Modelling of Reactive Non-Isothermal Mixture Flow and Its Simulation in COMSOL Multiphysics® Software

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Abstract

I introduce a model of fluidized reactor which, in presence of heterogeneous platinum-based catalyst, decomposes liquid formic acid producing gaseous mixture of carbon dioxide and hydrogen as the product. I treat the physical system as a (Class II) mixture of four constituents - namely formic acid (FA), Platinum micro-pellets (Pt), carbon dioxide (CO_2) and hydrogen (H_2) - which can be, without loss of generality, reduced to a binary mixture of continuous phase (Pt + FA) and dispersed phase (CO_2+H_2).

Physical interaction between the phases is modelled by the pressure-drag balance and chemical interaction undergoing Arrhenius kinetics. Since all the constituents (hence both phases) share one thermal field with thermal flux from warmer walls and thermal sink due to endothermal reactions, the thermal convection occurs driven by temperature gradient. Finally, we consider the gravitation and (constant) control volume of the reactor with open (top) boundary for gaseous outflow and formic acid inflow in the bottom. The computations are performed in COMSOL Multiphysics®.

Reference

K. Hutter, K. J\"ohnk, Continuum methods of physical modelling, Springer-Verlag Berlin-Heidelberg, 2004.
H.A. Jakobsen. Chemical Reactor Modeling: Multiphase Reactive Flows. Springer, 2008.
R. Clift, J.R. Grace, and M.E. Weber. Bubbles, Drops, and Particles. Dover Civil and Mechanical Engineering Series. Dover Publications, 2005.
E.A. Guggenheim. Thermodynamics: An Advanced Treatment for Chemists and
W.C. Yang. Handbook of Fluidization and Fluid-Particle Systems. Chemical Industries. Taylor & Francis, 2003.