A CFD-reactor model for an annular structured catalytic reactor for steam methane reforming: pilot scale testing and performance evaluation under commercial conditions

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Highlights

- CFD-reaction model for structured reactors developed and experimentally validated
- Transport phenomena experimentally studied in pilot-scale tests
- Reactor simulation and performance evaluation under commercial process conditions

1. Introduction

Steam methane reforming is the most widely practiced industrial process for the production of hydrogen and syngas from methane. The reactions are endothermic and conventionally carried out in packed bed reactors suspended in a furnace. The reactor performance is limited by heat transfer, pressure drop and intra-particle diffusion limitations. Structured catalytic reactors are a promising technology in order to intensify the process. When properly designed, the structure provides increased heat transfer efficiency and reduced pressure drop [1-2]. The use of a thin catalyst coating allows increased catalyst effectiveness factors. Reactor design, optimization and scale-up requires the development of a detailed reactor model accounting for transport phenomena and complex flow pattern.

2. Methods

To evaluate the performance of an annular structured catalytic reactor under typical commercial conditions, a detailed CFD-reaction model was developed. The Reynolds-Averaged Navier-Stokes (RANS) approach was adopted and turbulence was accounted for through the k-ε model. Thermal conduction in the walls and the internals of the reactor was accounted for and different radiation models were tested. The intrinsic reaction kinetics was coupled with the CFD code and catalyst effectiveness factors were independently estimated by solving intra-catalyst diffusion-reaction equation. Pressure drop data from cold flow pilot plant tests were used for the calibration of the parameters of the k-ε turbulence model [3]. Heat transfer and methane conversion data from pilot plant tests were used to further validate the CFD reactor model. This model was then used to perform simulations of the reactor under typical commercial conditions and optimization of the reactor design. Comparison with a conventional packed bed reactor was carried out.

3. Results and discussion

Cold flow pilot plant tests over a wide range of gas flow rates have shown that the annular structure provides a reduced pressure drop compared to pellet reactor. The semi-empirical parameters in the ε-equation of the turbulence model were optimized to have a good fit between CFD model and measured pressure drop, as shown in Figure 1(a). The turbulent kinetic energy profile in a cross section in the axial direction of the reactor, shown in Figure 1(b), indicates that turbulence is minimal inside the channels and considerably increased in the near-wall region, where abrupt changes of direction and velocity occur. This is responsible for the reduced pressure drop and efficient heat transfer between the reactor tube wall and the process gas.

Simulations along a commercial-sclae annular reactor under typical industrial conditions were carried out. The simulations were performed with an imposed constant furnace temperature of 1400K. For the configuration used in the cold flow pilot plant pressure drop tests (base case), predicted exit CH_4 conversion is close but slightly inferior to the one reported with a conventional packed bed reactor [4-5]. Simulations have shown that in the first part of the reactor, a superior performance in terms of CH_4 conversion is achieved with the structure, due to significant contribution of radiation, allowing heat transfer intensification.

In the second part of the reactor, pronounced interfacial mass transfer limitations lead to a somewhat inferior performance. A configuration with doubled amount of blades per unit length of reactor, that is doubled geometric surface area (GSA), was tested. The simulations shown an improved performance in the second part of the reactor and the predicted exit CH_4 conversion is similar to the one obtained with conventional technology, but with lower pressure drop.

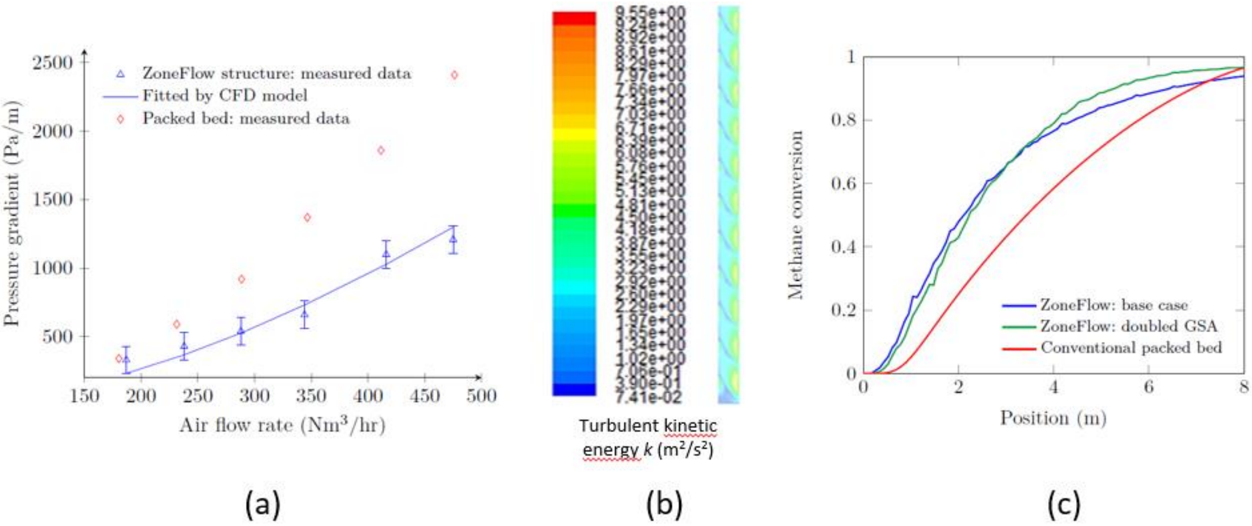

Figure 1. (a) Experimentally measured and fitted pressure drop in the annular structure, (b) turbulent kinetic energy in a cross section in the axial direction of the reactor and (c) predicted methane molar conversion under commercial operating conditions: comparison between annular structure and conventional packed bed reactor.

4. Conclusions

A CFD model was developed for an annular structured catalytic reactor. Experimental pressure drop, temperature and methane conversions data from a pilot plant allowed optimization and calibration of the parameters and model validation. The developed model was used to evaluate the performance of the reactor under typical commercial process conditions. Comparison with a conventional packed bed rector and optimization of the reactor design were made. The benefic contribution of radiation to heat transfer was revealed. Simulations shown that conversions similar to those obtained with a classical packed bed reactor can be obtained with significantly reduced pressure drop.

References

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Keywords
Structured catalytic reactor ; Steam methane reforming ; CFD reactor model ; Pilot plant tests