Modeling of Non-Isothermal Reacting Flow in Fluidized Bed Reactors

Vít Orava[1,2], Ondřej Souček[2], Peter Cendula[1]

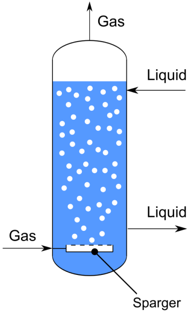
[1]Institute of Computational Physics, ZHAW, Switzerland
[2]Faculty of Mathematics and Physics, CUNI, Czech Republic

October 15, 2015

Orava et al., *Multi-phase modeling of non-isothermal reactive flow in fluidized bed reactors*, J. Comp. App. Math., 2015.

COMSOL CONFERENCE 2015 GRENOBLE

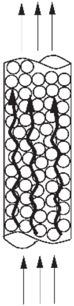
What is a fluidized bed reactor?



Bubble column reactor:

liquid ⇋ gas

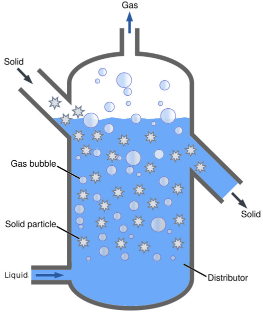
Dissolution of the gas into the liquid.



Packed bed reactor:

gas $\overset{solid}{\leftrightharpoons}$ gas

Heterogeneous catalysis in porous **immobilized** macro-structure



Fluidized bed reactor:

liquid $\overset{solid}{\leftrightharpoons}$ 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.

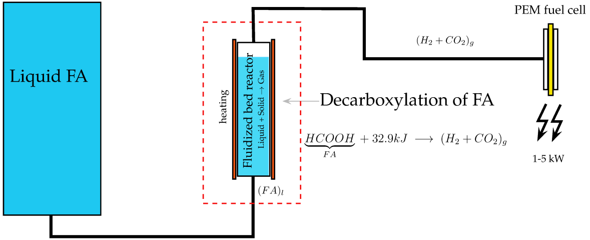


Figure : Scheme of the HyForm system.

- Purpose: Using formic acid as a fuel to generate $1 - 5kW$.
- Typical usage: back-up devices, i.e. start-up in a few minutes, works for many hours, comparable with diesel aggregate.

Constituents and phase transitions within the reactor

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

$$FA_{(l)}, FA_{(g)}, CO_{2(d)}, CO_{2(g)}, H_{2(d)}, H_{2(g)}, Cat_{(s)}.$$

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

$$FA_{(l)} \xrightarrow{23.1kJ} FA_{(g)}$$
$$H_{2(d)} \longrightarrow H_{2(g)}$$
$$CO_{2(d)} \longrightarrow CO_{2(g)}.$$

Other transformation processes are assumed to be negligible.

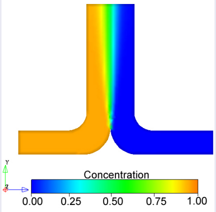
Model setting

- 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 $()_g$ - 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 $()_l$ - 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 $()_s$ - consists of $Cat_{(s)}$.

  (ii)* **Suspension:** denoted by $()_{ls}$ - mixture of liquid and solid where $\Phi_{ls} := \Phi_l + \Phi_s$.

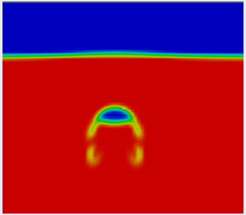
Mixture theory

- handling mass concentrations c_i
- no interfacial phenomena
- usually CPU friendly



Two-phase theory

- handling volume fractions Φ_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.

SLATTERY, J. C., *Momentum, Energy and Mass Transfer in Continua*, McGraw-Hill Book Co., 1972.

Full model

$$\partial_t(\Phi_{ls}\rho_{ls}^{true}) + \mathrm{div}\left(\Phi_{ls}\rho_{ls}^{true}\mathbf{u}_{ls}\right) = -\dot{m}_{gl} \tag{MaB.1}$$

$$\partial_t(\Phi_g\rho_g^{true}) + \mathrm{div}\left(\Phi_g\rho_g^{true}\mathbf{u}_g\right) = M_{CO_{2(d)}} r^{ev}_{CO_{2(d)}} + M_{H_{2(d)}} r^{ev}_{H_{2(d)}} + M_{FA} r^{ev}_{FA_{(l)}} \tag{MaB.2}$$

$$\partial_t(\Phi_s\rho_s^{true}) + \mathrm{div}(\Phi_s\rho_s^{true}\mathbf{u}_s) = 0 \tag{MaB.3}$$

$$\partial_t(\Phi_{CO_{2(d)}}\rho^{true}_{CO_{2(d)}}) + \mathrm{div}(\Phi_{CO_{2(d)}}\rho^{true}_{CO_{2(d)}}\mathbf{u}_l) + \mathbf{J}_{CO_{2(d)}} = M_{CO_{2(d)}} r^{ch} - M_{CO_{2(d)}} r^{ev}_{CO_{2(d)}} \tag{MaB.4}$$

$$\partial_t(\Phi_{H_{2(d)}}\rho^{true}_{H_{2(d)}}) + \mathrm{div}(\Phi_{H_{2(d)}}\rho^{true}_{H_{2(d)}}\mathbf{u}_l) + \mathbf{J}_{H_{2(d)}} = M_{H_{2(d)}} r^{ch} - M_{H_{2(d)}} r^{ev}_{H_{2(d)}} \tag{MaB.5}$$

$$\Phi_{ls}\rho_{ls}^{true}\frac{\mathrm{d}_{ls}\mathbf{u}_{ls}}{\mathrm{d}t} = -\Phi_{ls}\nabla p_{ls} + \Phi_{ls}\rho_{ls}^{true}\nu_{ls}\mathbb{D}_{ls} + \Phi_{ls}\rho_l^{true}\mathbf{g} - \dot{m}_{gl}\mathbf{u}_{ls} + \Phi_{ls}\Phi_g\frac{3}{8}\frac{C_d\rho_{ls}^{true}}{r_g}|\mathbf{u}^{lsg}_{slip}|\mathbf{u}^{lsg}_{slip} \tag{MoB.1}$$

$$\nabla\left(p_{ls}^{dyn} + \Phi_g\frac{2\sigma}{r_g}\right) + (\Phi_{ls}\rho_{ls}^{true} - \Phi_g\rho_g^{true})\mathbf{g} = -\Phi_{ls}C_d\frac{3}{8}\frac{\rho_{ls}^{true}}{r_g}|\mathbf{u}^{lsg}_{slip}|\mathbf{u}^{lsg}_{slip} \tag{MoB.2}$$

$$(\rho_l^{true} - \rho_s^{true})\nabla p_{ls}^{dyn} + (\rho_l^{true} - \rho_s^{true})\mathbf{g} = -\frac{9}{2}\frac{\Phi_{ls}\rho_{ls}^{true}\nu_{ls}}{r_s^2}\mathbf{u}^{ls}_{slip} \tag{MoB.3}$$

$$\rho C_p\frac{\mathrm{d}_u T}{\mathrm{d}t} - k\Delta T = -\frac{L^{ch}}{M_{FA}}r^{ch} - \frac{L^{ev}_{FA}}{M_{FA}}r^{ev}_{FA} - \frac{L^{diss}_{CO_{2(d)}}}{M_{CO_{2(d)}}}r^{ev}_{CO_{2(d)}} - \frac{L^{diss}_{H_{2(d)}}}{M_{H_2}}r^{ev}_{H_{2(d)}} \tag{EnB}$$

$$\partial_t n + \mathrm{div}(n\mathbf{u}_g) = R \tag{Pop}$$

Quasi-steady model

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

$$\partial_t(\Phi_{ls}\rho_{ls}^{true}) + \operatorname{div}\left(\Phi_{ls}\rho_{ls}^{true}\mathbf{u}_{ls}\right) = -M_{FA}r^{ch} \tag{MaB.1}$$

$$\partial_t(\Phi_{g}\rho_{g}^{true}) + \operatorname{div}\left(\Phi_{g}\rho_{g}^{true}\mathbf{u}_{g}\right) = M_{FA}r^{ch} \tag{MaB.2}$$

$$\partial_t(\Phi_{s}\rho_{s}^{true}) + \operatorname{div}(\Phi_{s}\rho_{s}^{true}\mathbf{u}_{s}) = 0 \tag{MaB.3}$$

$$\Phi_{ls}\rho_{ls}^{true}\frac{\mathrm{d}_{ls}\mathbf{u}_{ls}}{\mathrm{d}t} = -\Phi_{ls}\nabla p_{ls} + \Phi_{ls}\rho_{ls}^{true}\nu_{ls}\mathbb{D}_{ls} + \Phi_{ls}\rho_{l}^{true}\mathbf{g} - \dot{m}_{gl}\mathbf{u}_{ls} + \Phi_{ls}\Phi_g\frac{3}{8}\frac{C_d\rho_{ls}^{true}}{r_g}|\mathbf{u}_{slip}^{lsg}|\mathbf{u}_{slip}^{lsg} \tag{MoB.1}$$

$$\mathbf{g} = -\frac{3}{8}\frac{C_d}{r_g}|\mathbf{u}_{slip}^{lsg}|\mathbf{u}_{slip}^{lsg} \tag{MoB.2}$$

$$(\rho_l^{true} - \rho_s^{true})\mathbf{g} = -\frac{9}{2}\frac{\Phi_{ls}\rho_{ls}^{true}\nu_{ls}}{r_s^2}\mathbf{u}_{slip}^{ls} \tag{MoB.3}$$

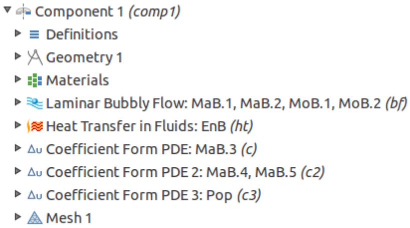
$$\rho C_p\frac{\mathrm{d}_u T}{\mathrm{d}t} - k\Delta T = -\frac{L^{ch}}{M_{FA}}r^{ch} \tag{EnB}$$

$$\partial_t n + \operatorname{div}(n\mathbf{u}_g) = R \tag{Pop}$$

where $\Phi_{ls} + \Phi_g = 1, \mathbf{u}_{slip}^{ls} = \mathbf{u}_s - \mathbf{u}_l, \mathbf{u}_{slip}^{lsg} = \mathbf{u}_{sl} - \mathbf{u}_l$

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

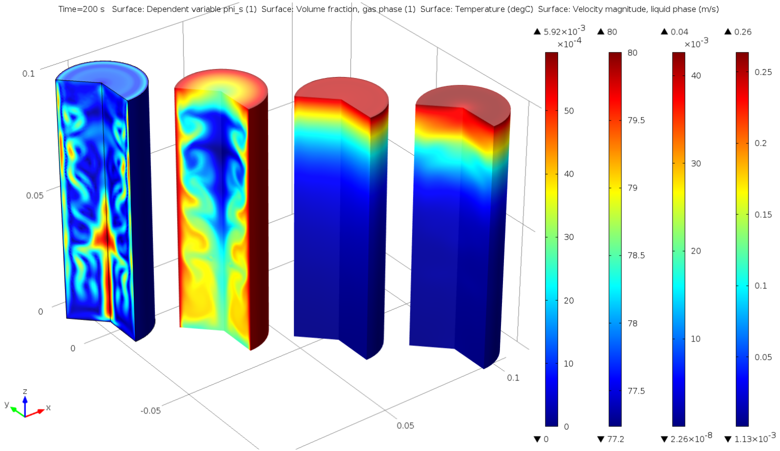


Figure : Velocity Field Liquid, Temperature, Gas Concentration, Solid Concentration.

The results: Traffic Jam Effect

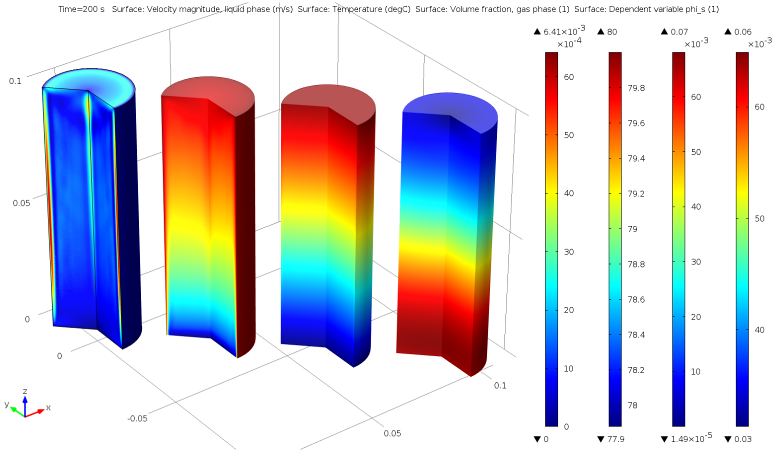


Figure : Velocity Field Liquid, Temperature, Gas Concentration, Solid Concentration.
Traffic Jam Effect: $\rho_s^{true} < \rho_l^{true}$

Game over!

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.