346e Comparison of Low Effectiveness Catalyst Particles in Fixed Beds Using CFD with Heat Sinks

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Modeling of fluid flow, heat transfer and reaction in fixed beds is an essential part of their design. This is especially critical for highly endothermic or exothermic reactions in low tube-to-particle diameter ratio (N) tubes, such as are used in steam reforming and partial oxidation. In our previous work, comparative studies were performed to show the effect of catalyst design on heat transfer performance in the near-wall region, in a steam reforming packed bed reactor tube. Computational Fluid Dynamics (CFD) was used to obtain detailed flow and temperature fields in a representative wall segment of the tube. Simulations in which inert packing was heated up showed that particles with no internal voids appeared to perform better than particles with internal voids, in the bed interior. However these simulations ignored the influence of catalyst geometry on the reaction heat effects. Present state-of-the-art in CFD does not permit the representation of species diffusion, conduction and reaction inside solid regions, such as catalyst particles. To approximate the heat effects in steam reforming, temperature-dependent heat sinks were introduced into the particles. This was complicated by the very low effectiveness factors in these catalysts, so that the particles behaved like egg-shell catalysts. This was especially challenging for particles with internal voids. Our approach to this problem implemented user-defined functions in the CFD code Fluent 6.1. Simulations were performed under realistic industrial conditions of high temperature, pressure and gas flow rate, with gas properties corresponding to those of steam reforming. A constant wall heat flux was imposed, and various shapes of particles studied with heat sinks to simulate the reforming endothermic reaction. When heat sinks were included in the particles to represent the thermal effects of chemical reaction, the heat effects of the particles were shown to change markedly, both qualitatively and quantitatively. The radial temperature profiles of the fixed bed were obtained for cylindrical catalyst particles with different sizes and numbers of internal voids. These profiles were interpreted by comparison to the related bed voidage and active region profiles, and it was found that both of the above factors interacted to affect the temperature profile. The 4-hole catalyst particle showed the best heat sink performance, and this observation was explained by considering the total surface area of the catalyst particles. Finally, the effect of wall conduction was analyzed utilizing all the catalyst particles for a typical industrial case. There were no significant differences observed with this inclusion.