AIDIC EFCE
ISCRE25 FLORENCE 2018
BRIDGING SCIENCE & TECHNOLOGY
The 25th International Symposium on Chemical Reaction Engineering
20-23 May 2018
Florence, Italy
www.aidic.it/iscre25

Design of a High Temperature Catalytic Wall Reactor: Synthesis of Hydrogen Cyanide

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Highlights

- Optimal reactor design based on fundamental physical insights instead of cost specifications and under uncertain product specification requirements
- Two stage reactor design based on optimisation of a rigorous reactor model.
- Inclusion of computational fluid dynamics and radiative heat transfer in reactor design

1. Introduction

Sustainability and climate change require carbon-reduced electricity generation and distribution but also substantially higher material and energy efficiencies. In the case of the chemical industry these objectives are directly linked to economic goals and competitiveness. While process design in this context is crucial to meet long-term future challenges, process optimisation and retrofitting of existing plants can boost resource efficiencies and ecological footprints of the chemical industry on the short term. Energy-intensive processes such as high-temperature gas phase synthesis reactions stand out in that context because small process improvements have a large impact on the ecological footprint of the industry. Typical examples are steam methane reforming and the synthesis of hydrogen cyanide (HCN). Their reactors consist typically of an outer oven compartment that generates heat e.g. via methane combustion for an inner compartment in which the endothermic synthesis reaction takes place at high temperature (1000-1500K). Providing the heat to the catalytically active sites in the inner compartment effectively leads directly to a reactor design problem that is tightly coupled to the resource and energy efficiency of the overall process. Optimisation in that context remains challenging due to high modelling complexity and coupling of transport mechanisms at different length- and timescales [1].

2. Methods

In this work reactor optimisation is performed with a steady, two-dimensional detailed catalytic channel reactor model using an in-house Matlab/CasADi computational fluid dynamics code based on a typical industrial reactor design used in the synthesis of HCN [2]. In this synthesis, methane and ammonia react on catalyst coated walls to form HCN and hydrogen [3]: $CH_4 + NH_3 \rightarrow HCN + 3H_2$ $\Delta_R h \approx 250 kJ/mol$.
In order to link the reactor geometry with energy efficiency for the optimisation, the model takes into account both compartments that are mentioned above – the oven and the reactor side. The compartments are separated by a ceramic wall. The design problem is then addressed in two consecutive steps: (i) design of the inner synthesis compartment at given constant specific boundary conditions; (ii) optimisation of the oven compartment is achieved using a coupled model consisting of a single compartment and an outer oven compartment while specifying the previously identified optimal single synthesis compartment of the first step.
Compressible boundary layer flow is assumed in both compartments where pronounced cross-channel gradients in temperature, mass and velocity exist. Modelling focus is on the synthesis compartment of the reactor. The conservation equations consist of a system of momentum, total continuity, partial continuity and energy balances combined with the radiative transfer equation (RTE). In order to minimise computational cost, combustion reactions on the oven side are omitted and approximated by a hot flue gas flow. Special emphasis is attributed to modelling all heat transfer modes including radiation in inner and outer compartments as the influence of different heat transfer mechanisms is crucial for the overall optimisation.

3. Results and discussion

The optimal reactor design depends essentially on the desired product specifications as well as fixed and operating costs: both may be uncertain or even unknown because the optimal operating point of the reactor depends on inlet conditions and downstream processing whereas costs solely represent a single isolated economic scenario. The reactor optimisation requires therefore weighing of different aspects according to the respective economic scenario in which the plant is operated. For these reasons a parameter sampling is presented containing optimal process scenarios that serve as decision support in order to maximize resource efficiency in a wide range of economic scenarios.

In the considered example, the reactant mixture flows through pipes that are suspended in an oven chamber where a methane-air mixture is combusted. Both the geometry of the single compartments – length and width – as well as the spacing among different pipes as well as chamber walls are degrees of freedom and key parameters in terms of energy efficiency. In order to obtain maximum fuel exploitation, modelling studies with different reactor geometries are carried out (Fig. 1) according to the two design stages explained above: First of all, reactor length and width of a single reaction compartment are optimised for a fixed outer temperature (Fig. 1 left). Consecutively, inner and outer compartments are coupled and the outer geometry is optimised for the best interior design (Fig. 1 right). The figures visualize parameter samplings where the horizontal plane illustrates a minimum normalized mass flow or conversion according to [2]. For the stage one optimisation product yield is either increased with smaller width or longer reactor designs whereas the stage two optimisation has the incineration chamber characteristics – flue gas velocity and oven width – as degrees of freedom. As a result, mass flow is maximized for high velocities and larger oven geometries compared to the synthesis compartment.

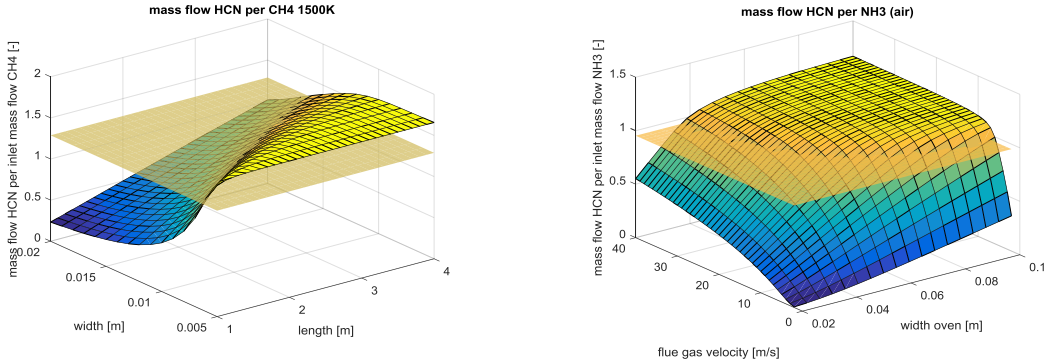

Figure 1: Results of the reactor optimisation as normalized mass flows versus decisive reactor design parameters (left : synthesis (inner) compartment, right : coupled (synthesis and oven) reactor model).

4. Conclusion

This work enables an optimal reactor design in uncertain circumstances – both economically and with unknown product specifications. This is achieved via a rigorous first principles model and optimization based on physico-chemical criteria that are more general than specific economic cost factors. In this manner, the results serve as decision support e.g. in modelling and optimization of the entire process chain.

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Keywords
Reactor Design, Two-stage Optimisation, Radiative Heat Transfer, Hydrogen Cyanide.