A multi-region model for reaction-diffusion process in a catalyst particle

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Zeolite catalysts have large applications in a variety of industrial sectors, such as FCC and MTO. In practice, catalyst particles used in industrial reactors have complicated porous structures, in which pores with hierarchical sizes may co-exist [1, 2]. As shown in Fig. 1(a), an industrial catalyst particle is composed of micro-pore zeolites and meso/macro-pore catalyst support. Despite the reaction–diffusion process inside the zeolites, the transport and thus the reaction in an industrial catalyst particle are also highly related to the fraction, size, and position of the micro-pore zeolites. Here, a multi-region model based on the unified Maxwell–Stefan diffusion theory was developed to investigate the reaction–diffusion processes within catalyst particles formed by micro-pore zeolites and meso/macro-pore support [3]. By simulating the process of alkylation of benzene over a single catalyst particle formed with H-ZSM-5 zeolites, the effects of volume fraction, size and spatial distribution of H-ZSM-5 zeolites on the effectiveness factor of the catalyst particle were then investigated and discussed.

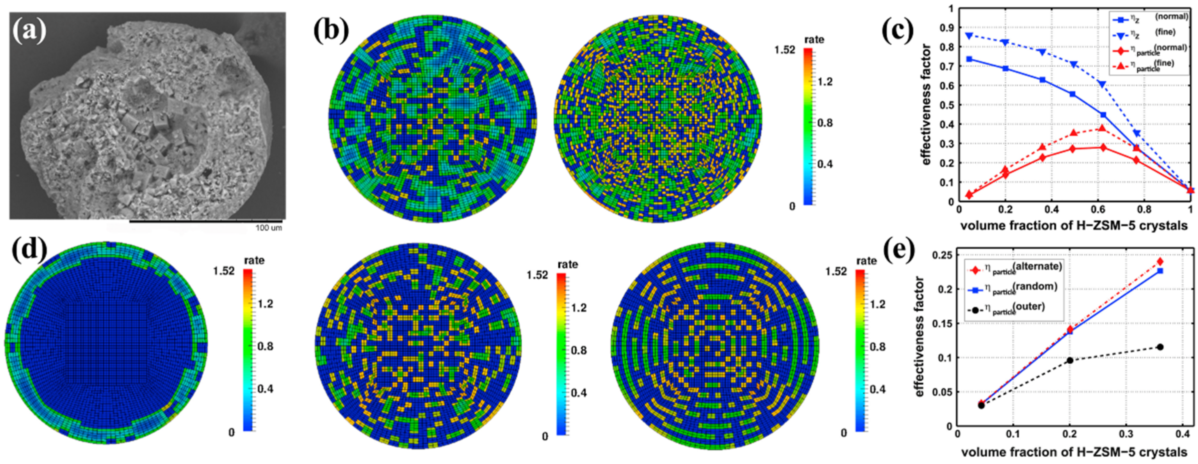

Figure 1: (a) Interior of catalyst particle used in industrial process. (b) The distribution of zeolite and reaction rate inside catalyst particle with volume fraction of H-ZSM-5 of 0.62. (c) Effectiveness factor as a function of volume fraction of H-ZSM-5 for both normal and fine crystal sizes. (d) The spatial distribution of zeolites and reaction rate inside catalyst particle. (e) Effectiveness factor for zeolites with different spatial distribution.

As shown in Fig. 1(b, c), our simulations verified that the catalyst particle composed by fine size of zeolites has higher effectiveness factor than that composed by normal size of zeolites. Our simulations suggest that the intracrystalline diffusion resistance within the zeolite region is decisive for the effectiveness factor of the catalyst particle. In Fig. 1(d, e), our simulations indicate that the effectiveness factor of outer distribution deviates significantly from that of the other two distributions when the volume fraction of zeolites is increased. The alternate distribution has the best catalytic performance when the volume fraction of zeolites is lower than 0.36.

It is shown that the multi-region model developed in this work is a potential bottom to up tool for reaction-diffusion processes inside a catalyst particle exhibiting multi-scale time characteristic. The possible applications include rational design for catalyst encountered in many industrial applications.

References

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