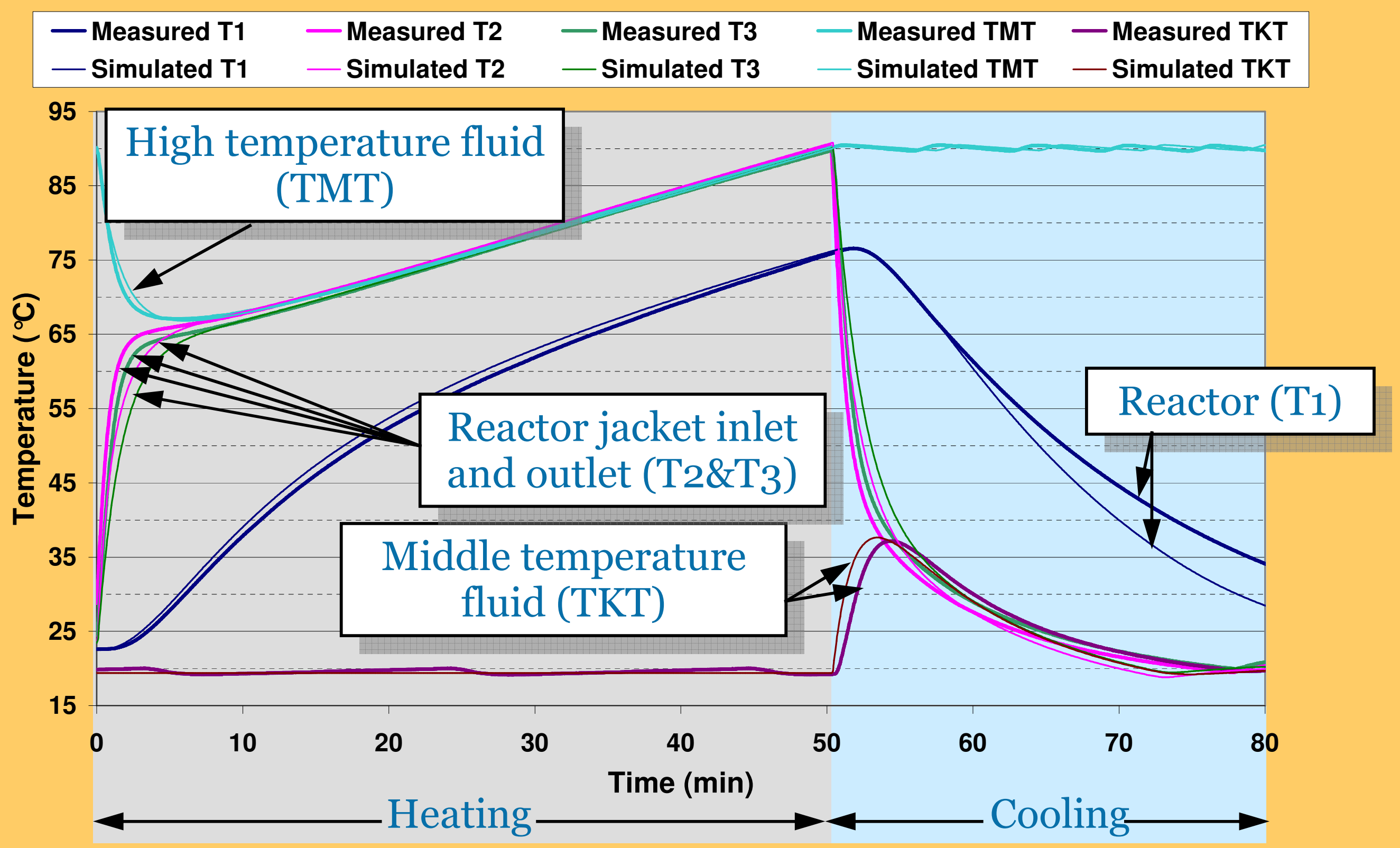
The simulator is made with Honeywell's UniSim™ Design Suite, which is based on HYSYS® software. It offers steady-state and dynamic simulation, design, performance monitoring, optimization and business planning for the oil and gas production, gas processing, petroleum refining and chemical industries.





Simple reactor model

We only used two different temperatures (hot and middle) of the three available. The simulated temperatures show good approximation compared to the measured data, except the reactors temperature on the cooling part, where increasing differences occur. This model doesn't contain any information about the viscosity of the fluid that is highly temperature dependant and affects the heat transfer coefficient significantly. This is the reason why the cooling part doesn't fit to the measured data (system parameters were fitted to the heating part).



<u>Used equations:</u>

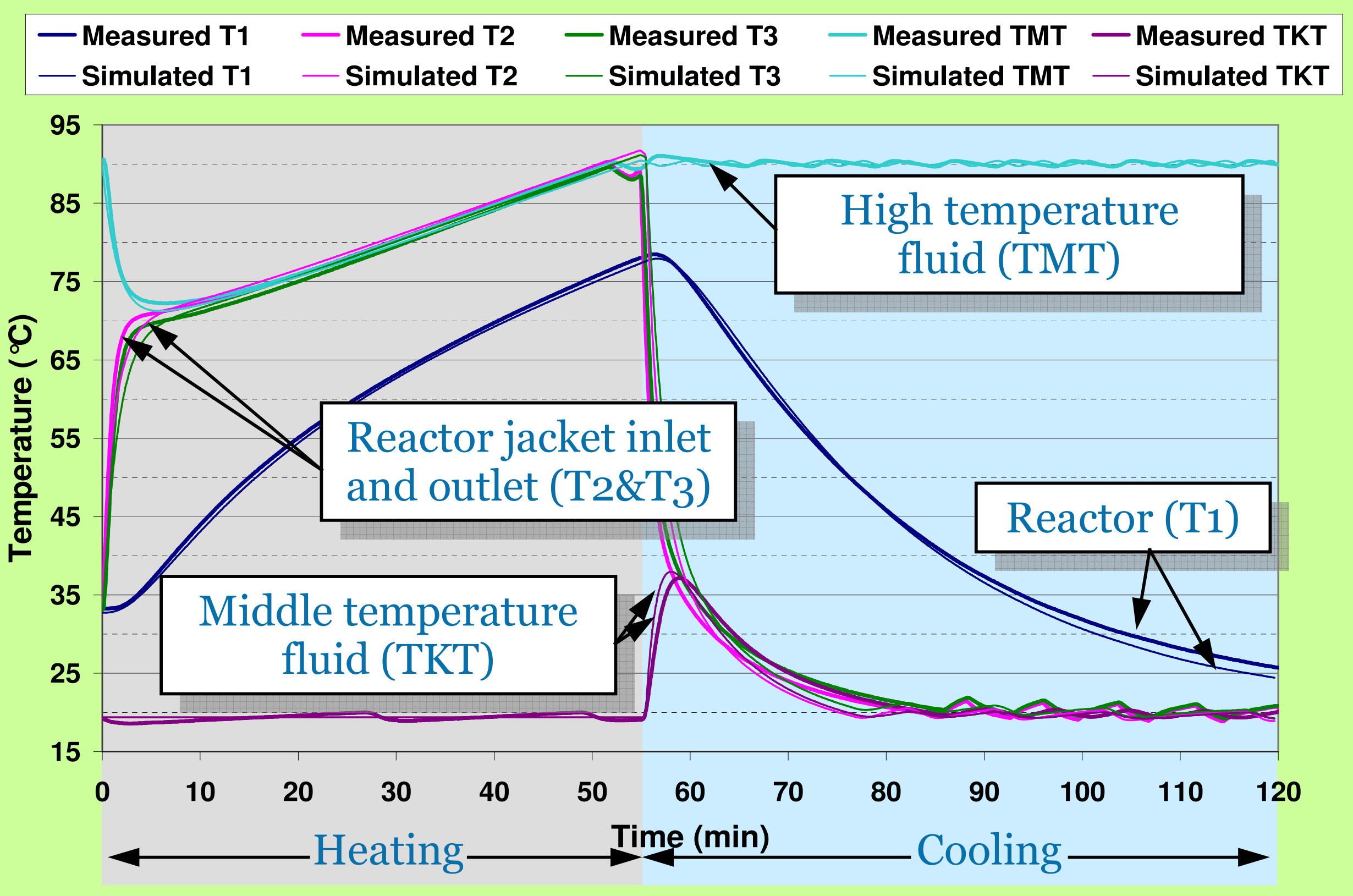
Transferred heat flow: $Q = \kappa A \Delta T_{LM} F_t$

Dynamic correction factors:

$$F_T = \frac{2 f_1 f_2}{f_1 + f_2} \quad f_1 = \left(\frac{M_{cs}}{M_{cs,ref}}\right)^{0,8} \quad f_2 = \left(\frac{M_k}{M_{k,ref}}\right)^{0,8}$$

Detailed reactor model

To eliminate the deficiencies of the simple model, we built a detailed model containing temperature dependent viscosity. It calculates the heat transfer coefficient in every time step from the constant physical dimensions and dynamic fluid properties of the system. We this change the constant overall heat transfer coefficient became dynamic.



<u>Used equations:</u>

Overall heat transfer coefficient:

$$\kappa = \frac{1}{\frac{1}{\alpha_{reactor}} + \frac{1}{\alpha_{jacket}} + \frac{\delta_{wall}}{\lambda_{wall}} + \frac{\delta_{glass}}{\lambda_{glass}}}$$

Reactor side heat transfer coefficient:

$$\alpha_{reactor} = Nu \cdot \frac{\lambda}{D_{inside}}$$

Nusselt number on reactor side (Chilton correlation):

$$Nu = C \cdot \mathrm{Re}^{2/3} \cdot \mathrm{Pr}^{1/3} \cdot \left(\frac{\mu}{\mu_{wall}}\right)^{0,14}$$

Jacket side heat transfer coefficient:

$$\alpha_{jacket} = Nu \frac{\lambda}{d_h}$$

Equivalent diameter in the jacket:

$$d_h = \frac{4 \cdot f}{U}$$

Nusselt number on jacket side (Sieder-Tate correlation): $Nu = 0{,}023 \cdot \mathrm{Re}^{4/5} \cdot \mathrm{Pr}^{1/3} \cdot \left(\frac{\mu}{\mu_{wall}}\right)^{0,14}$

Conclusion

In result we made a simulator responding likewise the real system; with this corrected model more accurate controllers can be designed. To connect the simulator with process control software through OPC (OLE for process control) interface Honeywell's UniSim™ Operations Suite is needed instead of UniSim™ Design. The connected dynamic simulator can be a useful tool for controller design and testing and for student laboratory practices.