EXPERIMENTS AND PARTICLE-RESOLVED CFD MODELING OF CATALYTIC PARTIAL OXIDATION IN A LAB SCALE PACKED BED REACTOR

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Abstract

The thermal behavior of a typical lab-scale reactor for an Oxidative Coupling of Methane was investigated using spatially-resolved experiments and particle-resolved Computational Fluid Dynamics (CFD). Temperature profiles were measured using both moving thermocouple and infrared camera techniques for a wide range of exothermal conditions corresponding to temperature rise (400- 900°C) under various operating conditions. A particle-resolved CFD model has been developed to understand the complex heat transfer within the preheat zone, catalytic fixed bed, and post reaction zone. The role of different heat transfer modes (conduction, convection, and radiation) are evaluated as a function of the different thermal environments and these results are used to understand the spatial temperature distribution and the contribution of heat loss on the performance of the packed-bed reactors.

Keywords

OCM, Particle-resolved CFD, Infrared Thermography, Packed Bed.

Introduction

Packed bed reactors are widely used for several industrial processes such as partial oxidations, hydrogenations, methanation, propane dehydrogenation, and methane steam reforming. Understanding heat transfer within a catalyst bed is crucial for safely operating the reactor at high productivity, and for achieving the optimum performance. Although numerous empirical correlations have been proposed for the energy transport phenomena between gas and solid phases, these correlations may deviate an order of magnitude from each other due to the difficulty in distinguishing the solid and gas temperatures under high temperature conditions (Kunii 1977).

Without relying on transport correlations, we used a particle-resolved Computational Fluid Dynamics (CFD) to model an actual catalytic fixed bed reactor. Simulation was validated against the spatial temperature measurements from an Infrared Camera and an axially moving thermocouple for Oxidative Coupling of Methane process.

Experimental

A simplified schematic of experimental setup is shown in Fig.1. The mixture gas comprising methane and oxygen was supplied to a quartz tube reactor. The test section was placed in an electrical furnace to maintain the operational temperature.

Part of the furnace was replaced with a sapphire windows for Infrared Camera measurement of catalyst surface temperature. A type R thermocouple was attached to a linear translational stage and was housed in a thermal well for gas temperature measurement. The exhausted gas composition was measured using a 490 Agilent Micro GC.

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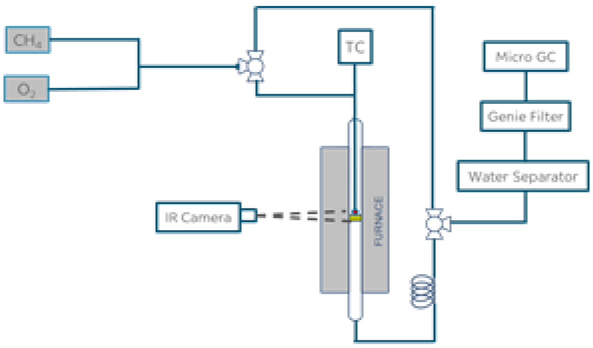

Figure 1. Schematic of reactor setup.

Particle-resolved CFD

A randomly packed bed of catalyst in a cylindrical reactor was generated using a DEM (Discrete Element Model) simulation by dropping particles into a reactor vessel and simulate till they are completely settled. Each catalyst pellet was treated as solid particles with conjugate heat transfer with gas phase. For reaction mechanism, a single step global reaction with the estimated stoichiometry from GC data was assumed on the surface of these particles. Thermodynamic and transport properties for the feed and product gases were taken from Chemkin database. To account for radiation heat transfer, Discrete Ordinates method was used.

Results

The thermal profiles show a hot zone on the catalyst surface at the beginning of the catalytic bed (Fig. 2a), while the temperature of the gas phase remains at significantly lower values (Fig. 3). The thermal behavior in this first zone can be explained considering the presence on the catalyst surface of highly exothermic total and partial oxidation reactions and heat transport limitations between the catalyst surface and the gas phase, that do not allow to equalize their temperatures. In the following part of the catalytic bed, the gas phase temperature increases reaching a maximum, with a corresponding decrease of that on the surface. Near to the end of the catalytic bed, the temperature of the catalyst surface is lower than that of the gas phase. The decrease of the surface temperature below the value in the gas phase in this zone is attributed to the axial and radial heat loss.

Although CFD simulations (Fig. 2b and 3) showed similar trends as that of experimental results, the discrepancy can be addressed to parameters estimation of a global kinetic model and also some inherent limitations in ascribing the heat source from the reactions to the particle surfaces. Additional details related to the role of radiation vs. convection/conduction for various peak temperatures in the reactor will be presented.

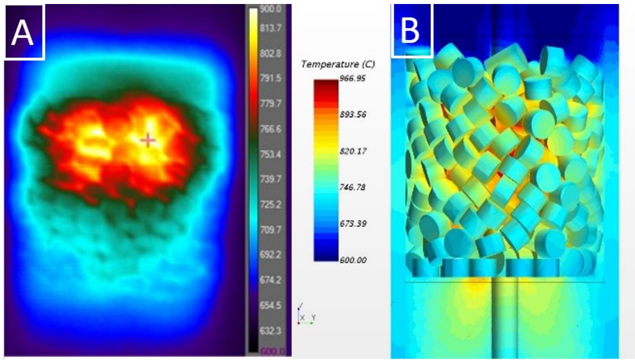

Figure 2. a) IR image of the peripheral catalyst surface temperature and b) CFD simulation results during the OCM test. Experimental conditions are residence time = 15 ms, $CH_4/O_2 = 7.4$

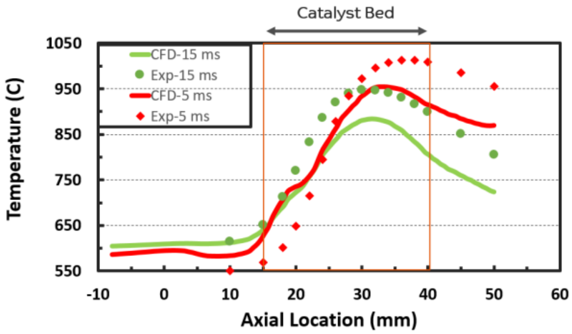

Figure 3. Axial temperature profiles measured by moving thermocouples were compared to the results simulated by CFD at $CH_4/O_2 = 7.4$, residence time = 15 ms and 5 ms respectively.

Conclusions

IR thermography and thermocouple measurements have shown large temperature gradients between surfaces and gaseous phases, as well as steep axial gradient temperature for OCM process. Comparisons between experimental temperatures and calculated CFD temperatures have shown the similar trends. Developing a detail micro kinetic mechanism and incorporating internal mass and heat transfers within particle are an ongoing work.

Acknowledgement

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References

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