Efficient and robust method for numerical analysis of dead zone in catalyst particle and packed bed reactor.

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Abstract

For two processes of large importance, catalysis and biocatalysis, were reported zones without reactants, so called dead zone (DZ). They results from diffusional transport limitations, when apparent reaction order is between (-1..1). Formation of DZ reduces effectiveness of catalyst and influence packed bed reactor productivity. For simple reaction kinetic model, a DZ width inside a pellet can be calculated analytically solving appropriate differential mass balance model. However, generally the analytical solution is unknown and only with using numerical method the position of DZ can be established. The problem with DZ appearance belongs to problems with moving boundaries. Its solution requires application of special numerical procedure and relatively long CPU time. In this work it was proposed a simple, very fast numerical method for calculation of DZ position inside pellet. The method proposed combined with orthogonal collocation on finite elements can be applied for analysis of work of packed bed reactor.

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