



# Multi-phase modeling of non-isothermal reactive flow in fluidized bed reactors

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## ABSTRACT

We investigate a model of a fluidized bed reactor decomposing liquid formic acid and producing gaseous mixture of carbon dioxide and hydrogen in the presence of microscopic solid catalytic particles. We describe the system, contained in a fixed control volume, as a mixture composed of four constituents—formic acid (*FA*), catalyst micro-particles (*Cat*), carbon dioxide ( $\text{CO}_2$ ) and hydrogen ( $\text{H}_2$ ). 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 four-constituents model to a binary mixture model of liquid phase (*Cat* + *FA*) and gaseous phase ( $\text{CO}_2$  +  $\text{H}_2$ ) which forms bubbles.

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. Physical interaction between the bubbles and the liquid is modeled under simplifying assumptions by the pressure-drag balance. The chemical rates satisfy mass-action law and undergo Arrhenius kinetics. The model was implemented numerically in COMSOL Multiphysics and we present several simulations addressing primarily the role of liquid viscosity and imposed wall temperature on the performance and flow regime inside the reactor.

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## 1. Introduction

In the recent years, proper understanding and optimization of the process of hydrogen production at the industrial scale has become a topic of utmost importance. This is mainly due to the primal role of hydrogen as a fuel in most types of fuel cells whose application in various industry segments has been growing rapidly, see [1]. Production of hydrogen by formic acid (*FA*) decomposition is one promising route to overcome inherently difficult and inefficient storage of hydrogen itself [2]. Different noble-metal catalysts and chemical aspects were reviewed for the *FA* decomposition [2], but the actual physical processes taking place in the reactor for *FA* decomposition were not yet investigated. In this work, we develop a mathematical model for the physical processes taking place in the fluidized bed reactor for *FA* decomposition. The liquid phase *FA* is decomposed to gaseous mixture of carbon dioxide ( $\text{CO}_2$ ) and hydrogen ( $\text{H}_2$ ) during the presence of the catalytic particles.

Although the liquid and gaseous phases are macroscopically distinguishable, we model the system in the framework of continuum multi-phase theory, employing volume-averaged properties and balance equations. In such description, all

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phases are equi-present in each point of the physical space (with possibly highly-variable concentration from place to place) and, consequently, the arising framework for the system description is the continuum mixture (multi-phase) mechanics and thermodynamics.

We start by formulating the partial balances of mass for all four constituents and then reduce the model to only two sub-phases (liquid and gas). We formulate the partial momentum balances for the two sub-phases and we conclude by postulating one common internal energy balance for the mixture as a whole. Finally, supplementing the system with constitutive relations leads to the desired closure of the system. The model is numerically implemented in COMSOL Multiphysics software and several numerical simulations are presented.

## 2. Partial mass balances

### 2.1. General form of partial mass balance

The multi-phase averaged partial balance equation for mass for  $\alpha$  constituent reads [3]:

$$\partial_t(\Phi_\alpha \rho_\alpha^{true}) + \text{div}(\Phi_\alpha \rho_\alpha^{true} \mathbf{u}_\alpha) = m_\alpha, \tag{1}$$

where  $\rho_\alpha^{true}$  denote the true material densities of the constituents (densities of the pure substances);  $\mathbf{u}_\alpha$  are their partial velocities and  $\Phi_\alpha$  stand for their volume fractions (i.e. local fraction of volume occupied by each phase per volume of the mixture);  $m_\alpha$  denote mass production rates due to chemical reactions. As a consequence of the mass conservation in the chemical reactions, the mass-production terms due to chemical reactions must sum up to zero:

$$\sum_\alpha m_\alpha = 0. \tag{2}$$

Invoking the standard stoichiometric description, it is convenient to rewrite the mass-production terms as

$$m_\alpha = \sum_{z=1}^Z M_\alpha \nu_\alpha^z r_z^{ch}, \tag{3}$$

where  $M_\alpha$  denotes the molar mass of the  $\alpha$  component,  $\nu_\alpha^z$  denotes the corresponding stoichiometric coefficient of the  $\alpha$  constituent in the  $z$ -th reaction (considered positive for the products and negative for the reactants);  $r_z^{ch}$  denotes the rate of the  $z$ -th chemical reaction, and  $Z$  denotes the number of the chemical reactions.

### 2.2. Particular setting—dissociation of formic acid on dispersed solid catalyst

In our particular setting, we consider a four-component system, the constituents being the (liquid) formic acid (FA),<sup>1</sup> the microscopic solid catalytic particles (e.g. palladium based [4] or ruthenium based [5]) (*Cat*), hydrogen ( $H_2$ ) and carbon dioxide ( $CO_2$ ). The only considered chemical reaction is the dissociation of the formic acid into carbon dioxide and hydrogen:



With the given notation for the mass-production terms, the system of partial mass balances for the four-component system undergoing the considered chemical reaction reads:

$$\partial_t(\Phi_{FA} \rho_{FA}^{true}) + \text{div}(\Phi_{FA} \rho_{FA}^{true} \mathbf{u}_{FA}) = -M_{FA} r^{ch}, \tag{5a}$$

$$\partial_t(\Phi_{Cat} \rho_{Cat}^{true}) + \text{div}(\Phi_{Cat} \rho_{Cat}^{mix} \mathbf{u}_{Cat}) = 0, \tag{5b}$$

$$\partial_t(\Phi_{CO_2} \rho_{CO_2}^{true}) + \text{div}(\Phi_{CO_2} \rho_{CO_2}^{true} \mathbf{u}_{CO_2}) = M_{CO_2} r^{ch}, \tag{5c}$$

$$\partial_t(\Phi_{H_2} \rho_{H_2}^{true}) + \text{div}(\Phi_{H_2} \rho_{H_2}^{true} \mathbf{u}_{H_2}) = M_{H_2} r^{ch}. \tag{5d}$$

Note that since

$$M_{FA} = M_{CO_2} + M_{H_2}, \tag{6}$$

the constraint (3) is satisfied.

### 2.3. Further simplifications

Now we introduce several simplifying physical assumptions which are specific to our desired experimental setting:

1. We assume that both gases ( $CO_2$  and  $H_2$ ) are always produced together (in the considered chemical reaction), forming bubbles of binary gaseous mixture. Consequently, neglecting the diffusion of the gas into the liquid across the walls of the

<sup>1</sup> In this setting we do not consider possible evaporation of FA, i.e. its gaseous phase.

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