Soft Sensor Methodology for the Precise Spatial and Temporal Prediction of Thermodynamic States Inside a Chemical Reactor

Fabian Zapf[1], Elisabeth Rammerstorfer[2], Erich Jeitler[2], Günther Holzer[2], Thomas Wallek[1]

Graz University of Technology

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Motivation

Inside a continuous chemical reactor (illustrated in figure 1), in which phase transitions occur during the reaction, thermodynamic conditions as well as compositions of the process stream are subjected to significant spatial and temporal changes.

As exothermic chemical reactions often show temperature peaks which are likely to destroy catalysts and components or adversely affect their service life, this limited information about internal reactor states poses a considerable risk with regard to product quality and process reliability. Therefore, this paper proposes a novel approach, which enables a more detailed prediction of the reaction progress in view of avoiding undesired temperature peaks, based on measured process parameters of the input and output streams only.

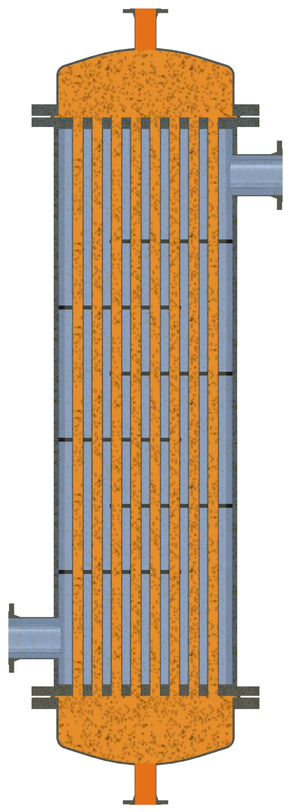


Figure 1: Reactor

Approach

As a reference model, a production plant for ethyl tert-butyl ether (ETBE) as part of the gasoline line of a refinery is chosen. The reactor configuration is shown in figure 2.

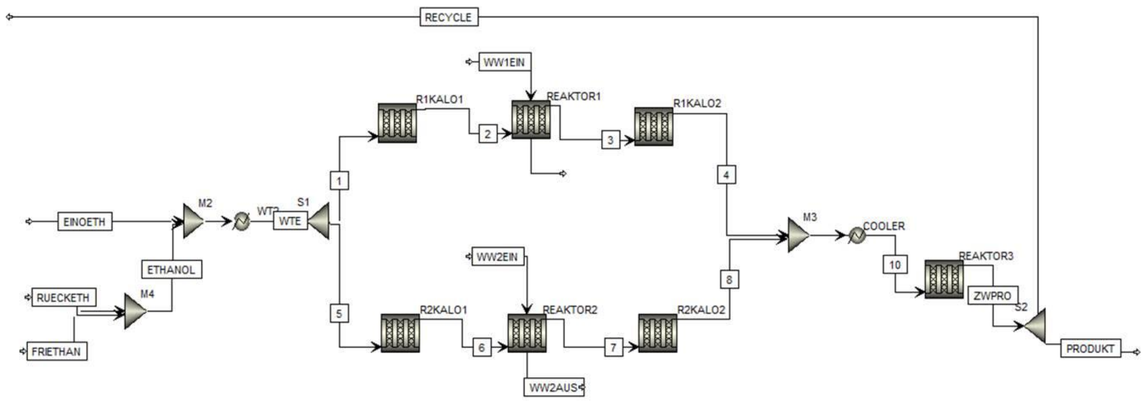


Figure 2: Reference model in Aspen Plus®

The liquid educts of the reaction, in particular ethanol and iso-butene, are fed into a cooled tubular reactor in a counterflow arrangement, and the products also leave the reactor in a liquid state. Although the exothermic nature of the reaction leads to partial evaporation inside the reactor, the reaction solely occurs in the liquid phase. The reaction network (see table 1) for this type of ETBE synthesis and its kinetics has most recently been published by [1] and [2]. The influence of the phase equilibrium on the kinetics has been described in literature [3].

Main reaction:

$$EtOH + IB \leftrightarrow ETBE$$

Side reactions:

$$2\,IB \leftrightarrow DIB$$

$$2\,EtOH \leftrightarrow DEE + H_2O$$

$$H_2O + NB \leftrightarrow ESBE$$

$$IB + H_2O \leftrightarrow TBA$$

Abbreviation	Name
ETBE	Ethyl-tert-butylether
EtOH	Ethanol
IB	iso-butene
NB	n-butene
DIB	Diisobutenes
DEE	Diethylether
ESBE	Ethyl sec-butylether
TBA	Tert-butyl alcohol

Table 1: Reactions and used abbreviations

Via a user kinetic extension, the kinetics for ETBE and related side reactions [3] are implemented into the commercial flow-sheet simulator KBC PetroSIM®, which allows for static and dynamic simulations. The combination of a user kinetic model with a commercial process simulation tool opens access to a broad variety of thermodynamic property models, i.e., activity coefficients and equations of state, which makes it possible to model reactions for practically all kinds of highly non-ideal systems.

Because the kinetic model for the reference reaction is based on activities, the liquid phase fugacities in the course of vapor-liquid equilibrium calculations are described by the NRTL activity coefficient model [4], where missing binary parameters are estimated using the modified UNIFAC (Dortmund) group contribution approach [5].

Results

The resulting output of the model is a real-time visualization of the key process parameters, including the precise spatial and temporal prediction of temperatures inside the reactor as well as wall surface temperatures. Figure 3 and Figure 4 show the calculated temperature and reactant concentration profile inside the reactor for a reference case. Figure 5 shows the byproduct concentrations for two different C4 feed streams and a 1:1 mixture of them. Based on this information, destructive temperature peaks as well as undesired byproduct formation can be avoided and plant throughputs can be optimized precisely, taking into account material life and catalyst life cycle. For the reference plant at hand, the throughput-related catalyst life cycle could be increased by up to 10%.

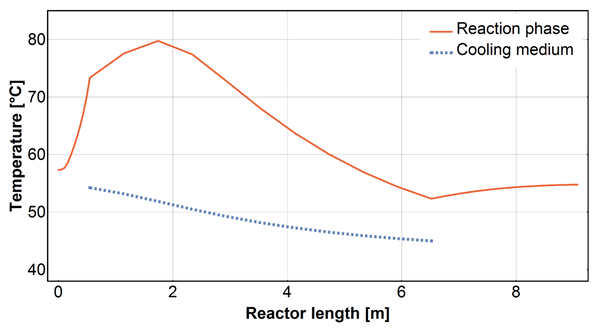


Figure 3: Temperature profile

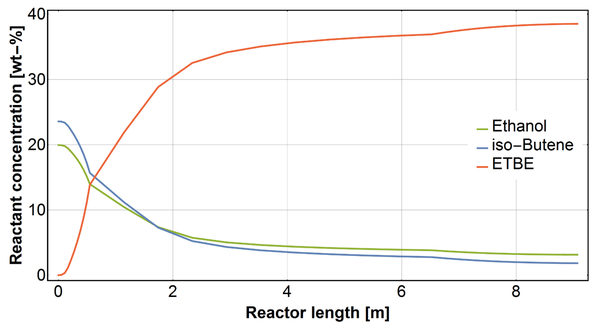


Figure 4: Reactant concentration

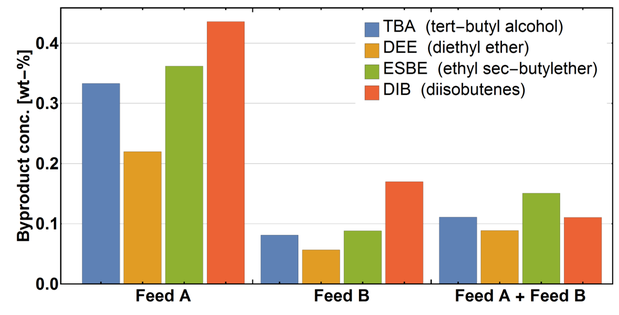


Figure 5: Byproduct formation for different feeds streams

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[1] Institute of Chemical Engineering and Environmental Technology, Graz University of Technology, Austria

[2] Prozess Optimal CAP GmbH, Vorau, Austria

Prozess Optimal CAP GmbH
Impulszentrum 1
8250 Vorau
AUSTRIA
www.prozess-otpimal.at
holzer@prozess-otpimal.at

Institut of Chemical Engineering and Environmental Technology
Graz University of Technology
8010 Graz
www.ceet.tugraz.at
fabian.zapf@tugraz.at

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