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

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What are we investigating?

We are studying a model of fluidized bed reactor which, in presence of heterogeneous platinum-based (solid) catalytic particles, decomposes liquid formic acid producing gaseous mixture of carbon dioxide and hydrogen as the product.

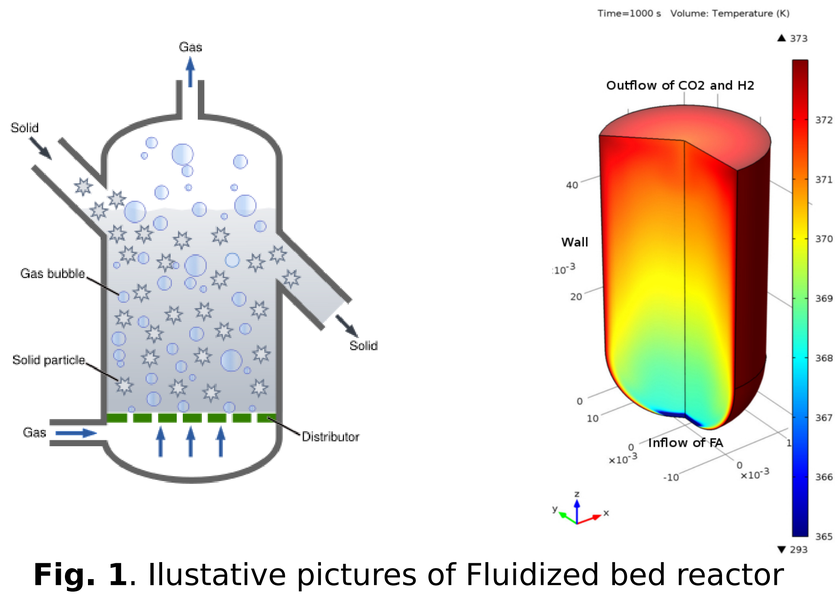


Fig. 1. Ilustative pictures of Fluidized bed reactor

How do we model that?

- We treat the system as a (Class II) mixture where we distinguish partial densities and velocities sharing one thermal field.
- First of all, we consider four constituents, namely formic acid (FA), Platinum micro-pellets (Pt), carbon dioxide (CO_2) and hydrogen (H_2).
- Secondly, we reduce the four-constituent model to a binary mixture model of “liquid” phase (Pt + FA) and gaseous phase ($CO_2 + H_2$) which forms bubbles.
- Liquid phase is considered as non-Newtonian fluid satisfying compresible Navier-Stokes equation with temperature-dependent density and viscosity modelled by Boussinesq approximation and Williams-Landel-Ferry model.
- Physical interaction between the bubbles and liquid is modelled under equilibrium assumption by the pressure-drag balance.
- Chemical rates satisfy mass-action law and undergo Arrhenius kinetics.

The model

$$\partial_t \Phi_g + \mathrm{div}(\Phi_\mathrm{g}\mathbf{u}_\mathrm{g}) = \frac{\mathrm{m_{dc}}}{\rho_\mathrm{g}^\mathrm{true}} \qquad (\mathrm{CE.1})$$

$$\partial_t\left(\Phi_l\rho_l^{true} + \Phi_g\rho_g^{true}\right) + \mathrm{div}(\Phi_\mathrm{l}\rho_\mathrm{l}^\mathrm{true}\mathbf{u}_\mathrm{l} + \Phi_\mathrm{g}\rho_\mathrm{g}^\mathrm{true}\mathbf{u}_\mathrm{g}) = 0 \qquad (\mathrm{CE.2})$$

$$\frac{\rho_l^{true} - \rho_g^{true}}{\rho_l^{true}}\nabla p_l = -\frac{18}{d_g^2}\mu_l\mathbf{u}_{slip} \qquad (\mathrm{MB.1})$$

$$\Phi_l\rho_l^{true}\frac{\mathrm{d}\mathbf{u}_\mathrm{l}}{\mathrm{dt}} = -\nabla p + \mathrm{div}\left(\Phi_\mathrm{l}\mu_\mathrm{l}\left(2\mathbb{D}_\mathrm{l} - \frac{2}{3}\mathrm{div}\mathbf{u}_\mathrm{l}\mathbb{I}\right)\right) + \Phi_\mathrm{l}\rho_\mathrm{l}^\mathrm{true}\mathbf{g} \qquad (\mathrm{MB.2})$$

$$\rho C_p\partial_t T + \rho C_p\mathbf{u}\cdot\nabla T = \mathrm{div}(\mathrm{k}\nabla\mathrm{T}) - \frac{\mathrm{H}}{\mathrm{M_{FA}}}\mathrm{m_{dc}} \qquad (\mathrm{HE})$$

$$\rho := \rho_g^{mix} + \rho_l^{mix} := \Phi_g\rho_g^{true} + \Phi_l\rho_l^{true},\ \rho\mathbf{u} := \rho_g^{mix}\mathbf{u}_g + \rho_l^{mix}\mathbf{u}_l$$

$$m_{dc} = \Phi_{FA}\rho_{FA}^{true}\,Ae^{-\frac{E_a}{RT}},\ \Phi_{FA} = \frac{(\Phi_l\rho_l^{true} - \Phi_{Pt}\rho_{Pt}^{true})}{\rho_{FA}^{true}}$$

$$\Phi_g + \Phi_l = 1, k = \Phi_g k_g + \Phi_l k_l, C_p = c_l C_l + (1 - c_l)C_g$$

$$\rho_l^{true} = \rho_{c,STP}^{true}\Big(1 - \alpha(T - 273)\Big),\ \frac{p}{\rho_g^{true}T} = \frac{p_{atm}}{\rho_{d,STP}^{true}\,273}.$$

Numerical simulations

Numerical simulations were performed in COMSOL Multiphysics® with CFD Module. Since the devices has usually simple tube-like geometry we employ axial symmetry.

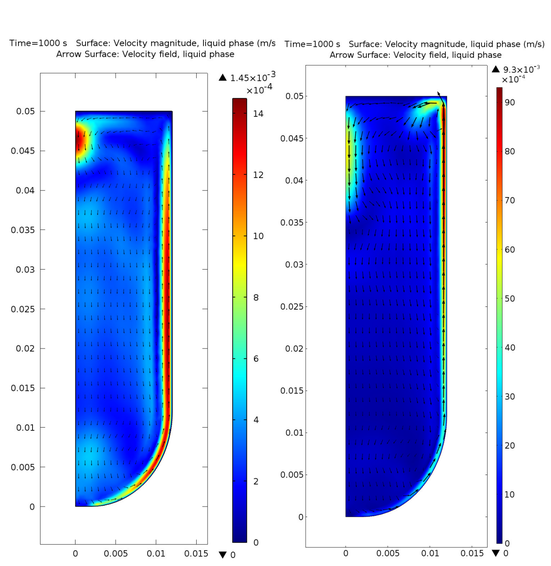


Fig. 2. $\mu_l^0 = 0.005$ Pa·s, $A = 10^8$ s^{-1}

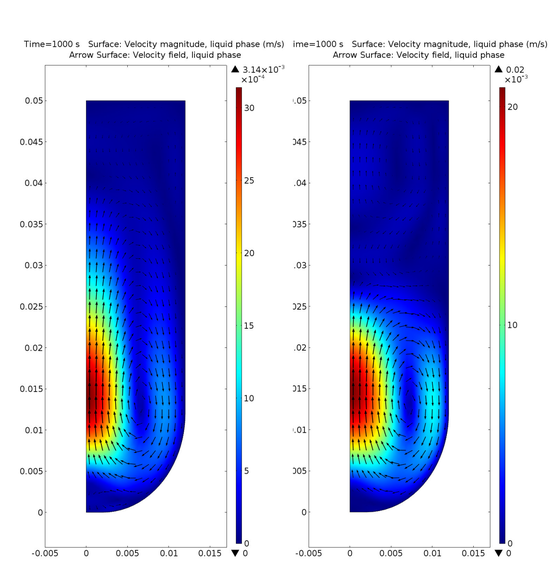
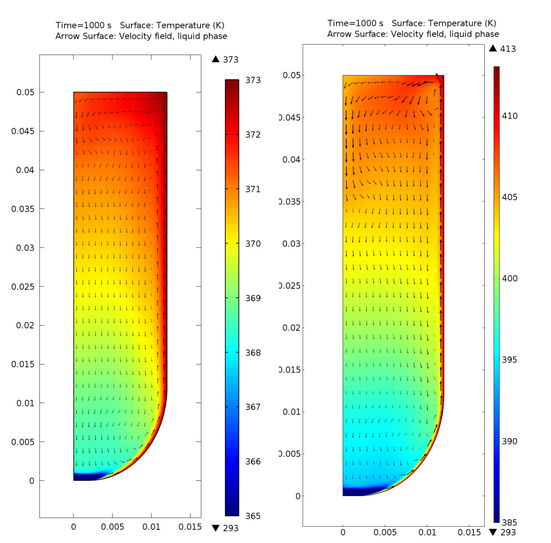
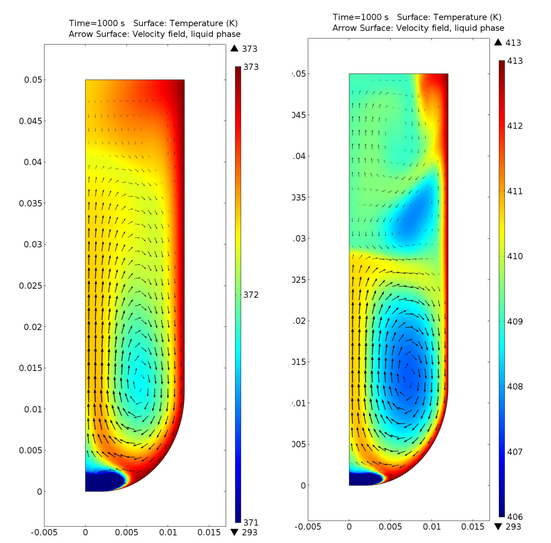


Fig. 3. $\mu_l^0 = 0.1$ Pa·s, $A = 10^7$ s^{-1}





Conclusions

- As we would expect from the physical model, there are two phenoma which influence the flow. First, thermal convection which is caused by temperature gradient and, second, a flow caused by ascending bubbles. These two phenomena drive the flow of the liquid phase in opposite directions and the resulting flow regime depends on the setting of parameters, mainly values of frequency factor A, activation energy E_a , viscosity μ_l and volumetric expansion coefficient α.
- Moreover, if the viscosity and the reaction parameters (A, E_a) are certainly high then the production of the gas is higher than possible outflow and rapid blow up of the liquid surface occurs which could lead to possible explosion of the reactor.

References

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