Modeling and optimization of a methanol synthesis loop with deactivating catalyst

Ingvild Løvik and Terje Hertzberg
Department of Chemical Engineering
Norwegian University of Science and Technology, Trondheim

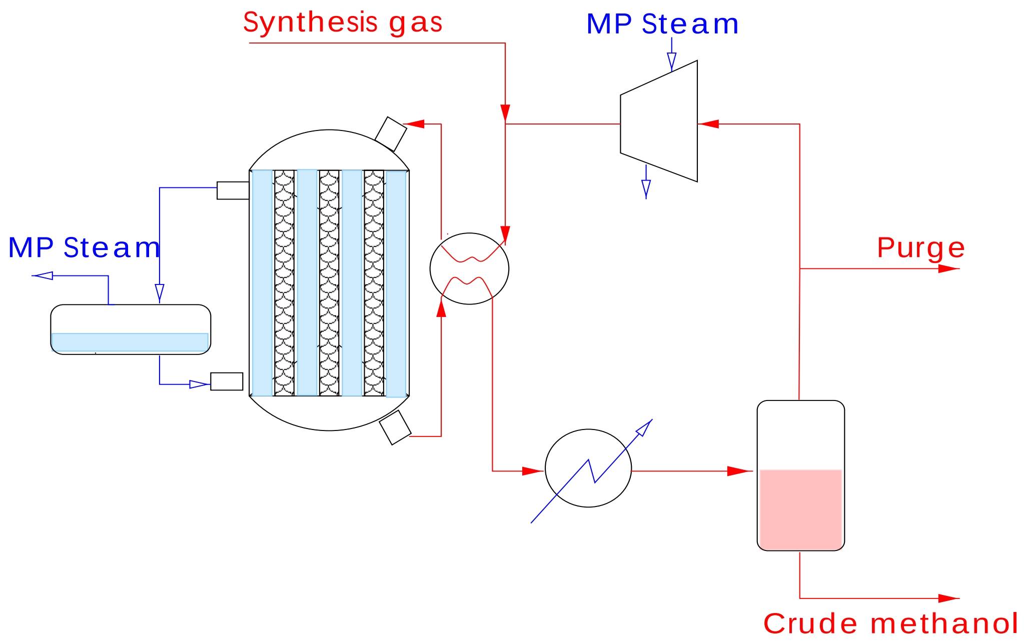
Magne Hillestad
Statoil R&D Centre, Trondheim

PROCESS DESCRIPTION

Synthesis gas is converted to methanol over a Cu/Zu/Al_2O_3 catalyst:

$$CO_2 + 3H_2 \Leftrightarrow CH_3OH + H_2O$$
$$CO + H_2O \Leftrightarrow CO_2 + H_2$$

Typical operating conditions: 250^o C, 80 bar



OPTIMIZATION PROBLEM

Maximize:

$$Profit = \int_{t_o}^{t_l} (F_{MeOH} \cdot P_{MeOH} + F_{Steam} \cdot P_{Steam})dt$$

Subject to:

$$T_{reactor}^{max} \leq 543K$$

$$513K \leq T_c \leq 533K$$

$$Q_{comp} \leq 1.2 \cdot Q_{comp}^{ref}$$

$$2 \leq R \leq 5$$

the process model

Prices (Metanex -98, Edgar and Himmelblau-89):

$$P_{MeOH} = 115\text{USD/ton} \ , P_{Steam} = 11\text{USD/ton}$$

SOLUTION APPROACH

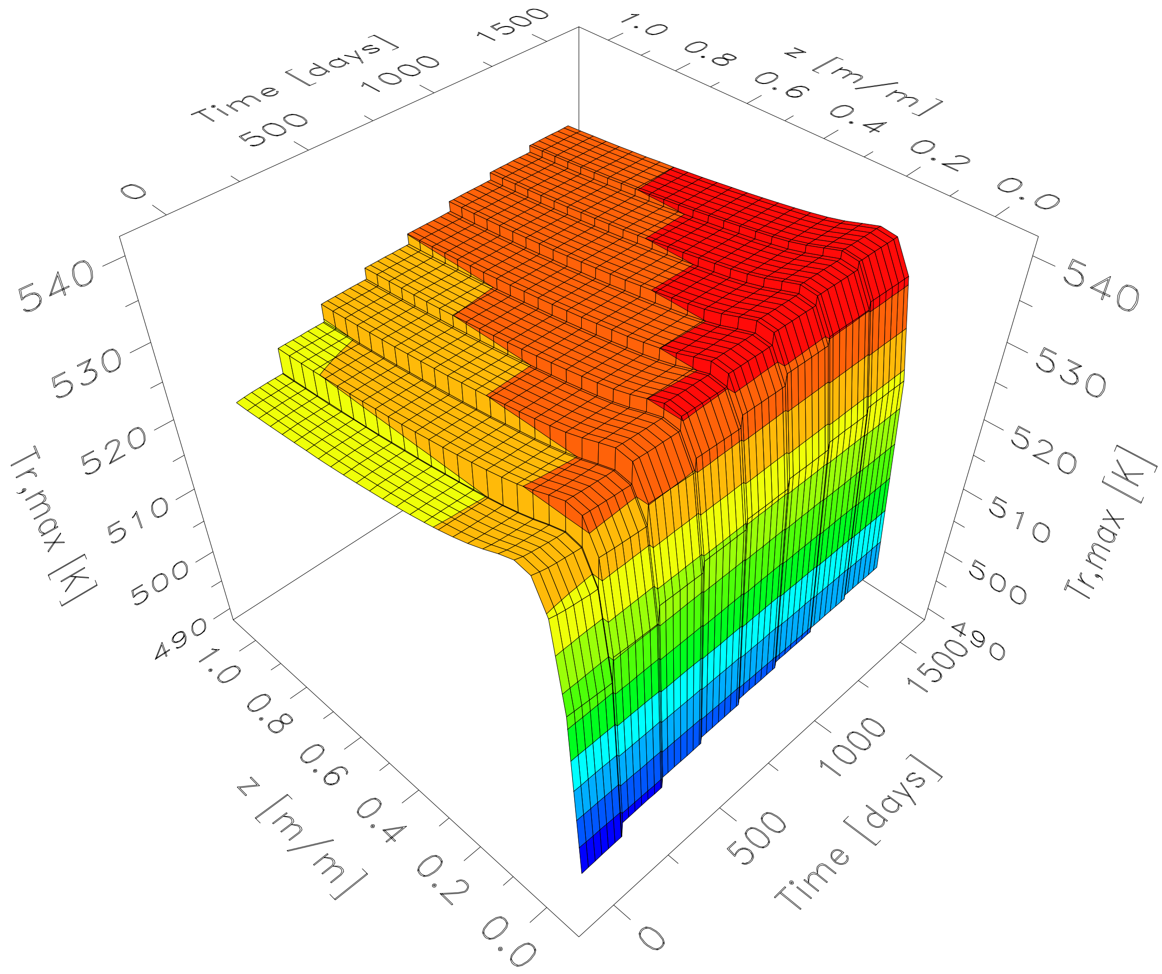
Control vector parameterization

- T_c and R discretized as piecewise constant profiles
  - easy to implement in real operation
- 8 intervals used
- the path constains was converted to end point constrains by integrating the constraint violation
- interior point constrains used to improve convergence

Implemented in gPROMS and gOPT

RESULTS

Maximum reactor temperature - below 543 K:



CONCLUSIONS

- The methanol synthesis reactor system was modeled and optimized
- Total profit can be increased by 3. 2$\pm$ 0.8*10^6 USD or 0.8$\pm$0.2 percent if the process is operated optimal
- Important to consider the reactor system, not only the reactor (Løvik et. al. -98)
- The method applies to all fixed-bed reactor systems

Future work:

- Implementing issues :

  -update activity from process data

  -repeated optimization