Modeling of Non-Isothermal Reacting Flow in Fluidized Bed Reactors

Vít Orava$^{1,2}$, Ondřej Souček$^2$, Peter Cendula$^1$

$^1$Institute of Computational Physics, ZHAW, Switzerland
$^2$Faculty of Mathematics and Physics, CUNI, Czech Republic

October 15, 2015

What is a fluidized bed reactor?

**Bubble column reactor:**
- Liquid $\rightleftharpoons$ Gas
- Dissolution of the gas into the liquid.

**Packed bed reactor:**
- Solid $\rightleftharpoons$ Gas
- Heterogeneous catalysis in porous immobilized macro-structure

**Fluidized bed reactor:**
- Liquid $\rightleftharpoons$ Gas
- Heterogeneous catalysis on moving micro-structure.
The application: Hydrogen generator coupled to PEM FC

Hydrogen (gas) is produced by endothermal decarboxylation of formic acid (liquid) - in presence of a (solid) catalyst.

Purpose: Using formic acid as a fuel to generate $1 - 5\, kW$.

Typical usage: back-up devices, i.e. start-up in a few minutes, works for many hours, comparable with diesel aggregate.

Figure: Scheme of the HyForm system.
Constituents and phase transitions within the reactor

- We treat the system, contained in a fixed control volume, as a mixture of 7 constituents:

  \[ FA(l), FA(g), CO_2(d), CO_2(g), H_2(d), H_2(g), Cat(s). \]

  Subscripts "(l), (g), (s)" denote liquid, gas, solid phase and "(d)" refers to dissolved phase.

- Along the decarboxylation of formic acid

  \[ FA(l) \xrightarrow{32.9kJ} H_2(d) + CO_2(d) \]

  we consider four phase transitions (evaporation) mechanisms

  \[ FA(l) \xrightarrow{23.1kJ} FA(g) \]

  \[ H_2(d) \rightarrow H_2(g) \]

  \[ CO_2(d) \rightarrow CO_2(g). \]

  Other transformation processes are assumed to be negligible.
Distinguishing partial densities and momenta, we consider one common temperature field - so called Class II model.

There is a natural division of the constituent within two groups forming, so called, pseudo phases where:

(i) **Gaseous phase:** denoted by \( (\cdot)_g \) - consists of \( CO_2(g) \), \( H_2(g) \) and \( FA(g) \) which share one common velocity field \( \mathbf{u}_g \) and \( \Phi_g := \Phi_{CO_2(g)} = \Phi_{H_2(g)} = \Phi_{FA(g)} \).

(ii) **Liquid phase:** denoted by \( (\cdot)_l \) - consists of \( FA(l) \) and dissolved \( CO_2(d) \), \( H_2(d) \) which share one common velocity field \( \mathbf{u}_l \) and \( \Phi_l \approx \Phi_{FA} \).

(iii) **Solid phase:** denoted by \( (\cdot)_s \) - consists of \( Cat(s) \).

(ii)* **Suspension:** denoted by \( (\cdot)_{ls} \) - mixture of liquid and solid where \( \Phi_{ls} := \Phi_l + \Phi_s \).
**Mixture theory**
- handling mass concentrations $c_i$
- no interfacial phenomena
- usually CPU friendly

**Two-phase theory**
- handling volume fractions $\Phi_i$
- tracking of interfaces
- **CPU-costly**, steady solution (?!)

**Our approach: Multi-phase (scale-up averaging) theory**
- Geometry of interfaces follow the mixture approach.
- Interfacial phenomena are caught in the model.

\[
\partial_t (\Phi_{ls} \rho^{true}_{ls}) + \text{div} \left( \Phi_{ls} \rho^{true}_{ls} \mathbf{u}_{ls} \right) = -\dot{m}_g \\
\partial_t (\Phi_g \rho^{true}_g) + \text{div} \left( \Phi_g \rho^{true}_g \mathbf{u}_g \right) = M_{CO_2(d)} r^{ev}_{CO_2(d)} + M_{H_2(d)} r^{ev}_{H_2(d)} + M_{FA} r^{ev}_{FA(l)} \\
\partial_t (\Phi_s \rho^{true}_s) + \text{div} (\Phi_s \rho^{true}_s \mathbf{u}_s) = 0 \\
\partial_t (\Phi_{CO_2(d)} \rho^{true}_{CO_2(d)}) + \text{div} (\Phi_{CO_2(d)} \rho^{true}_{CO_2(d)} \mathbf{u}_l) + \mathbf{J}_{CO_2} = M_{CO_2(d)} r^{ch} - M_{CO_2(d)} r^{ev}_{CO_2(d)} \\
\partial_t (\Phi_{H_2(d)} \rho^{true}_{H_2(d)}) + \text{div} (\Phi_{H_2(d)} \rho^{true}_{H_2(d)} \mathbf{u}_l) + \mathbf{J}_{H_2} = M_{H_2(d)} r^{ch} - M_{H_2(d)} r^{ev}_{H_2(d)} \\
\Phi_{ls} \rho^{true}_{ls} \frac{d \mathbf{u}_{ls}}{dt} = -\Phi_{ls} \nabla \mathbf{p}_{ls} + \Phi_{ls} \rho^{true}_{ls} \nu_{ls} \mathbf{I}_{ls} + \Phi_{ls} \rho^{true}_l \mathbf{g} - \dot{m}_g \mathbf{u}_{ls} + \Phi_{ls} \Phi_g \frac{3 \cdot C_d \rho^{true}_{ls}}{8 r_g} |\mathbf{u}_{slip}||\mathbf{u}_{slip}^{ls}|
\]

\[
\nabla \left( \rho^{dyn}_{ls} + \Phi_g \frac{2 \sigma}{r_g} \right) + (\Phi_{ls} \rho^{true}_{ls} - \Phi_g \rho^{true}_g) \mathbf{g} = -\Phi_{ls} C_d \frac{3 \rho^{true}_{ls}}{8 r_g} |\mathbf{u}_{slip}||\mathbf{u}_{slip}^{ls}|
\]

\[
(\rho^{true}_l - \rho^{true}_s) \nabla \rho^{dyn}_{ls} + (\rho^{true}_l - \rho^{true}_s) \mathbf{g} = -\frac{9}{2} \Phi_{ls} \rho^{true}_{ls} \nu_{ls} \mathbf{u}_{slip}^{ls}
\]

\[
\rho C_p \frac{d u}{dt} - k \Delta T = -\frac{L_{ch}}{M_{FA}} r^{ch}_{FA} - \frac{L^{ev}_{FA}}{M_{FA}} r^{ev}_{FA} - \frac{L^{diss}_{CO_2(d)}}{M_{CO_2(d)}} r^{ev}_{CO_2(d)} - \frac{L^{diss}_{H_2(d)}}{M_{H_2}} r^{ev}_{H_2(d)}
\]

\[
\partial_t n + \text{div} (n \mathbf{u}_g) = R
\]
Quasi-steady model

Performing parameter analysis and neglecting of some minor terms, we look for variables $\Phi_g, \Phi_{sl}, u_g, u_{ls}, p_{ls}, T$ and $n$ such that the following holds:

$$\partial_t (\Phi_{ls} \rho_{ls}^{true}) + \text{div} (\Phi_{ls} \rho_{ls}^{true} u_{ls}) = -M_{FA} r^{ch} \quad \text{(MaB.1)}$$

$$\partial_t (\Phi_g \rho_{g}^{true}) + \text{div} (\Phi_g \rho_{g}^{true} u_{g}) = M_{FA} r^{ch} \quad \text{(MaB.2)}$$

$$\partial_t (\Phi_s \rho_{s}^{true}) + \text{div} (\Phi_s \rho_{s}^{true} u_{s}) = 0 \quad \text{(MaB.3)}$$

$$\Phi_{ls} \rho_{ls}^{true} \frac{d_{ls} u_{ls}}{dt} = -\Phi_{ls} \nabla p_{ls} + \Phi_{ls} \rho_{ls}^{true} \nu_{ls} \nabla \Phi_{ls} + \Phi_{ls} \rho_{g}^{true} \Phi_g - \dot{m}_{gl} u_{ls} + \Phi_{ls} \Phi_g \frac{3}{8} \frac{C_d \rho_{ls}^{true}}{r_g} |u_{slg}| u_{slg} \quad \text{(MoB.1)}$$

$$g = -\frac{3}{8} \frac{C_d}{r_g} |u_{slg}| u_{slg} \quad \text{(MoB.2)}$$

$$(\rho_{g}^{true} - \rho_{s}^{true}) g = -\frac{9}{2} \frac{\Phi_{ls} \rho_{ls}^{true} \nu_{ls}}{r_s^2} u_{sl} \quad \text{(MoB.3)}$$

$$\rho C_p \frac{d u_T}{dt} - k \Delta T = -\frac{L^{ch}}{M_{FA}} r^{ch} \quad \text{(EnB)}$$

$$\partial_t n + \text{div} (nu_{g}) = R \quad \text{(Pop)}$$

where $\Phi_{ls} + \Phi_g = 1, u_{sl}^{ls} = u_s - u_l, u_{sl}^{slip} = u_{sl} - u_l$
COMSOL implementation

1. Full model:
   - Laminar Bubbly Flow (CFD Module):
     - MaB.1, MaB.2, MoB.1, MoB.2
   - Heat Transfer in Fluids: EnB
   - Coefficient Form PDE:
     - MaB.3, MaB.4 + MaB.5, Pop
   - explicit form: MoB.3

2. Quasi-steady model:
   - Laminar Bubbly Flow (CFD Module):
     - MaB.1, MaB.2, MoB.1, MoB.2
   - Heat Transfer in Fluids: EnB
   - Coefficient Form PDE:
     - MaB.3, Pop
   - explicit form: MoB.3
The results: Floating

Figure: Velocity Field Liquid, Temperature, Gas Concentration, Solid Concentration.
The results: Traffic Jam Effect

Figure: Velocity Field Liquid, Temperature, Gas Concentration, Solid Concentration.

Traffic Jam Effect: $\rho_s^{true} < \rho_l^{true}$
Thank you for your attention!

Details on my poster.

Acknowledgement

- We thank M. Grasemann, A. Dalebrook G. Laurenczy a J. Schumacher for providing preliminary experimental observations and fruitful discussions during the investigation of the problem.

- This work was supported by CCEM and Swisselectric Research under project Hy-Form and by MŠMT CZ under project SVV 260220/2015.