JOHANNES KEPLER UNIVERSITÄT LINZ | JKU

Polymer injection molding simulations in OpenFOAM®

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Institute of
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and Process Automation

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Introduction

- Injection molding
  - Communication
  - Medicine
  - Automotive
  - Packaging
  - etc…

- Expensive development stage
  - high pressure
  - high clamping forces
  - high viscosity
- Simulation
  - PolyFlow, Sigmasoft, Moldex3D, …
  - OpenFOAM®
- Model implementation
  - compressibility (pvT)
  - viscosity (non-Newtonian)

Incompressible models:

powerLaw:

$$\nu(\dot{\gamma}) = \nu_0 \dot{\gamma}^{n-1}$$

CrossPowerLaw:

$$\nu(\dot{\gamma}) = \frac{\nu_0 - \nu_\infty}{1 + (m\dot{\gamma})^n} + \nu_\infty$$

BirdCarreau:

$$\nu(\dot{\gamma}) = \nu_\infty + (\nu_0 - \nu_\infty)\left(1 + (m\dot{\gamma})^a\right)^{\frac{n-1}{a}}$$

$$\boldsymbol{\nu = \nu(\dot{\gamma}, T, p)}$$

Compressible models:

perfectFluid:

$$\rho(p) = \rho_0 + \frac{p}{RT}$$

adiabaticPerfectFluid:

$$\rho(p) = \rho_0 \left(\frac{p + B}{p_0 + B}\right)^{\frac{1}{\gamma}}$$

$$\boldsymbol{\rho = \rho(T, p)}$$

VOF:

$$\rho = \alpha\rho_l + (1-\alpha)\rho_g$$

$$\frac{\partial\alpha}{\partial t} + \nabla\cdot(\alpha\boldsymbol{u}) + \nabla\cdot(\alpha(1-\alpha)\boldsymbol{u}_r) = S_p + S_u$$

Continuity equation:

$$\frac{\partial\rho\boldsymbol{u}}{\partial t} + \nabla\cdot(\rho\boldsymbol{u}) = 0$$

Momentum equations:

$$\frac{\partial\rho\boldsymbol{u}}{\partial t} + \nabla\cdot(\rho\boldsymbol{u}\boldsymbol{u}) = -\nabla p + \nabla\cdot\tau + \rho\boldsymbol{g} + \boldsymbol{F}_\sigma$$

Energy equation:

$$\frac{\partial\rho T}{\partial t} + \nabla\cdot(\rho\boldsymbol{u}T) =$$

$$\Delta\left(\bar{k}T\right) + \tau:\nabla\boldsymbol{u}\cdot\left(\frac{\alpha}{c_{v_1}}\right) + [\nabla\cdot(p\boldsymbol{u})]\left(\frac{\alpha}{c_{v_1}} + \frac{(1-\alpha)}{c_{v_2}}\right)$$

tempPowerLaw (first order):

$$\nu(\dot{\gamma}, T) = \nu_0 \dot{\gamma}^{n-1} e^{c \cdot (T - T_0)}$$

$$\boldsymbol{\nu = \nu(\dot{\gamma}, T, p)}$$

CarreauYasudaWLF:

$$\nu(\dot{\gamma}, T) = \nu_\infty \cdot a_T(T) + (\nu_0 - \nu_\infty) a_T(T) \left(1 + (\lambda a_T(T) \dot{\gamma})^a\right)^{\frac{n-1}{a}}$$

$$\log a_T(T) = \frac{8.86 \cdot (T_0 - T_S)}{101.6 + (T_0 - T_S)} - \frac{8.86 \cdot (T - T_S)}{101.6 + (T - T_S)}$$

CrossArrhenius:

$$\nu(\dot{\gamma}, T) = \frac{\nu_0(T)}{1+\left(\frac{\nu_0(T)\dot{\gamma}}{\tau^*}\right)^{1-n}}$$

$$\boldsymbol{\nu = \nu(\dot{\gamma}, T, p)}$$

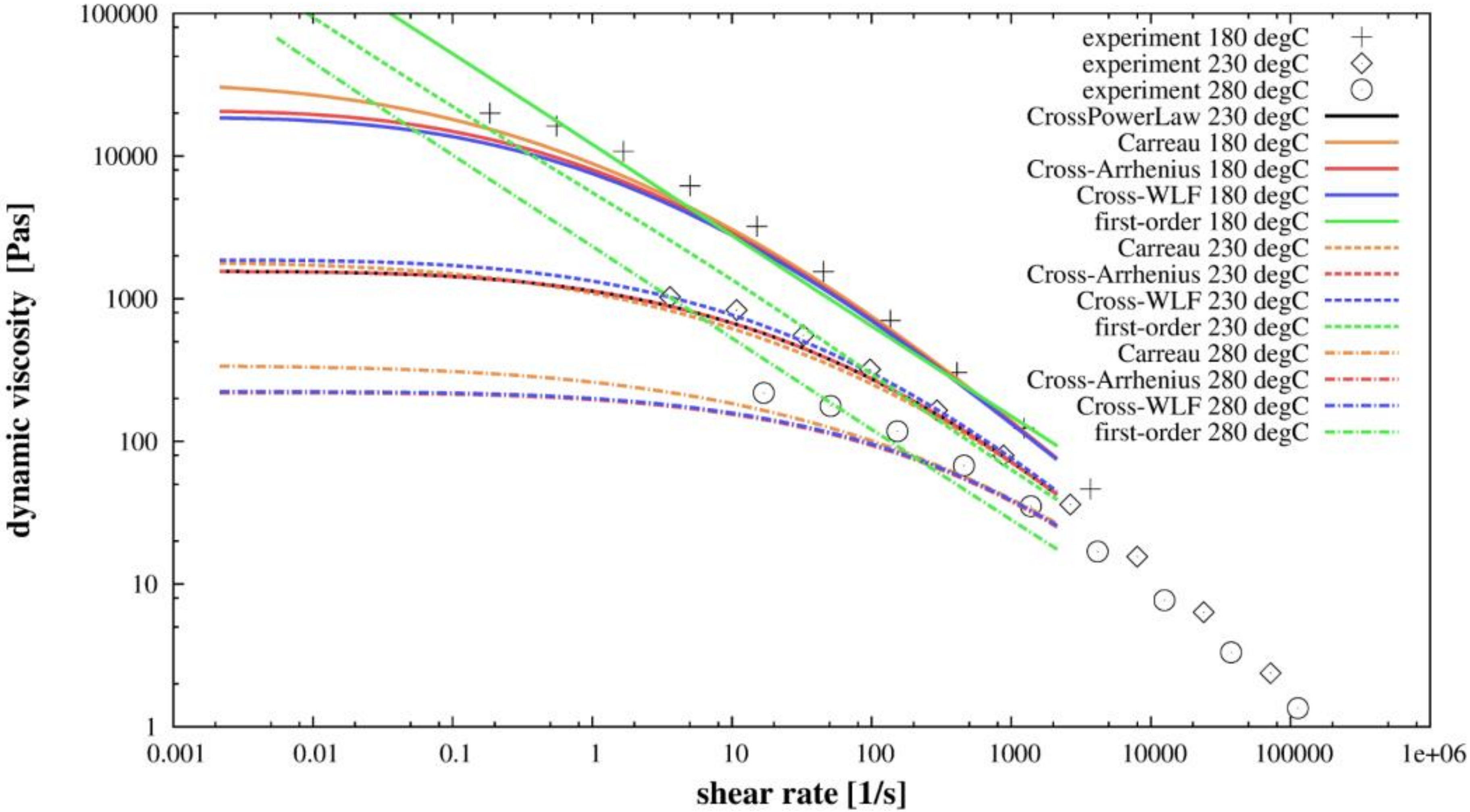
$$\nu_0(T) = B \cdot e^{T_b/T}$$

CrossWLF:

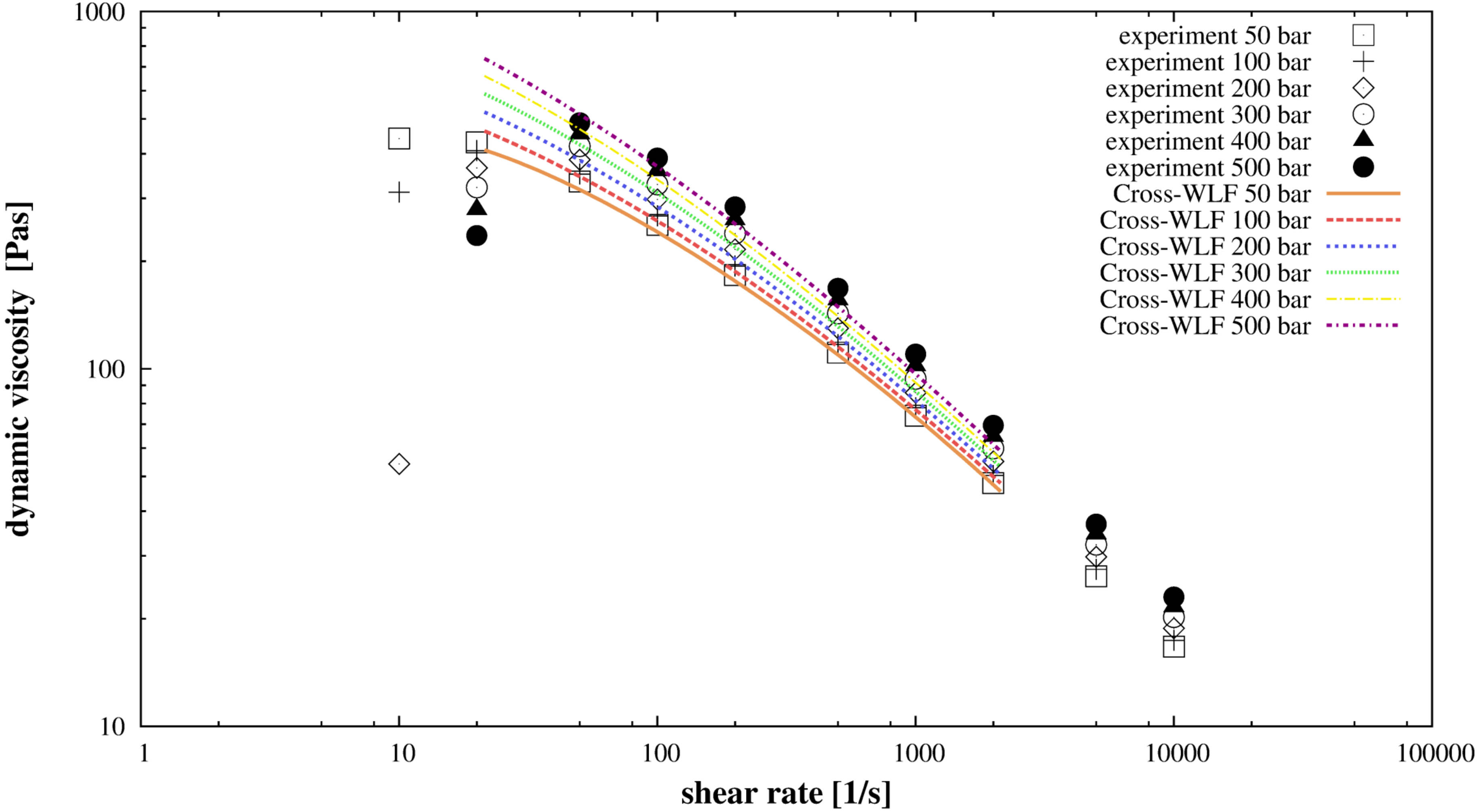
$$\nu(\dot{\gamma}, T, p) = \frac{\nu_0(T,p)}{1+\left(\frac{\nu_0(T,p)\dot{\gamma}}{D_4}\right)^{1-n}}$$

$$\nu_0(T) = D_1 \cdot \exp\left(\frac{(-A_1)\cdot(T-D_2-D_3\cdot p)}{A_2+T-D_2-D_3\cdot p}\right)$$

PS – 145D


dynamic viscosity [Pas]
shear rate [1/s]
100000
10000
1000
100
10
1
0.001
0.01
0.1
1
10
100
1000
10000
100000
1e+06
experiment 180 degC
experiment 230 degC
experiment 280 degC
CrossPowerLaw 230 degC
Carreau 180 degC
Cross-Arrhenius 180 degC
Cross-WLF 180 degC
first-order 180 degC
Carreau 230 degC
Cross-Arrhenius 230 degC
Cross-WLF 230 degC
first-order 230 degC
Carreau 280 degC
Cross-Arrhenius 280 degC
Cross-WLF 280 degC
first-order 280 degC

PP – HG313MO



1000
100
10
1
10
100
1000
10000
100000
dynamic viscosity [Pas]
shear rate [1/s]
experiment 50 bar
experiment 100 bar
experiment 200 bar
experiment 300 bar
experiment 400 bar
experiment 500 bar
Cross-WLF 50 bar
Cross-WLF 100 bar
Cross-WLF 200 bar
Cross-WLF 300 bar
Cross-WLF 400 bar
Cross-WLF 500 bar

Schmidt:

$$v(p,T) = \frac{PF1}{PF4+p} + \frac{PF2 \cdot T}{PF3+p} \qquad T \leq T_{trans}$$

$$v(p,T) = \frac{PS1}{PS4+p} + \frac{PS2 \cdot T}{PS3+p} \qquad T \geq T_{trans}$$

$$T_{trans} = PK1 + PK2 \cdot p$$

$$\boldsymbol{\rho = \rho(T,p)}$$

Tait:

$$v(p,T) = \left\{v_s(T) \cdot \left[1 - C \cdot \ln\left(1 + \frac{p}{B_s(T)}\right)\right] + W_s(T)\right\} \quad T \leq T_{trans}$$

$$v_s(T) = b_{1s} + b_{2s} \cdot (T - b_5)$$

$$B_s(T) = b_{3s} \cdot e^{-b_{4s} \cdot (T - b_5)}$$

$$W_s(T) = b_7 \cdot e^{b_8 \cdot (T - b_5) - b_9 \cdot p}$$

$$v(p,T) = \left\{v_m(T) \cdot \left[1 - C \cdot \ln\left(1 + \frac{p}{B_m(T)}\right)\right]\right\} \quad T \geq T_{trans}$$

$$v_m(T) = b_{1m} + b_{2m} \cdot (T - b_5)$$

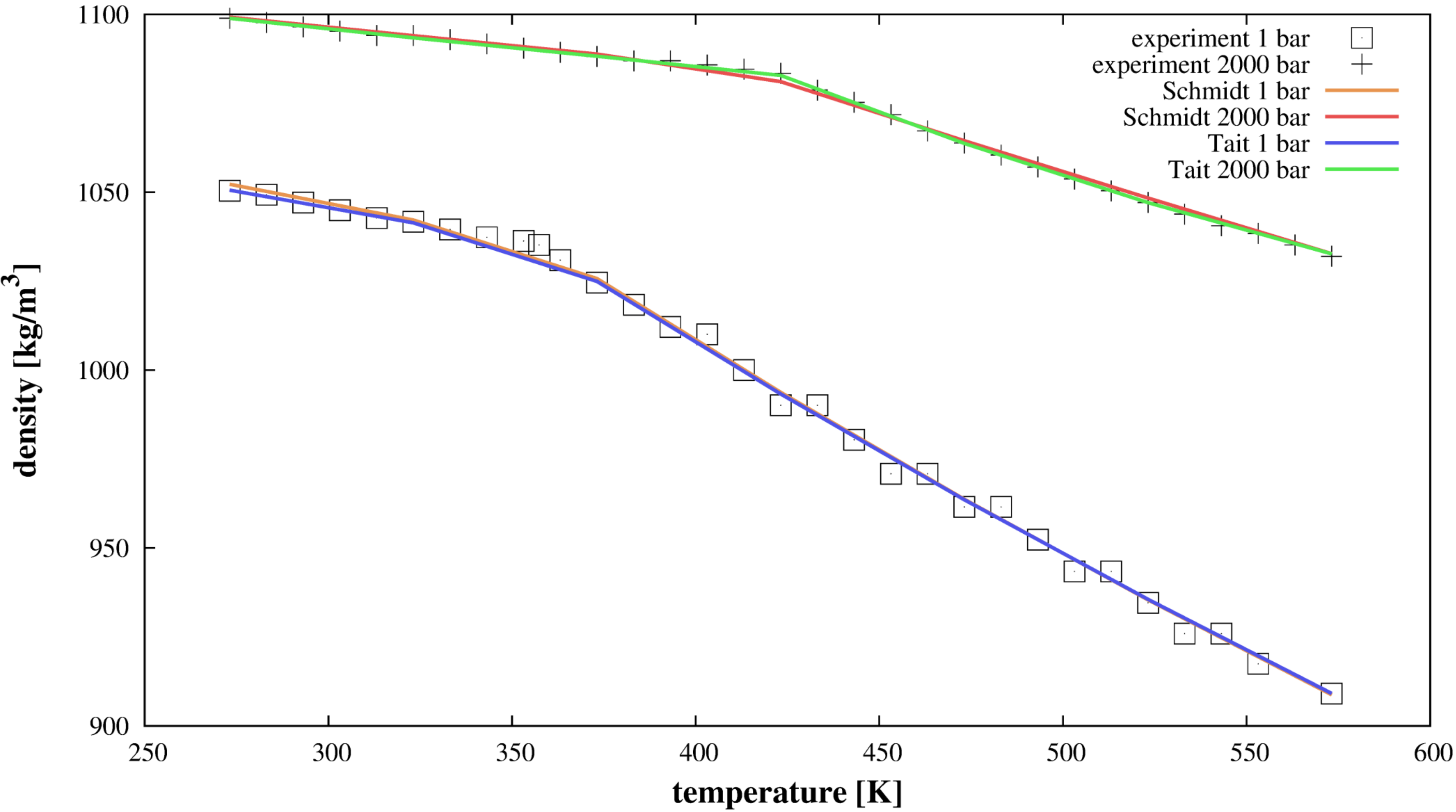
$$B_m(T) = b_{3m} \cdot e^{-b_{4m} \cdot (T - b_5)}$$

$$T_{trans} = b_5 + b_6 \cdot p$$

$$\boldsymbol{\rho = \rho(T,p)}$$

$$C = 0.0894$$

PS – 145D



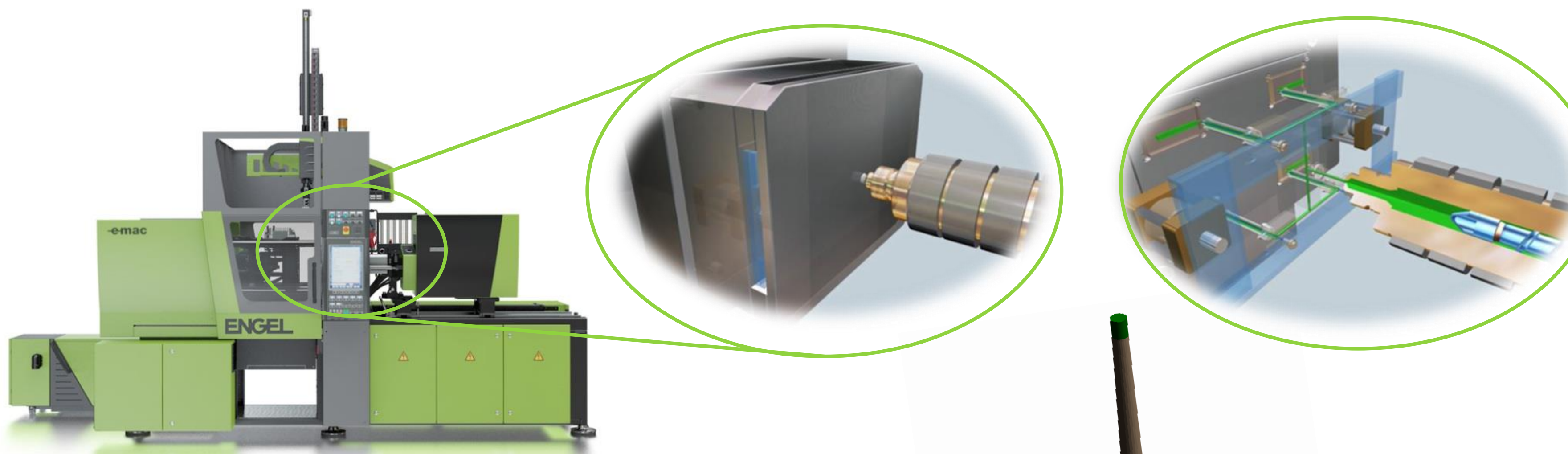
experiment 1 bar
experiment 2000 bar
Schmidt 1 bar
Schmidt 2000 bar
Tait 1 bar
Tait 2000 bar
density [kg/m³]
temperature [K]
1100
1050
1000
950
900
250
300
350
400
450
500
550
600

Drug delivery system

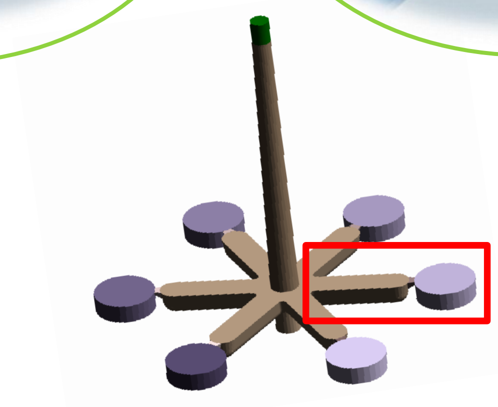
Discontinuous processing technique for polymer-additive systems

Injection molding machine:

- Plasticizing the polymer-additive system with single screw
- Shaping of the melt within the cavities in the mold
- One-stop production

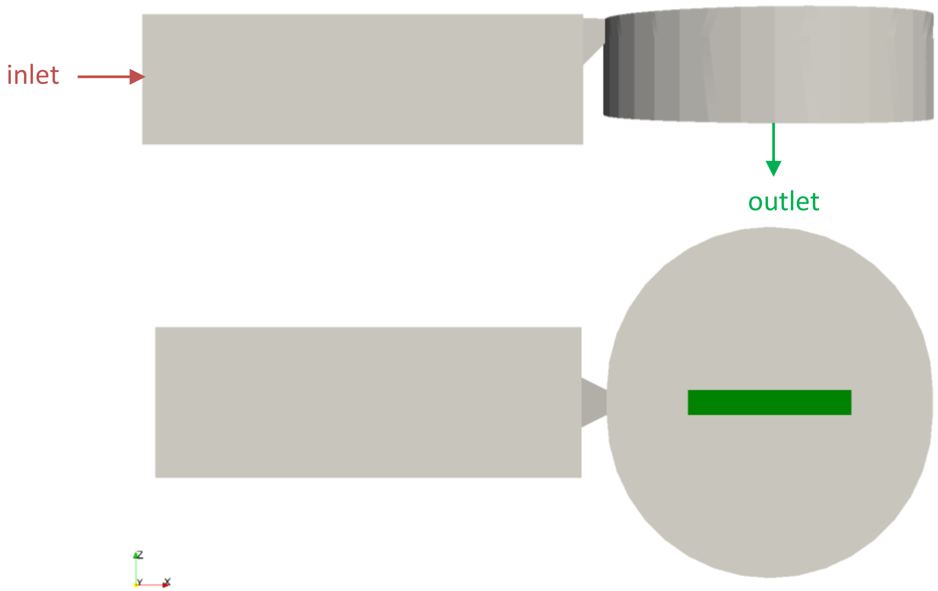


Injection Molding Machine type e-mac; Source: ENGEL Austria GmbH

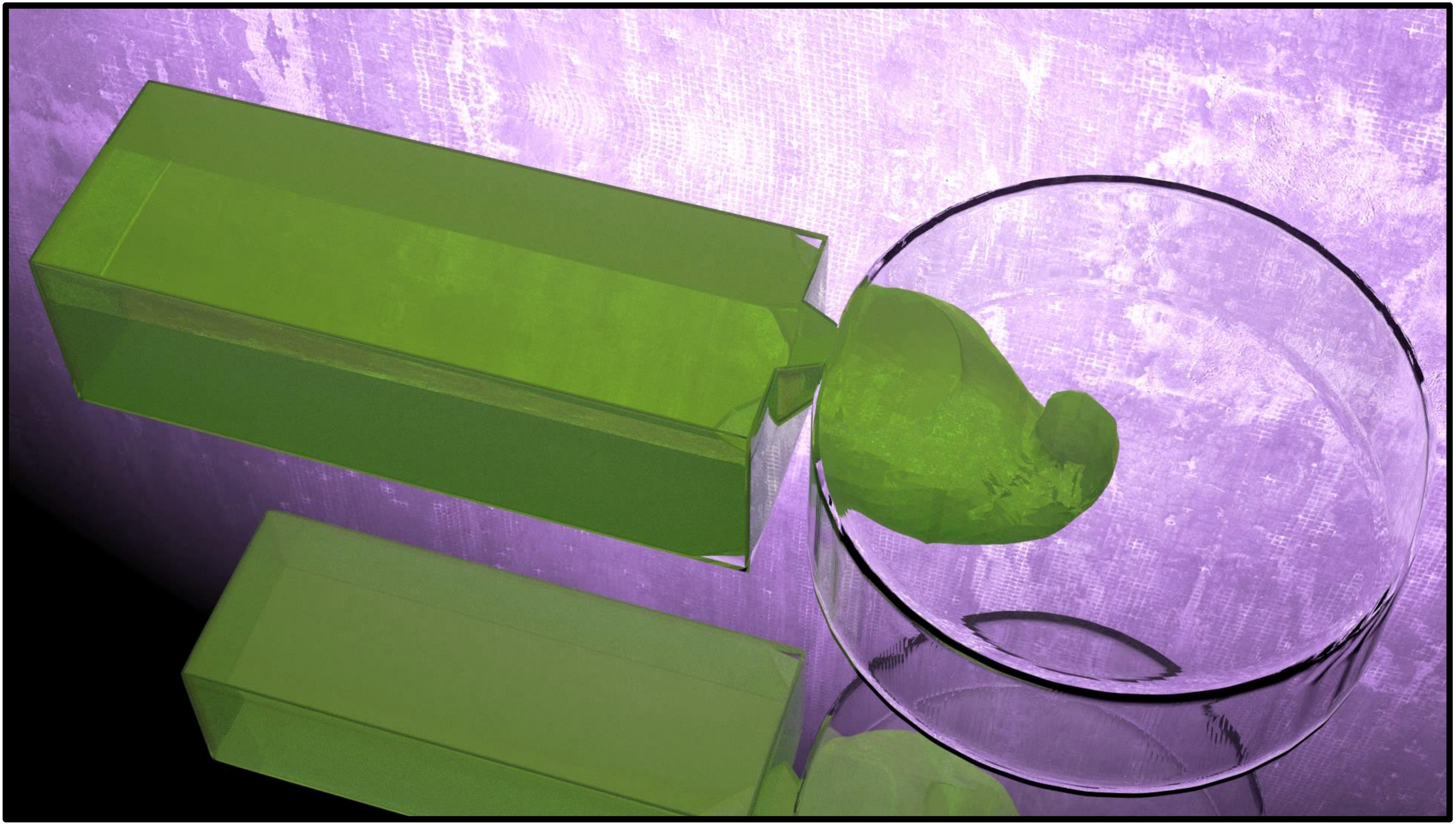


Problem setting – injection molding process

- Trial simulation of injection process (coarse mesh)
  - Influence of strain rate, density, temperature, pressure, viscosity etc.
  - Back coupling
- Geometry – 1 tablet cavity
- Fill time of **1 s**
- Wall temperature of **503 K**
- Inlet temperature of **553 K**
- Tait, CrossWLF for PS 145D

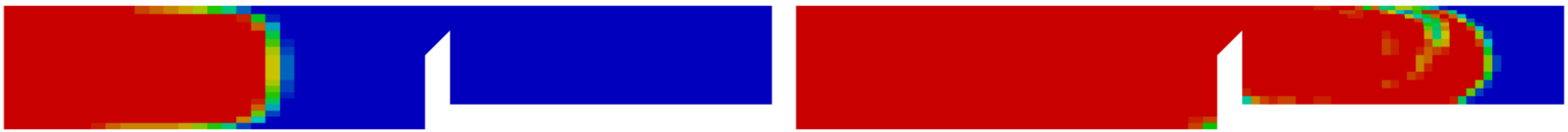


Injection molding process

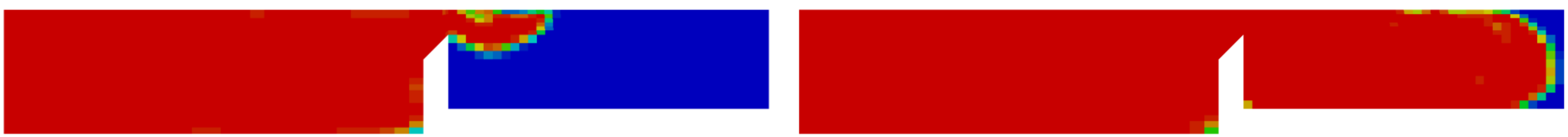


Liquid phase fraction

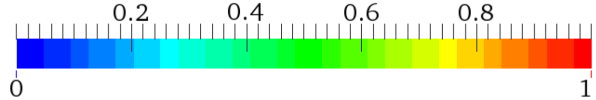
t = 0.25 s   t = 0.75 s



t = 0.5 s   t = 1 s

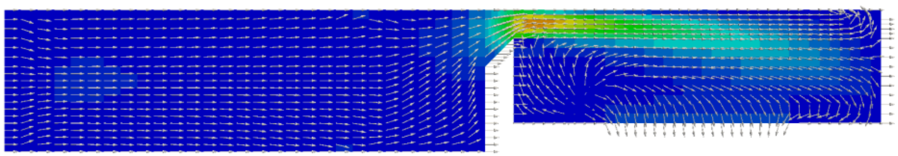


liquid phase fraction [-]

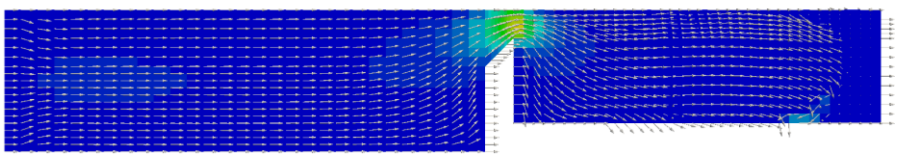


Velocity magnitude and vectors

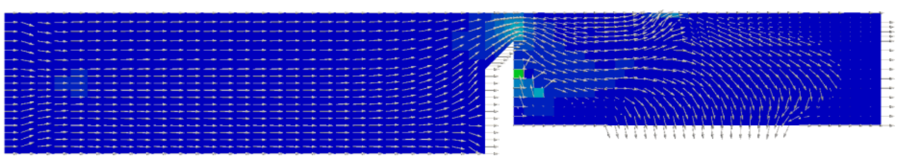
t = 0.25 s



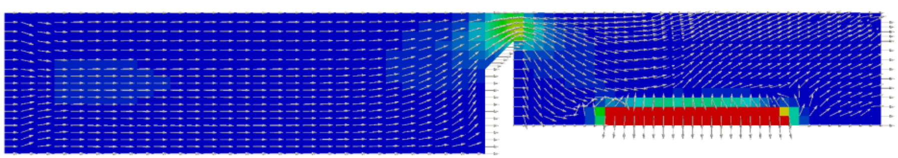
t = 0.75 s



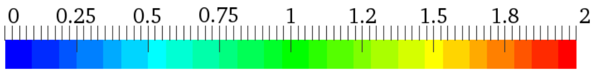
t = 0.5 s



t = 1 s

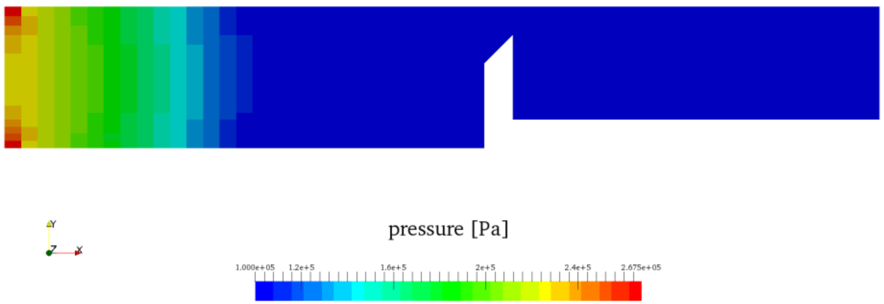


velocity magnitude [m/s]

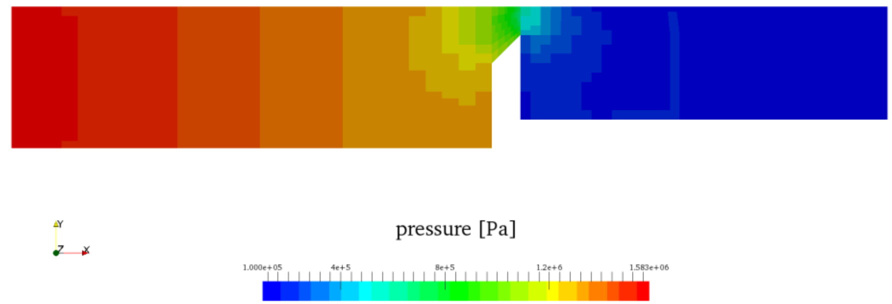


Pressure

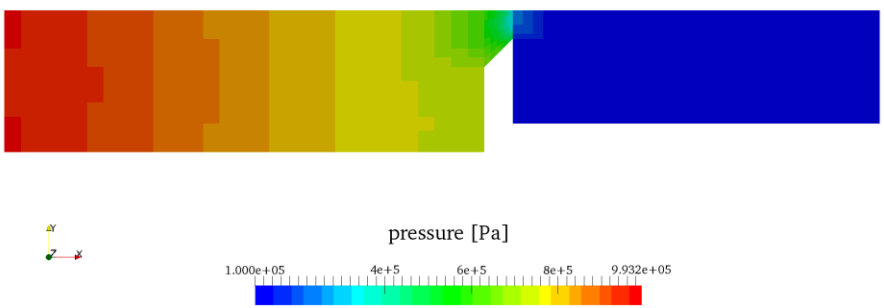
t = 0.25 s



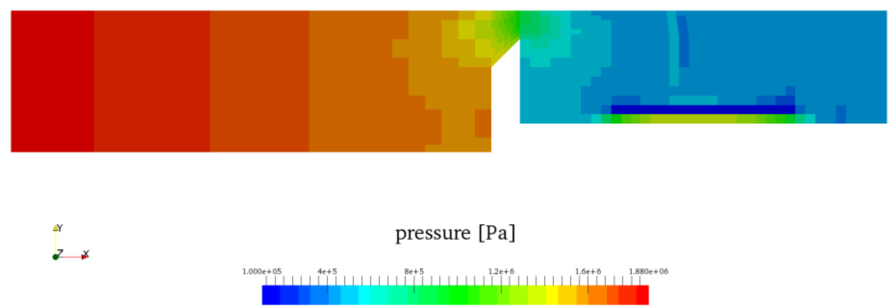
t = 0.75 s



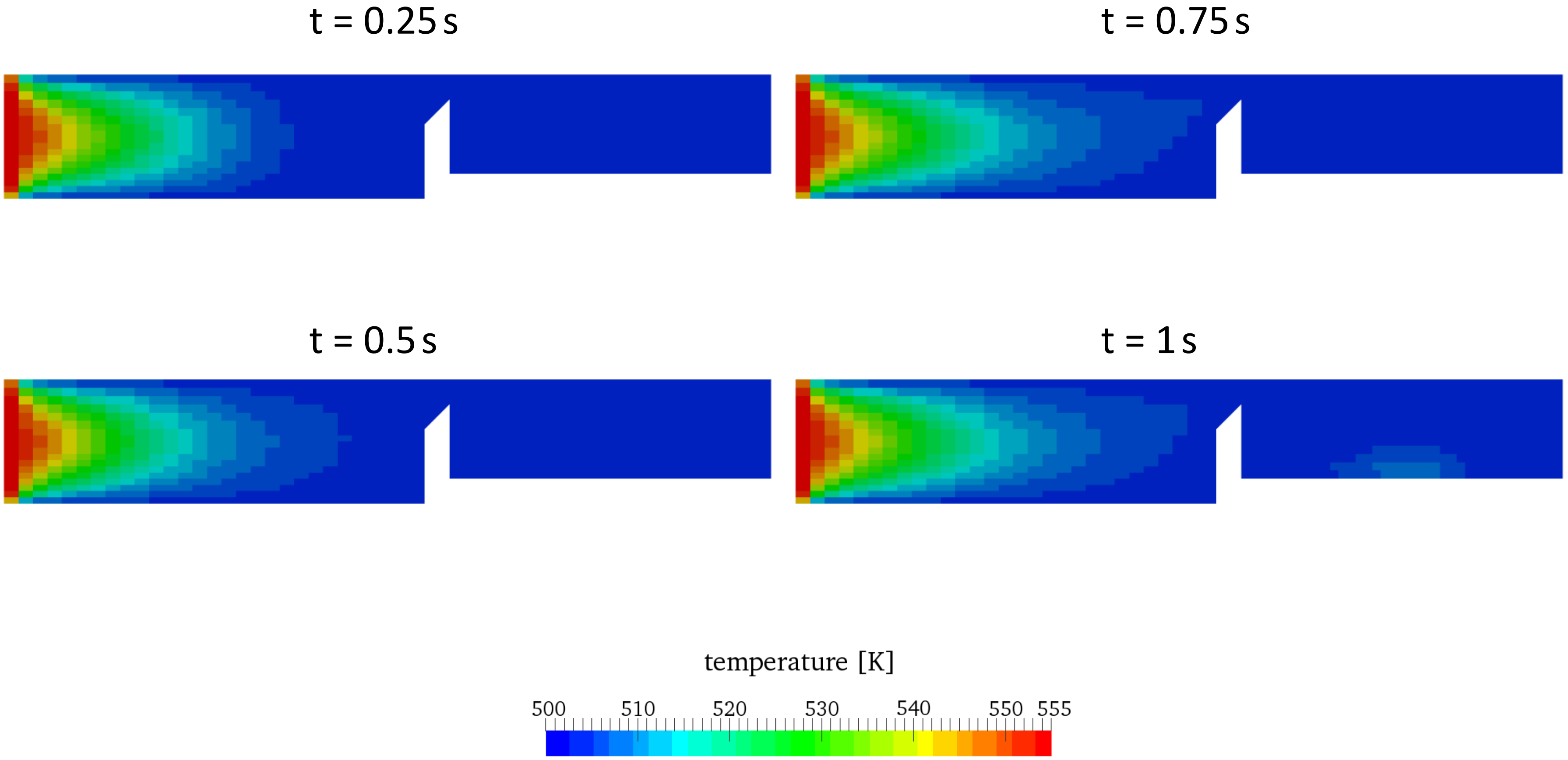
t = 0.5 s



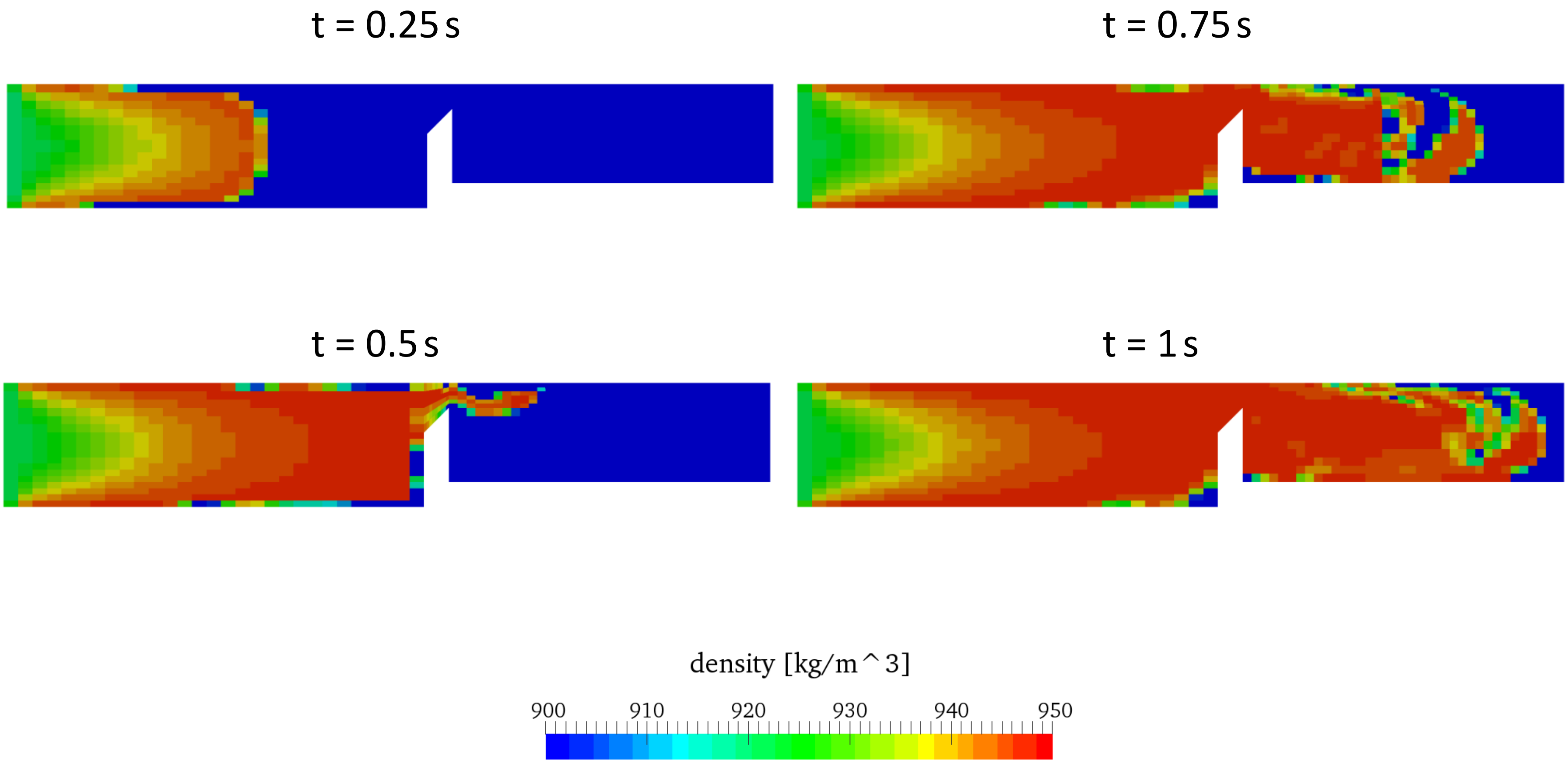
t = 1 s



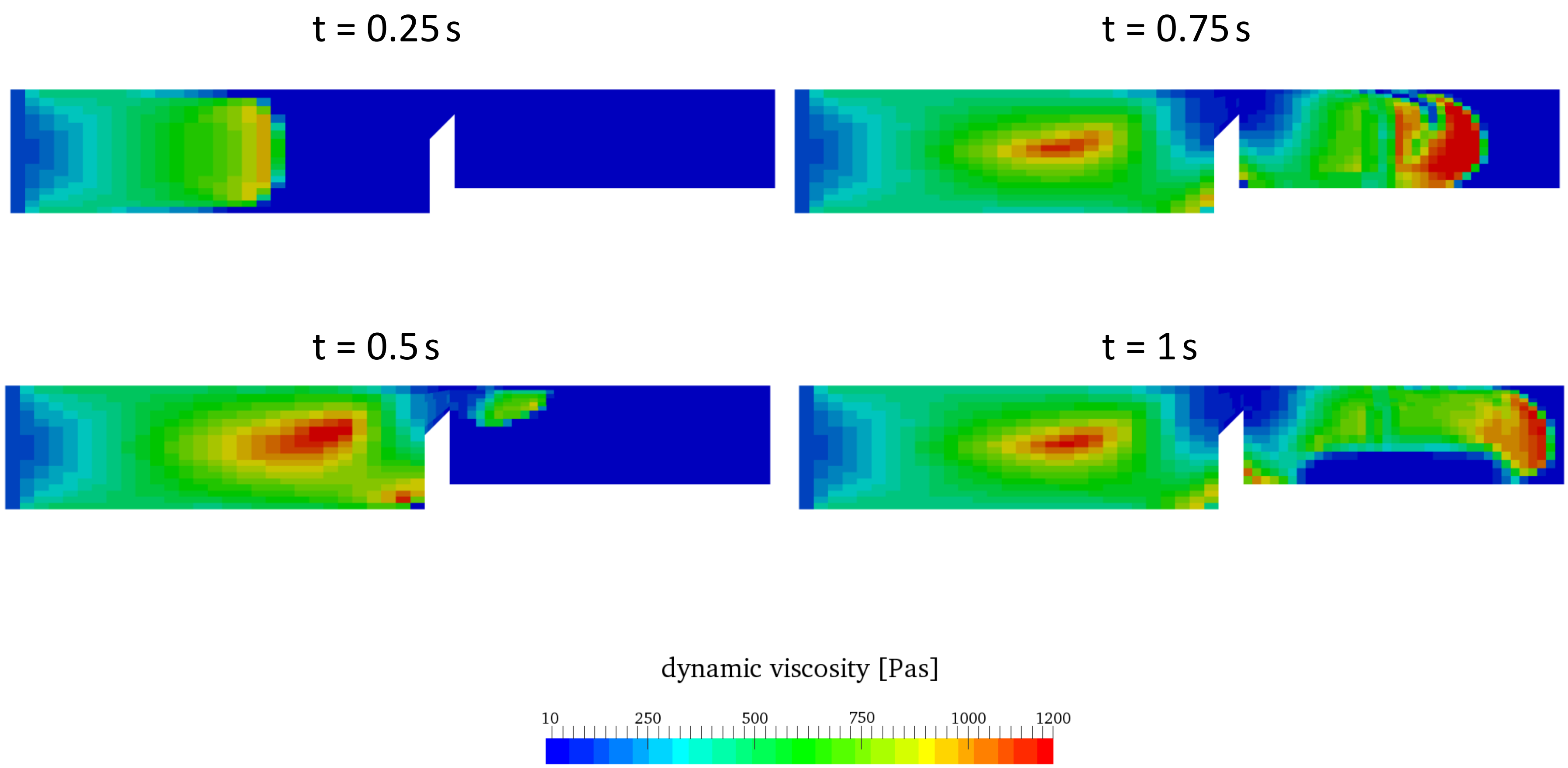
Temperature



Density



Dynamic viscosity



Conclusions and outlook

- Injection molding process in OpenFOAM®
- Implemented viscosity models
  - tempPowerLaw (first order)
  - CarreauYasudaWLF
  - CrossArrhenius
  - CrossWLF
- Implemented compressibility models
  - Schmidt
  - Tait
- Adaptation of compressibleInterFoam
- Next steps
  - crystallization
  - fiber orientation
  - cure
  - etc…

Thank you for your attention!

FFG
FORSCHUNG WIRKT.

ENGEL

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Introduction to injection molding technique and its simulation

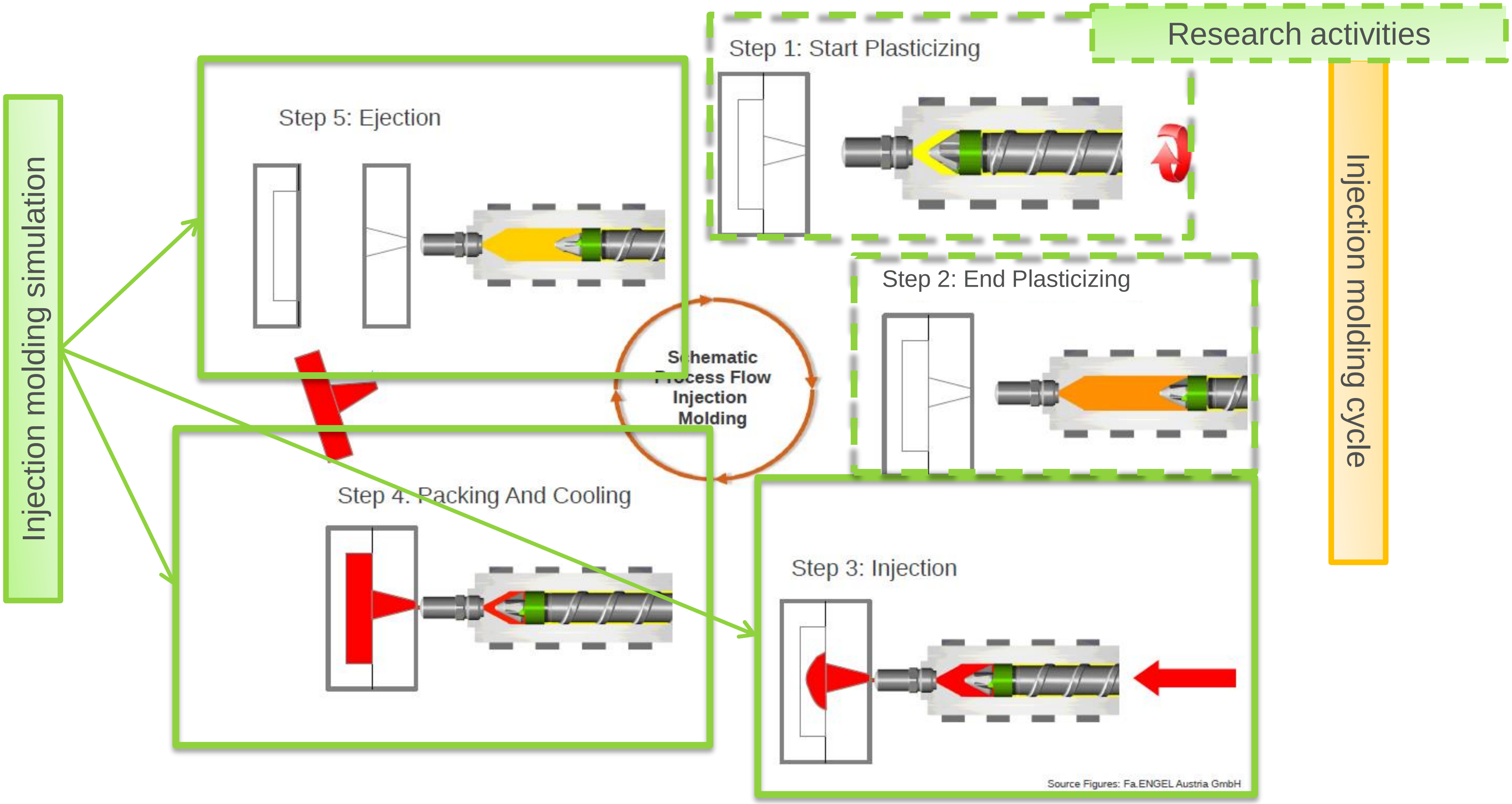

Figure 2: Injection molding cycle