CFD Analysis of the Zoneflow^{TM} Reactor for Methane Steam Reforming

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Abstract

Reactor concept

The *ZoneFlow^{TM}* Reactor (J.J. Feinstein, 2007 - *Tribute Creations LLC*) uses a structured packing in which two major and interconnected zones can be distinguished, the wall zone and the core zone (Figure 1). The core zone consists of layers comprising alternating perforated smooth and corrugated cones. The corrugated cones do not extend to the central axis of the tube, leaving there a circular opening permitting a fraction of the gas to flow directly from smooth cone to smooth cone. The perforations in the smooth and the corrugated cones are not positioned on the same vertical to avoid channeling of the gas. The wall zone consists of alternating sectors containing blades which direct the flow either centrifugally or centripetally. Radial fins separate the centrifugal and the centripetal sectors. The radial fins do not abut the wall of the reactor, leaving a gap through which the centrifugally and centripetally orienting wall zone sectors communicate. The structured packing is coated with a conventional Ni based catalyst.
The *ZoneFlow^{TM}* Reactor optimizes the heat transfer near the wall via relatively higher velocities in the wall zone and by directing the flow towards the reactor wall. Furthermore, the *ZoneFlow^{TM}* Reactor increases the effective amount of catalyst per unit reactor volume via a higher geometric surface area. It also optimizes the flow distribution and the residence time distribution in the reactor, with in particular a shorter residence time in the relatively hotter and more reactive wall zone than in the core zone of the reactor.

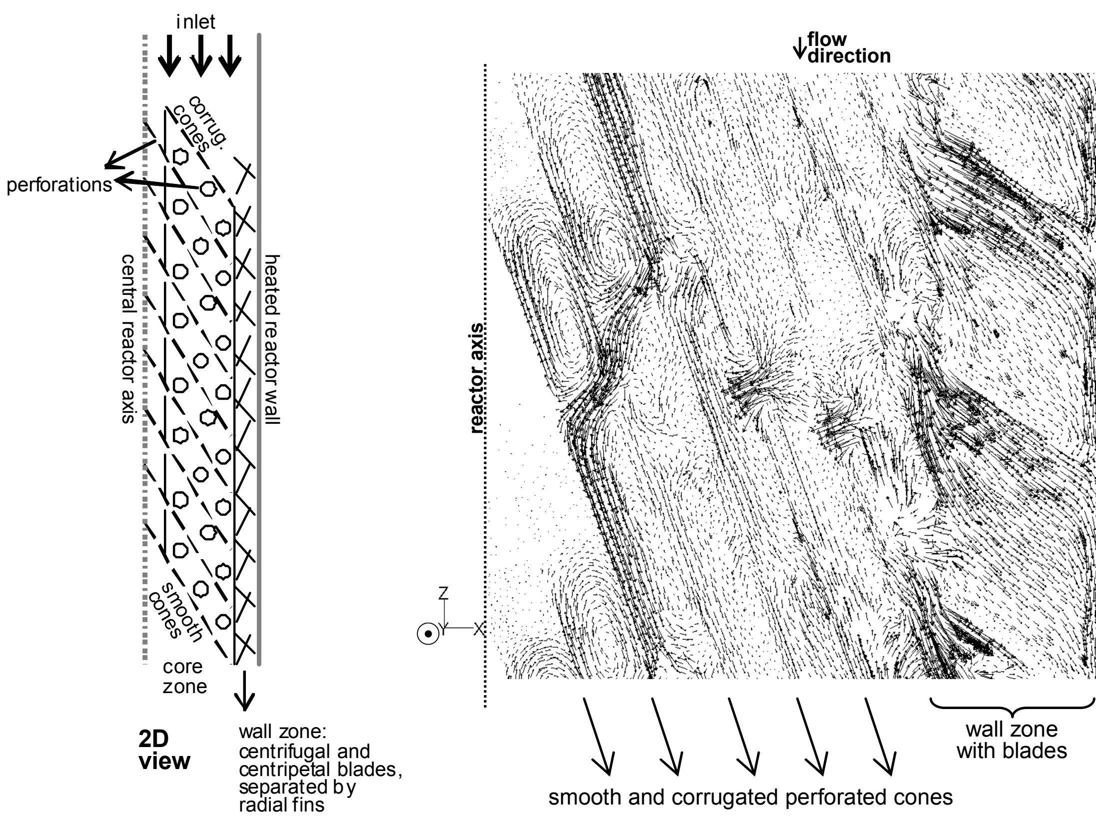
Application to methane steam reforming

The performance of the *ZoneFlow^{TM}* Reactor for methane steam reforming was evaluated via 3D computational fluid dynamics (CFD) simulations. The industrial operating conditions of Xu and Froment (1989b) were used and a comparison with conventional fixed bed reactor technology was made. For the complex *ZoneFlow^{TM}* Reactor geometry, a 10° sector of a 1 meter reactor length was simulated. The flow pattern was fully developed after 30 cm (Figure 1(b)). Turbulence, heat transfer by convection and radiation, detailed reaction kinetics including coking, and the compressibility of the gas phase were accounted for. A Reynolds Averaged Navier Stokes (RANS) approach was taken. Turbulence was modeled by introducing the turbulent kinetic energy k and the turbulence dissipation ε, for which extra transport equations were solved. A gray radiation model was used and the Rosseland or diffusion approximation for radiation was adopted. The fundamental kinetic model for steam reforming of methane of Xu and Froment (1989) was used. The coking reactions were accounted for using the kinetic model of Snoeck et al. (2002, 2003). Internal diffusion limitations were shown to be very

important in methane steam reforming (Xu and Froment, 1989b) and were accounted for via the catalyst effectiveness factor. To increase the catalyst effectiveness factor and to limit the pressure drop over the reactor, the catalyst layer thickness was limited to 80 µm in the present simulations.

Results and discussion

The simulations show that the flow field is complex (Figure 1(b)) and the velocity gradients in the reactor are important, both in the core and wall zone of the reactor. Furthermore, most of the flow is directed through the wall zone of the reactor. In the core zone, the flow jetting through the perforations results in vortex formation and generates both downward and upward flow in between the cones (Figure 1(b)). The position of the perforations in the cones is of importance to prevent channeling. The high velocity gradients resulting from the presence of the cones, the perforations in the cones, the blades, and the radial fins cause significant turbulence. The latter is the most pronounced in the wall zone of the reactor, improving the heat transfer between the heated reactor wall and the catalyst surfaces. Heat transfer resistance between the bulk gas and the catalyst surfaces was found to be important. The axial pressure gradient in the *ZoneFlow*^{TM} Reactor was found to be only slightly higher than in the conventional fixed bed reactor.



(a) (b)

Figure 1: (a) Schematic 2D representation of the *ZoneFlow*^{TM} Reactor; (b) Velocity vector profile in a cross section with centrifugal blades in the wall zone.

Two compensating effects allow obtaining radially uniform methane conversion and product concentration profiles in the *ZoneFlow*^{TM} Reactor: 1) Most of the flow is directed towards the wall zone, resulting in longer gas-catalyst contact times in the core zone and, for most of the gas, shorter gas-catalyst contact times in the wall zone. 2) Significantly higher temperatures in the wall than in the core zone, implying higher reaction rates in the former. Further optimization of the reactor concept is possible, for example by a radially non-uniform distribution of the catalyst.
Compared to the conventional reactor technology (Xu and Froment, 1989), the *ZoneFlow*^{TM} Reactor shows reaction and heat transfer rates that are increased significantly, due to flow patterns improving heat transfer near the wall and to a significantly higher geometric surface area providing a greater amount of effective catalyst per cubic meter of reactor.
Finally, for the operating conditions investigated in the present work, the coke gasification easily equals the coke formation at steam to carbon ratios significantly lower than those used in conventional steam reformers, even at the heated wall.

<u>References</u>

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