Modeling of Non-isothermal Reacting Flow in Fluidized Bed Reactors

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Abstract

Abstract:
We investigate a prototype concept of a back-up electricity device where we use liquid formic acid (FA) to produce a mixture of carbon dioxide (CO2) and hydrogen (H2) which is used in a PEM fuel cell, Fig. 1. In the fluidized bed reactor the liquid FA is decomposed to a gaseous mixture of CO2 and H2 in the presence of microscopic floating solid catalytic particles. We describe the system, contained in a fixed control volume, as a mixture composed of five constituents - liquid FA, gaseous FA (FAg), catalyst micro-particles (Cat), CO2 and H2. For the individual mixture components, we distinguish partial densities and momenta, while we only consider one common temperature field for the mixture as a whole. We reduce the five-constituents model to a binary mixture model of liquid phase (Cat + FA) and gaseous phase (CO2 + H2 +FAg) which forms bubbles. The liquid phase is considered as a compressible viscous fluid with temperature-dependent density and viscosity depending on both the temperature (Arrhenius model) and the volume fraction of the catalyst particles. The gaseous phase is considered as an ideal gas mixture where the molar-ratio of H2 and CO2 is 1:1. Since we assume local gas/liquid equilibrium where the liquid is already saturated by all three gaseous constituents, the amount of FAg in the bubbles depends on the saturation pressure (i.e. temperature and ambient pressure) and any interfacial mass flow is neglected. Chemical rates satisfy mass-action law and follow the Arrhenius kinetics. The quasi-steady model was implemented numerically in COMSOL Multiphysics and we present several simulations addressing primarily the role of saturation pressure and another important dependencies.

Keywords: multi-phase flow, fluidized bed reactor, gas-liquid equilibrium, bubbly flow, bubble growth

Use of COMSOL Multiphysics®:
We implemented the model using combination of "Laminar Bubble Flow" and "Heat Transfer in Fluids" Physics both included in CFD module. We defined material properties of the two phases, i.e. gaseous mixture (FA, H2, CO2) and mixture of liquid FA with catalytic particles. Their material properties were defined in way to realistically describe various dependencies. Furthermore, we redefine the bubble flow model according to Karamanev and we introduced some implicit constitutive relations. Here we have to introduce additional step in segregated solver by adding auxiliary PDE's - this can be also understand as additional stabilization.

Reference

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Figures used in the abstract

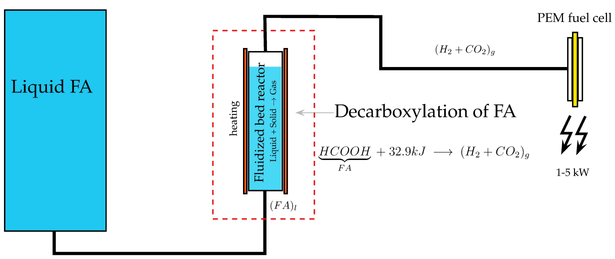

Figure 1: Schema of the device.

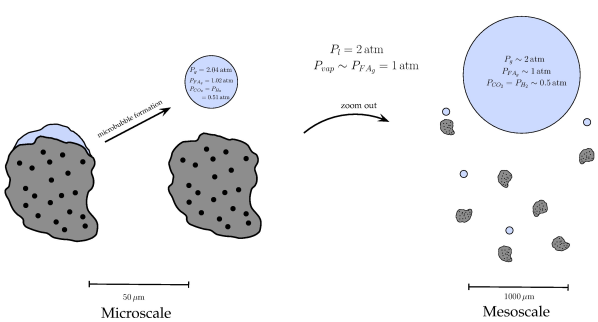

Figure 2: Bubble formation.