A multiscale model of packed-bed catalytic reactors

김다모아, 김세영, 박홍목†
서강대학교
(hmpark@sogang.ac.kr†)

The packed-bed may be viewed as consisting of two distinct fields, i.e., one existing on the macroscale and the other existing on the microscale levels. The macroscale temperature and concentration fields are found from a hypothetical continuum model of particle-fluid heterogeneous media. Each macroscale differential volume element contains several catalyst pellets, each of which is a microscale continuum embedded in a gross macroscale external fields. The boundary conditions of the microscale fields at the catalyst pellets are provided by the solution of the macroscale model equations, while the heat and mass source terms of the macroscale model equations are determined by the heat and mass transfer and chemical reactions within the catalyst pellets. In the present investigation, we have considered the HPPO process in which the propene oxide is produced by oxidizing propene with hydrogen oxide using the titanium silicalite-1(TS-1) catalysis. The set of six partial differential equations for the macroscale field coupled with the set of five partial differential equations for the microscale field at each macroscale point is solved employing the numerical Green's function technique to overcame the inherent numerical instability in this coupled PDE system.