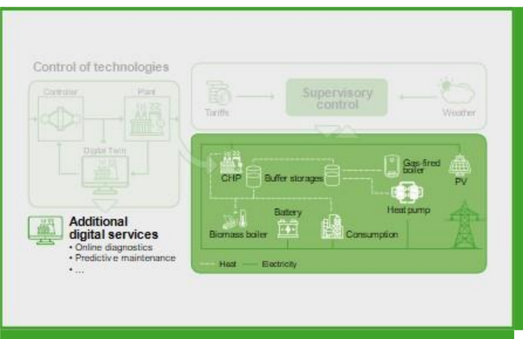

Fischer Tropsch Reactor

Mathematical model for soft sensor development

Ines Kirsten
Uwe Poms
Thomas Steiner
Theresa Köffler
Thomas Reiter-Nigitz
Gerald Weber
Markus Gölles

AREA 2.2 Automation and Control

Motivation

As part of the **Syngas Platform Vienna** the **Fischer-Tropsch pilot plant** is used to produce sustainable (bio)refinery products from syngas. The highly complex reaction network, allows for the production of different products (paraffins, olefins) of varying chain length in one reactor. Measuring the product composition in real time is hardly possible with established analytic methods (Simdist-GC analysis). Process control needs to rely on more readily available measurements. Since the reactions occurring are exothermic, a correlation between reactor temperature and product distribution can be established.

Correlation model

Instead of trying to formulate individual reaction rates with high uncertainty in this complex network, an alternative approach was chosen: describing the product distribution by the **Anderson-Schulz-Flory (ASF) distribution** and its extensions. The mole fractions y_n in the product are given by

$$y_n = (1-\alpha)\cdot\alpha^{n-1}$$

where α is the probability of chain growth, independent of chain length, and n the chain length. Higher alpha values shift the product distribution towards higher chain hydrocarbons, as shown in Figure 1.

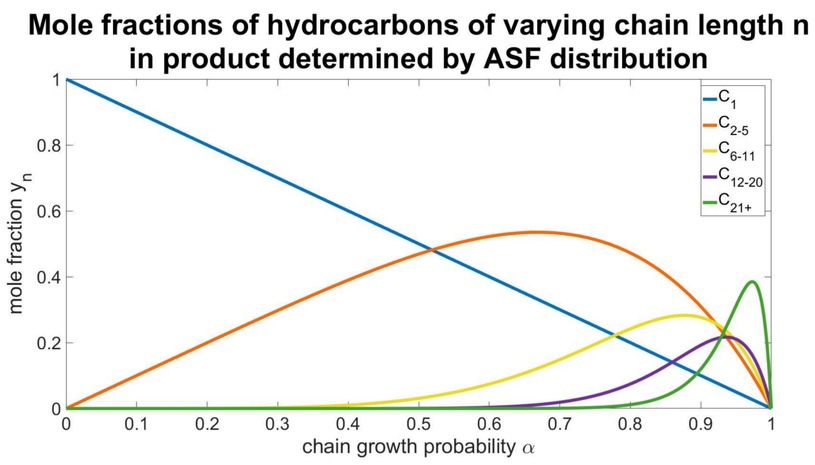

Figure 1: Product composition given by ASF distribution, products have been grouped

Subsequently the heat of reaction can be calculated and the results for three different α-values are visualized in Figure 2.

Dynamic Model of Heat Transfer

To distinguish the heat set free by the reaction in the reactor from other heat sinks and sources the development of a thermodynamic model of the reactor is needed. To account for the heat transfer through the different materials the reactor was divided into several subsystems, presented in Figure 3.

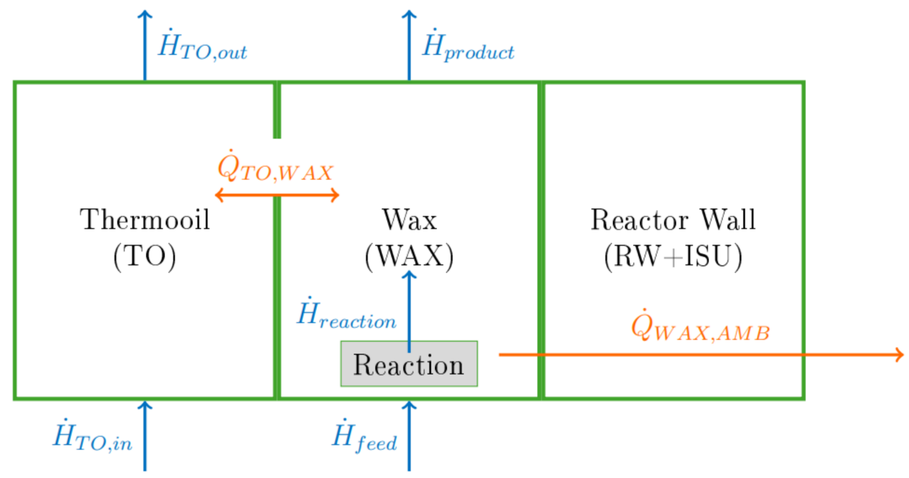

Figure 3: Subsystems and energy streams

Heat of reaction Δh_R^0

The heat of reaction can be calculated given the chemical equation and the heat of formation of the components

$$\Delta h_R^0 = \sum_i^{components} \nu_i \cdot \Delta h_{f,i}^0$$

assuming only the production of alkanes from syngas:

$$n\,CO + (2n+1)H_2 \rightarrow C_nH_{2n+2} + nH_2O$$

This requires the heat of formation of the hydrocarbon mixture, which can be determined from the mole fractions y_n and the heat of formation of the individual hydrocarbons $\Delta h_{f,C_nH_{2n+2}}^0$.

$\Delta h_{f,C_nH_{2n+2}}^0$ is found by setting the calorific value of the fuel, determined by an empirical correlation, equal to the standard enthalpy of combustion.

Combustion of alkanes:

$$C_nH_{2n+2} + \frac{3n+1}{2}O_2 \rightarrow nCO_2 + \frac{2n+2}{2}H_2O$$

Figure 2: Normalized enthalpies of reaction for selected α-values

BEST – Bioenergy and Sustainable Technologies GmbH

Firmensitz Graz
Inffeldgasse 21b
A 8010 Graz

T +43 5 02378-9201
office@best-research.eu
www.best-research.eu

FFG Forschung wirkt. · Bundesministerium Arbeit und Wirtschaft · Bundesministerium Klimaschutz, Umwelt, Energie, Mobilität, Innovation und Technologie · wirtschaftsagentur wien · Für die Stadt Wien · Das Land Steiermark – Wirtschaft, Tourismus, Regionen, Wissenschaft und Forschung · SFG – Neues Denken. Neues Fördern.