Alternative Haber Bosch Ammonia Reactor Concept

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Highlights

- A new reactor concept for ammonia production is proposed
- An improved temperature profile reduces the reactor size
- Temperature control using pinch does not require active controllers
- Significant reactor cost reduction

1. Introduction

The Haber-Bosch reaction for ammonia production is a well-known example for exothermal reactions. The reaction temperature profile needs to consider both kinetics and equilibrium limitations [1, 2]. In the standard reactor with a few adiabatic stages and intercoolers, there are limited degrees of freedom to adapt the temperature profile to the optimum profile. The typical zig-zag profile shows a large deviation to the optimum temperature near the inlet and outlet of each stage (fig. 2, left). An alternative concept is proposed, which allows a temperature profile closer to optimum.

2. Methods

The proposed approach is to use a cooled fixed bed with coils removing heat of reaction simultaneously with reaction progress. The cooling medium is the feed gas, which is thereby preheated. Simulations predict the temperature and concentration profiles in the cooled fixed bed. As multiple steady states can be reached potentially, the startup procedure is investigated by dynamic simulation. All simulations have been setup from scratch as C++-Code.

3. Results and discussion

For counter-current flow configuration, heat is captured at the hot end of the apparatus and the reaction temperature is exceeding the maximum temperature. To overcome that problem, an alternative flow configuration was applied. A permutation of the passages of the heat exchanger tubes as sketched in figure 1 causes a pinch, which limits the maximum reaction temperature and results in a temperature profile close to the optimum temperature profile (fig. 2, right).

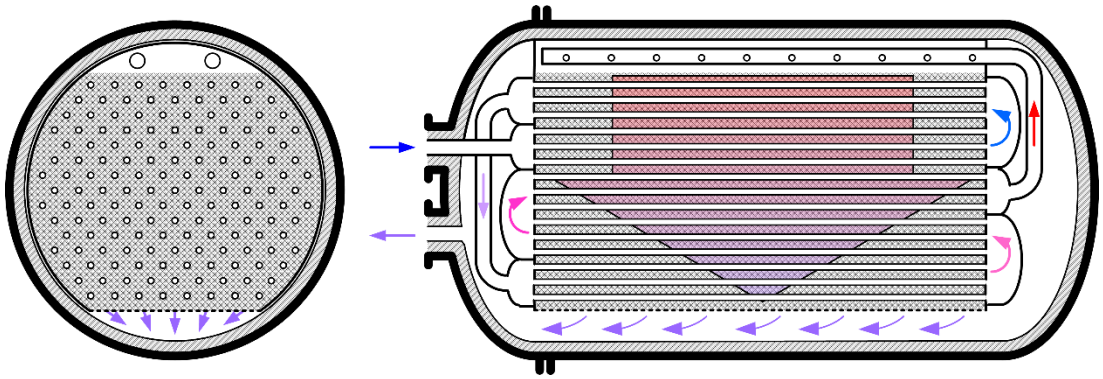

Figure 1. Setup of the cooled fixed bed reactor with feed preheating using permutated tube passages

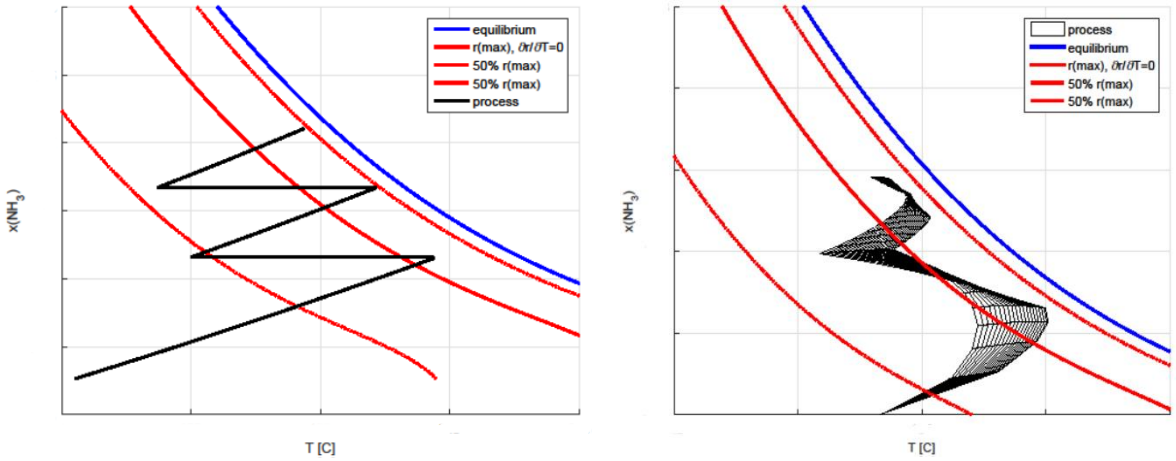

Figure 2. Temperature vs. NH_3 mole fraction profile in the classical Haber Bosch process (left) and in the proposed modification (right).

The reactor simulation is based on a 2D domain decomposition into control volumes and the solution of the heat and mass balances with reaction. The steady state model uses a Newton solver to solve the algebraic equation. In a dynamic version, numerical integration is used to get the time development of the reactor state.

4. Conclusions

Due to the improved temperature profile, the reactor volume is reduced compared with the standard Haber Bosch reactor. A second advantage is a simpler reactor control, as no active controllers are required. The temperature profile is adjusted by an internal temperature pinch. Therefore, no effort needs to be taken for controllers including measurements and actuators in a high-pressure environment.

References

[1] J.A. Moulijn, M. Makkee, A, van Diepen, Chemical Process Technology, Wiley 2001.
[2] U. Onken, A. Behr, Chemische Prozesskunde Band 3, Wiley 1996.

Keywords
Ammonia; Haber-Bosch; Reactor Simulation