SimParTurS – work report 2009–03–23

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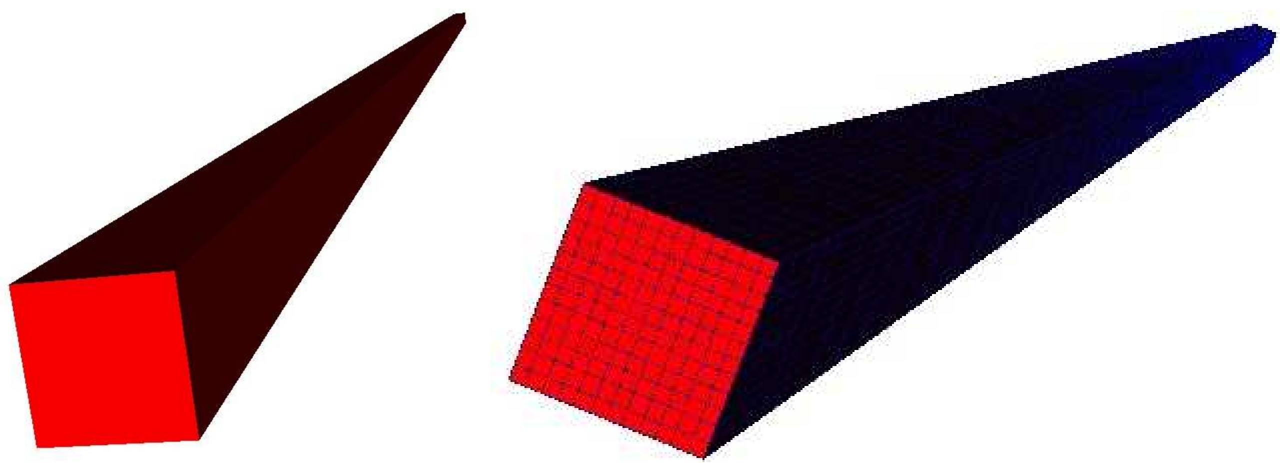
Population balance system in a channel with squared cross section

- based on the report by Christian Borchert and the discussions on March 23, 2009
- domain Ω
  - length $1.25\ m$
  - width $0.01\ m$
  - height $0.01\ m$



- reference length

$$l_\infty = 0.01\ m \quad \text{diameter of the channel}$$

- anisotropic grid in streamwise direction
  - aspect ratio increases towards the outflow
  - aspect ratio up to 30 (at the outflow)
- about 250 000 degrees of freedom

Flow equations

- dimensionless Navier–Stokes equations

$$\begin{aligned} \frac{\partial \mathbf{u}}{\partial t} - \frac{\nu}{l_\infty u_\infty}\Delta \mathbf{u} + (\mathbf{u}\cdot\nabla)\mathbf{u} + \nabla p &= \mathbf{0} \\ \nabla\cdot\mathbf{u} &= 0 \end{aligned}$$

- gravitation force include into pressure gradient
- parameters
  - kinematic viscosity (ethanol) $\nu = 1.361\ 10^{-6}\ m^2/s$
  - density (ethanol) $\rho = 789\ kg/m^3$
- reference quantities
  - velocity: $u_\infty = 0.01\ m/s$
  - time: $t_\infty = l_\infty/u_\infty = 1\ s$
  - pressure: $p_\infty = \rho u_\infty^2 = 7.89e - 5\ N/m^2$
- Reynolds number

$$Re = \frac{l_\infty u_\infty}{\nu} \approx 73.475386$$

Flow equations (cont.)

- inlet:

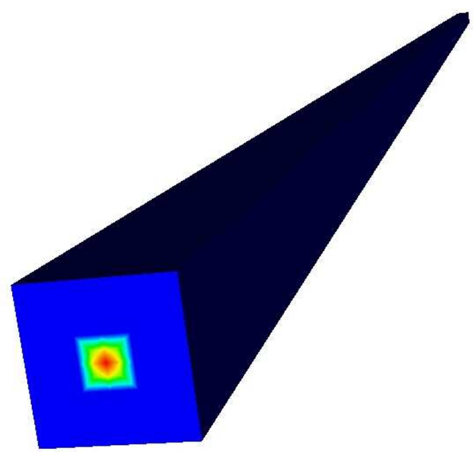
$$I = 0 \times \left[\frac{1}{3}, \frac{2}{3}\right] \times \left[\frac{1}{3}, \frac{2}{3}\right]$$

- inflow:

$$\begin{pmatrix} 2.5\ cm/s \\ 0 \\ 0 \end{pmatrix} \overset{\text{dimensionless}}{\Longrightarrow} \begin{pmatrix} u_{\text{in}} \\ 0 \\ 0 \end{pmatrix}$$

  with u_{in} solution of

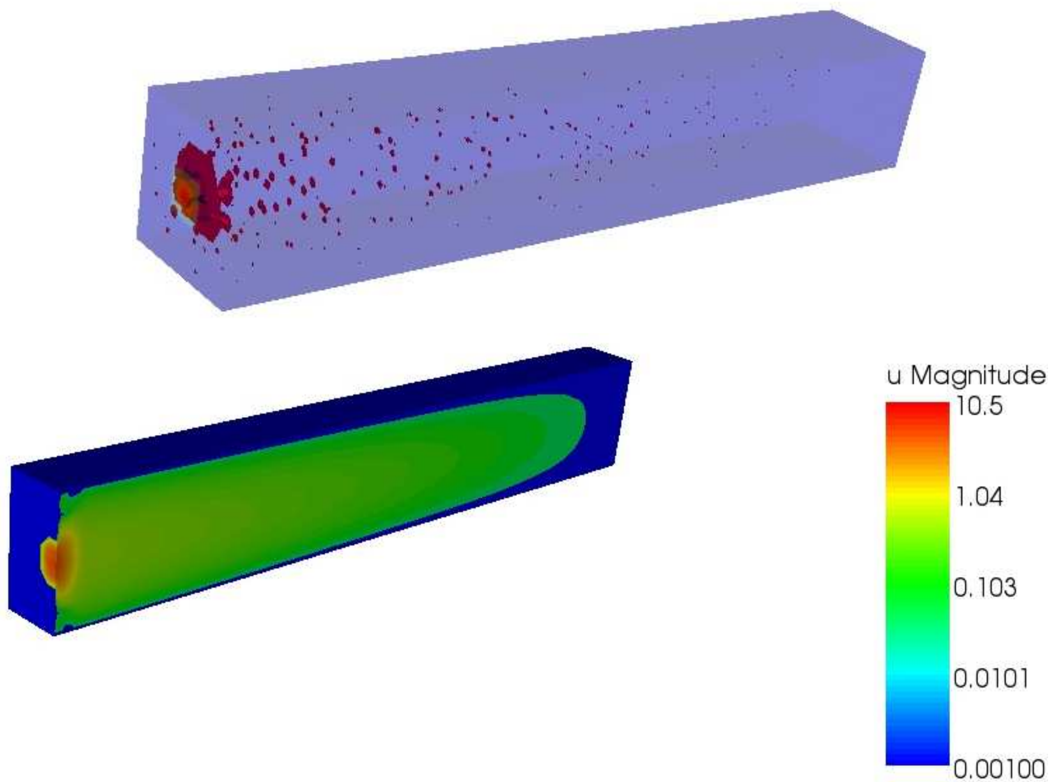
$$-\Delta u_{\text{in}} = 2.5 \text{ in } I, \quad u_{\text{in}} = 0 \text{ on } \partial I$$



- outlet $x = 125$: outflow boundary conditions

Flow equations (cont.)

- flow is probably time–dependent
  - stationary Navier–Stokes equations: solver stagnates
- Crank–Nicolson Galerkin FEM
- instantaneous flow field



  - grid dependence of result clearly visible, recirculation zone not sufficiently resolved

Energy balance

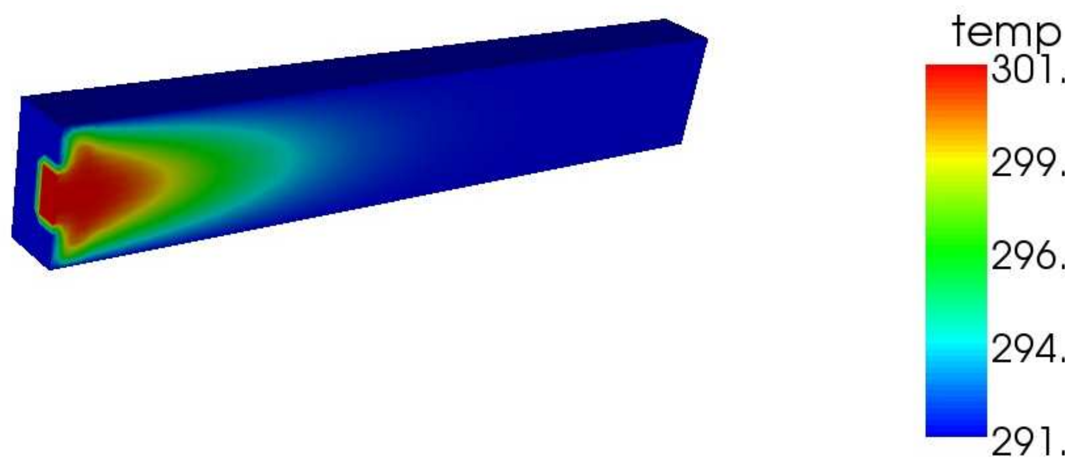
- dimensionless equation

$$
\begin{aligned}
\frac{\partial T}{\partial t} - \frac{\lambda}{l_\infty u_\infty \rho c_p}\Delta T + \mathbf{u}\cdot\nabla T &= \frac{l_\infty \Delta h_{\mathrm{U,cryst}}}{u_\infty T_\infty \rho c_p}\left(\sigma_{\mathrm{U,nuc}} + \sigma_{\mathrm{U,growth}}\right) \\
T(t,\partial\Omega) &= \begin{cases} 301.15 & \text{at the inlet} \\ 291.15 & \text{at the walls save inlet and outlet} \end{cases} \\
\frac{\lambda}{l_\infty u_\infty \rho c_p}\frac{T(t,\partial\Omega)}{\partial \mathbf{n}} &= 0 \quad \text{at the outlet} \\
T(0,\Omega) &= 298.15
\end{aligned}
$$

- parameters
  - thermal conductivity (ethanol) $\lambda = 0.167\ W/(K\ m)$
  - heat capacity (ethanol) $c_p = 2441.3\ J/(kg\ K)$
  - heat of solution (in ethanol) $\Delta h_{\mathrm{U,cryst}} = 216.45\ J/kg$
  - $\sigma_{\mathrm{U,nuc}}$, not yet implemented
  - $\sigma_{\mathrm{U,growth}}$, nonlinear term, not yet implemented

Energy balance (cont.)

- reference quantities
  - temperature: $T_\infty = 1\ K$
- $\Longrightarrow$ non–dimensional diffusion coefficient $\dfrac{\lambda}{l_\infty u_\infty \rho c_p} \approx 8.669984e-4$
- temperature only necessary for computing the growth rate of the particles
- Crank–Nicolson linear Finite–Element–Method Flux–Corrected–Transport (FEM–FCT) scheme
- instantaneous temperature distribution



  - discontinuous Dirichlet boundary condition

Mass balance for solute

- changed to equation for concentration

$$c = \frac{\rho_j^c}{m_{\mathrm{mol}}}, \quad m_{\mathrm{mol}}(\mathrm{urea}) = 60.06e-3\ \frac{kg}{mol}$$

- dimensionless equation

$$\frac{\partial c}{\partial t} - \frac{D_j}{l_\infty u_\infty}\Delta c + \mathbf{u}\cdot\nabla c + \frac{3\rho^d k_V G f_\infty L_\infty^3 l_\infty}{m_{\mathrm{mol}} c_\infty u_\infty}\int_{L_{\min}/L_\infty}^{L_{\max}/L_\infty} L^2 f\, dL = 0$$

$$\begin{aligned} c &= 71.09/m_{\mathrm{mol}} \approx 1183.65 \quad \text{at the inlet} \\ \frac{D_j}{l_\infty u_\infty}\frac{\partial c}{\partial \mathbf{n}} &= 0 \quad \text{else} \\ c(0,\Omega) &= 0 \end{aligned}$$

- parameters
  - diffusion coefficent (urea in ethanol) $D_j = 1.35e-9\ m^2/s$
  - density of dispersed phase based on phase volume $\rho^d = 1323\ kg/m^3$
  - $k_V = \pi/6$
- $\Longrightarrow$ non–dimensional diffusion coefficient $\dfrac{D_j}{l_\infty u_\infty} = 1.35e-5\ m^2/s$

Mass balance for solute (cont.)

- growth rate

$$G = \begin{cases} k_g \left(\dfrac{c m_{\mathrm{mol}} - \rho^{\mathrm{c}}_{\mathrm{j,sat}}(T)}{\rho^{\mathrm{c}}_{\mathrm{j,sat}}(T)} \right)^g & \text{if } \rho^c_j - \rho_{\mathrm{j,sat}} > 0 \\ 0 & \text{else} \end{cases}$$

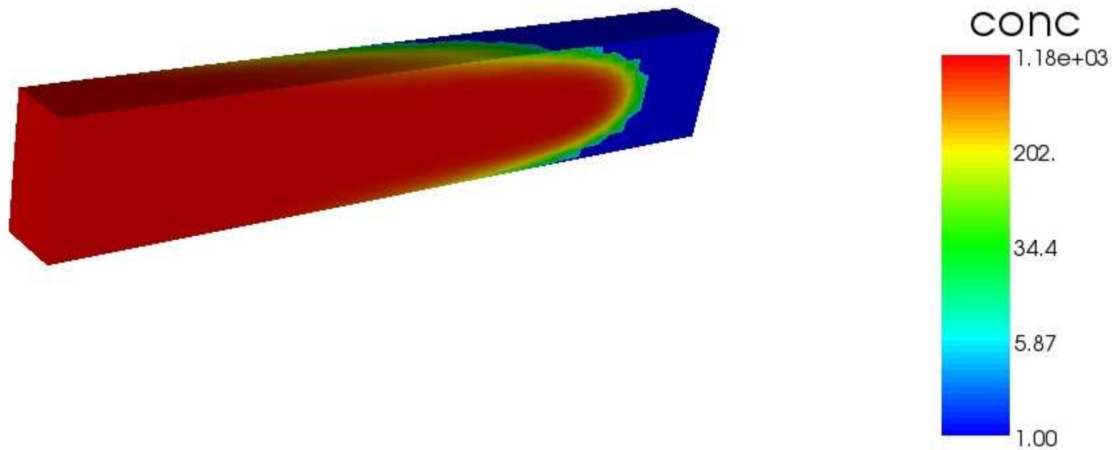
  - $k_g \approx 1e-7$
  - $g \approx 0.5$
  - solubility of urea in ethanol

$$\rho^{\mathrm{c}}_{\mathrm{j,sat}}(T) = 35.364 \, \frac{kg}{m^3} + 1.305 \, \frac{kg}{m^3 K} (T - 273.15) \, K$$

- reference quantities
  - concentration: $c_\infty = 1 \; mol/m^3$
  - particle diameter: $L_\infty = L_{\mathrm{max}}$
  - particle size distribution: $f_\infty = 1 \; m^{-4}$

Mass balance for solute (cont.)

- Crank–Nicolson linear FEM–FCT scheme
- instantaneous concentration distribution (with $f \equiv 0$)



Particle size distribution

- dimensionless equation

$$\frac{\partial f}{\partial t} + \frac{l_\infty G}{u_\infty L_\infty}\frac{\partial f}{\partial L} + \mathbf{u}\cdot\nabla_{\mathbf{x}} f \quad = \quad \frac{l_\infty}{u_\infty f_\infty}\,\text{rhs}$$

- reference quantities
  - $L_{\min} = 1e - 8\ m$
  - $L_{\max} = 2e - 5\ m$
- implementation started (without right hand side)
  - forward Euler upwind finite difference scheme
  - backward Euler upwind finite difference scheme
  - Crank–Nicolson linear FEM–FCT scheme

Next goals

- include PSD (until middle of April)
- better grid necessary (this week)
- link library for breakage and agglomeration (as soon as possible)