FLUID – Simulation of complex fluid flows for industrial applications.

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Outlook.

- Short description of fluid flow equations
- How to solve it ?
- Simple simulation examples
- FLUID – software solution for industrial applications.
- Industrial driven applications with examples.
- Summary.

- Flow equations are modeled with Navier – Stokes system of equations. Here, we assume incompressible, isothermal case:

$$\nabla \cdot v = 0$$

$$\frac{\partial \rho v}{\partial t} + \nabla \cdot (\rho v v) = -\nabla p + \nabla \cdot \sigma,$$

where $\boldsymbol{\rho}$ – density, v – velocity, p – pressure, $\boldsymbol{\sigma}$ – stress, μ – fluid viscosity.

- First equation is mass conservation equation.
- Second equation is momentum conservation equation.
- For Newtonian fluids we can assume that $\sigma = \mu(\nabla v + \nabla v^T)$ with constant viscosity μ, but
- In many cases fluids are not Newtonian.
- Non-Newtonian fluids posses more complicated stress – shear rate dependency, viscosity might be shear – rate, temperature dependent, can posses yield stress, can be composed of fluid and particles (suspensions), etc.

- For discretization finite volume method is used.
- Navier – Stokes is a system of equations that are solved for velocity v and pressure p.
- In a discrete form we can write the system in following form:

$$\begin{bmatrix} A & B \\ B^T & 0 \end{bmatrix} \begin{bmatrix} v \\ p \end{bmatrix} = \begin{bmatrix} f \\ 0 \end{bmatrix}$$

Where B is discrete gradient operator, B^T discrete divergence operator and A contain velocity related discretization terms from momentum equation.

- Problem is that this system is not easy to solve directly (saddle point problem). We cannot apply preconditioners directly.
- Therefore, so called splitting methods are used (Chorin, SIMPLE, SIMPLEC, PISO).

- Chorin method splits solution of one iteration into few steps:
  - Step 1: Solve momentum equations with pressure from previous iteration to get velocity prediction:

$$\frac{v^* - v^k}{dt} + Cv^* + Dv^* = Bp^k$$

Where A is decomposed to time derivative, convection C and D diffusion parts respectively

  - Step 2: Use continuity equation to build pressure correction equation:

$\frac{v^{k+1} - v^*}{dt} = Bp^c$ with $p^c = p^{k+1} - p^k$, applying B^T on equation we get: $-B^T v^* = dt \cdot B^T B p^c$

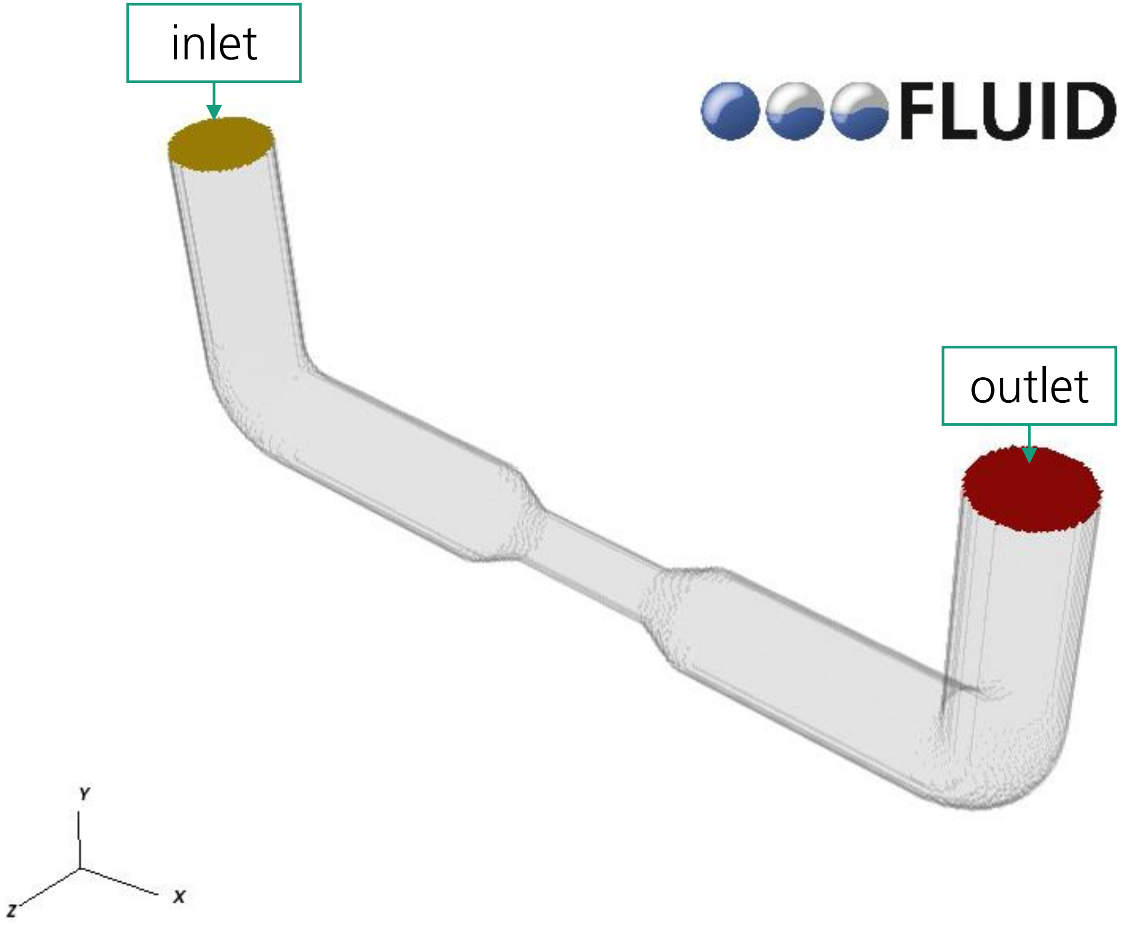
  - Step 3: Correct pressure and velocities.
  - Step 4: go to the next time step iteration.
- In Step 1, and Step 2 we can use preconditioners to speedup simulation.
- Pressure correction equation is of diffusion type, therefore multigrid methods are preferable to solve it fast.

CFD fluid flow simulations.

Simple example – Venturi pipe.

- Single phase flow.
- Pre – defined inlet velocity.
- 2 simulation performed for:
  - Case 1: constant low viscosity $\mu = 0.01\ (pas)$
  - Case 2: higher viscosity shear rate dependent (Carreau model)
    - $\mu_0 = 25\ [pa\ s]$.
    - $\mu_\infty = 0\ [pa\ s]$
    - $A_0 = 0.1315\ [1/s]$
    - $A_1 = 0.4814[-]$

$$\mu(\dot{\gamma}) = (\mu_0 - \mu_\infty)(1 + (A_0\dot{\gamma})^2)^{\left(\frac{A_1-1}{2}\right)} + \mu_\infty$$



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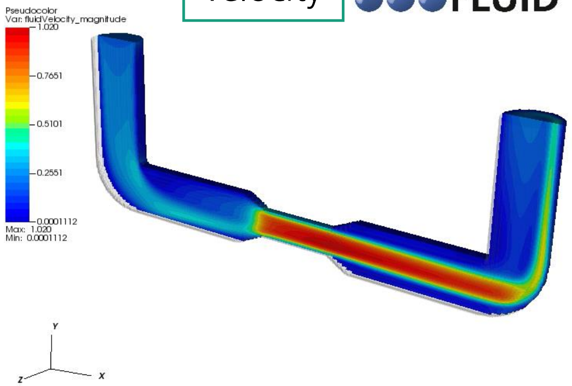
CFD fluid flow simulations.

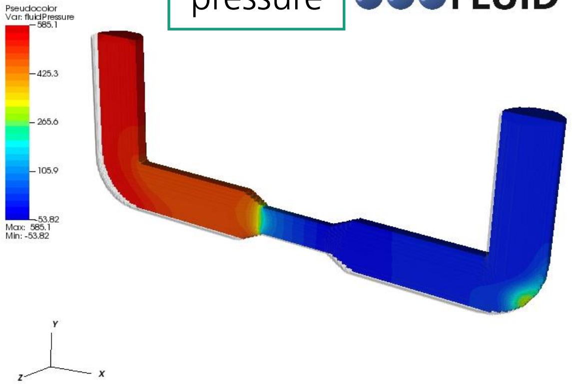
Simple example – Venturi pipe.

- Case 1:

velocity

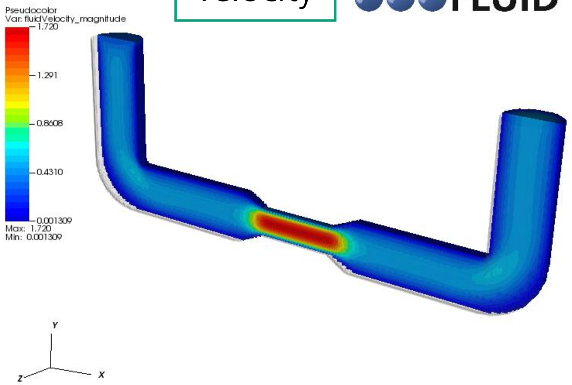


pressure

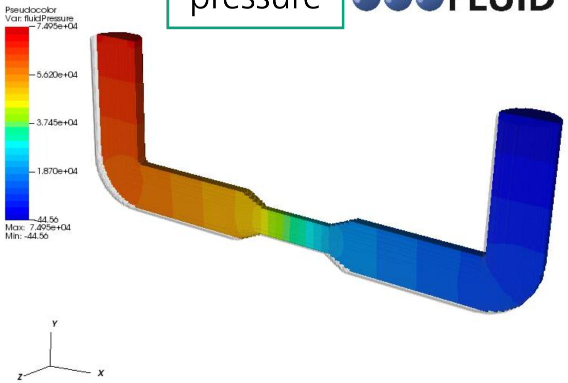


- Case 2:

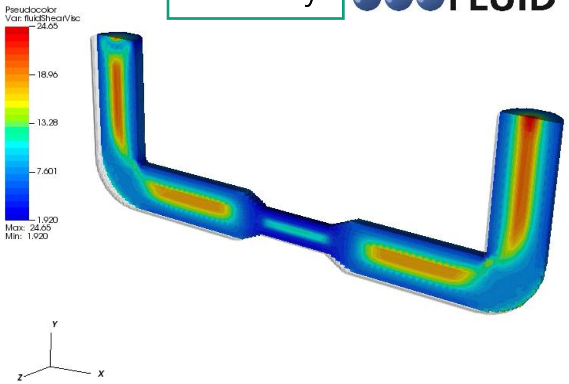
velocity



pressure



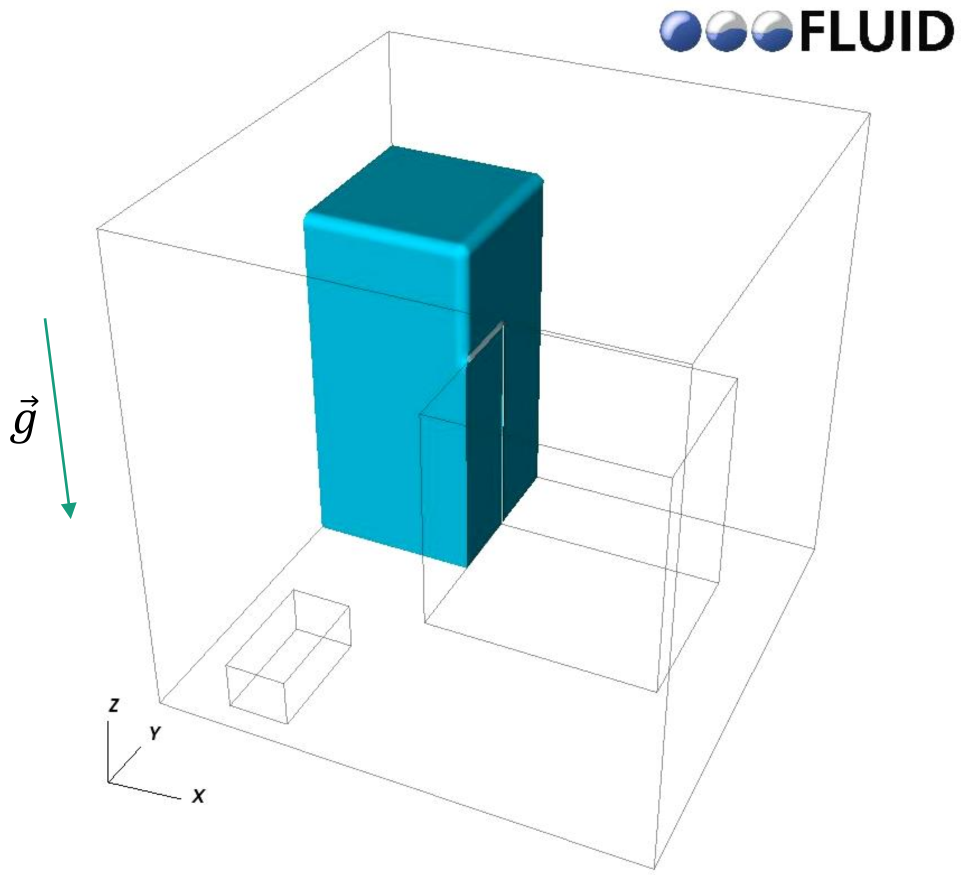
viscosity



CFD fluid flow simulations.

Simple example – dam break.

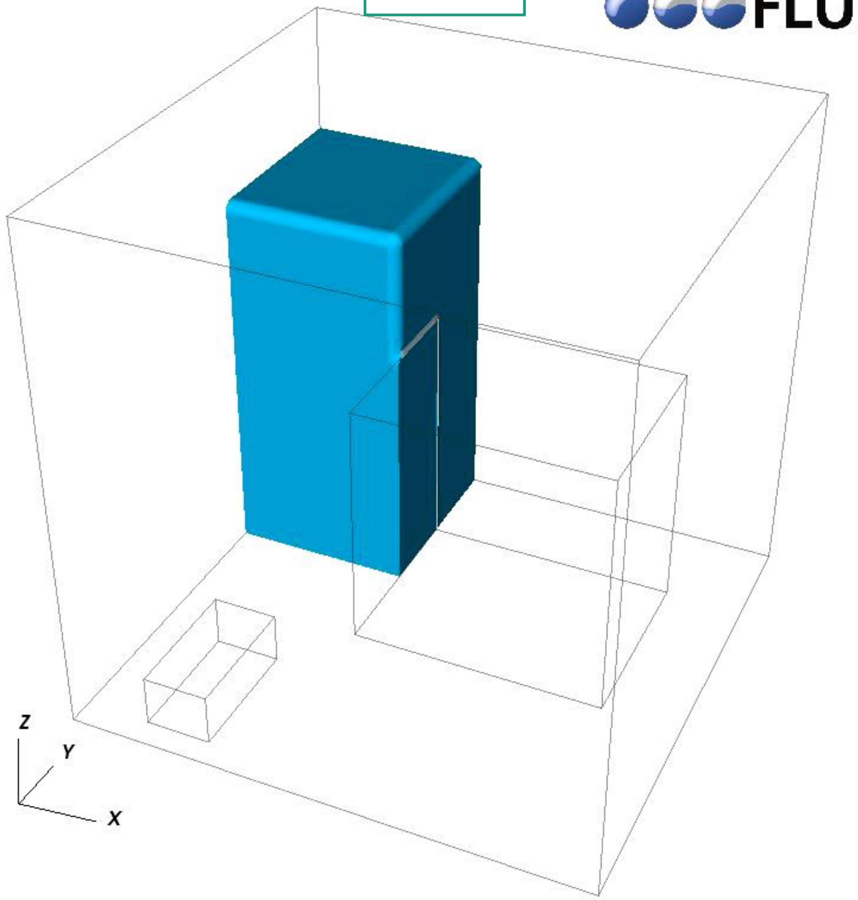
- Breaking dam example and effect of viscosity.
- We initialize block of fluid and release it.
- Fluid starts to flow down due to gravity force
- No – slip velocity boundary conditions applied on walls
- Friction forces depend on viscosity value.
- 2 simulation performed for:
  - low viscosity $\mu = 0.001\ (pas)$ (water)
  - higher viscosity $\mu = 2.5 (pas)$ (honey)



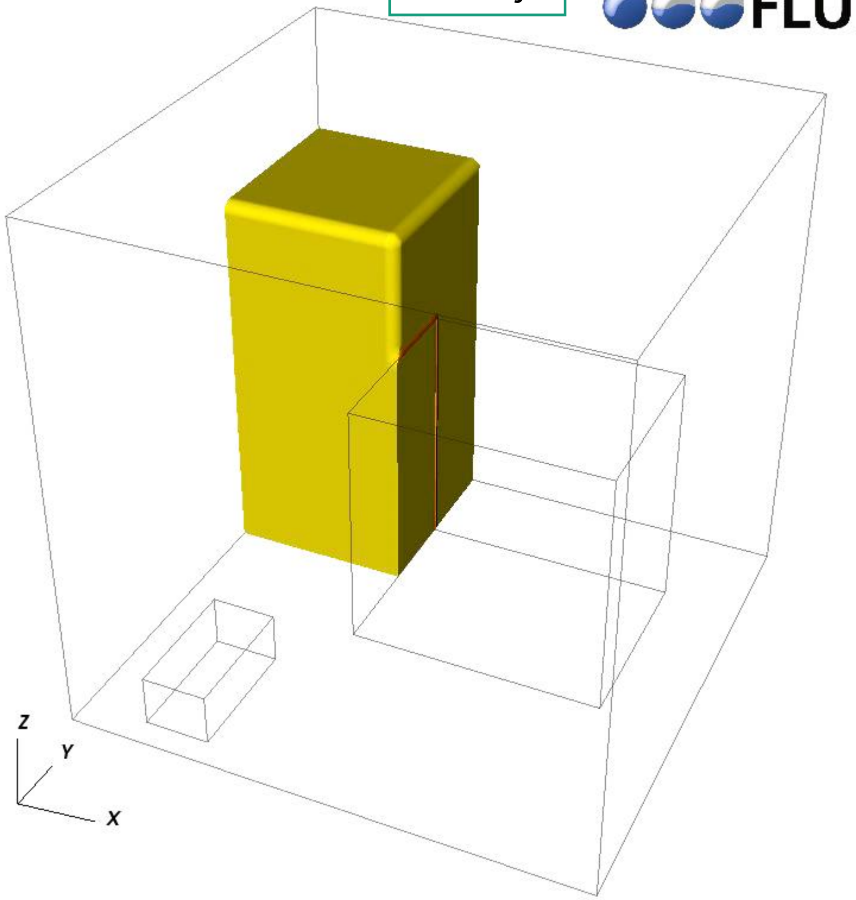
CFD fluid flow simulations.

Simple example – dam break.

water



honey



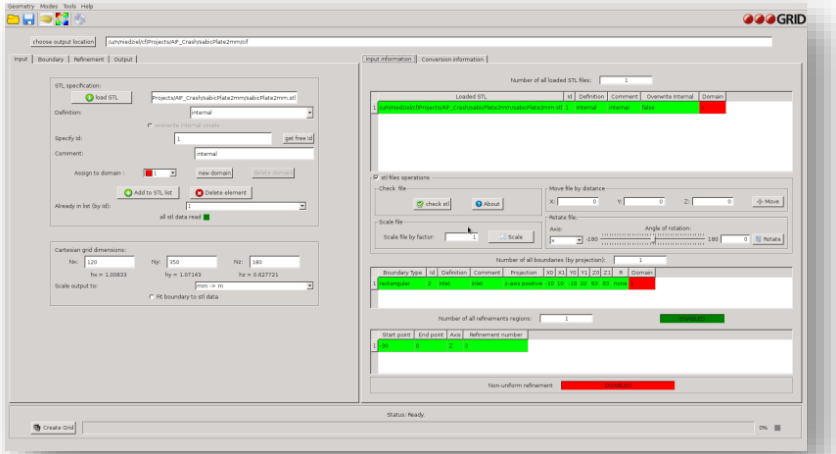
- **FLUIDsinglephase** (single phase complex fluid flow simulations; Newtonian, non-Newtonian fluids. Flow in porous media.)
- **FLUIDinjection** (injection molding process simulations of Newtonian, non-Newtonian fluids)
- **FLUIDmultiphase** (two phase complex fluid flow simulations; Newtonian, non-Newtonian fluids. Flow in porous media);
- Additional modules
  - Fluid thermal flow - temperature equation.
  - Fiber suspension - fiber orientation dynamics.
  - Particle suspension - particle concentration dynamics.
  - Scalar equations - convection-diffusion-reaction equations (up to 10). Scalar equations alse as separate stay alone solver module.

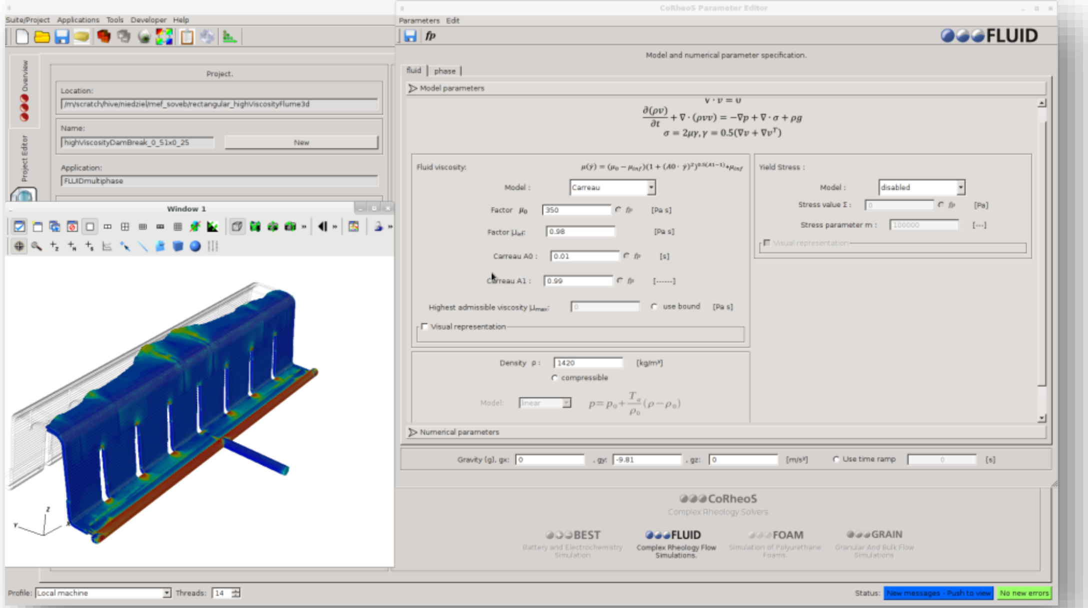
FLUID: Simulation of complex rheology flows.

Solvers for industrial applications.

FLUID

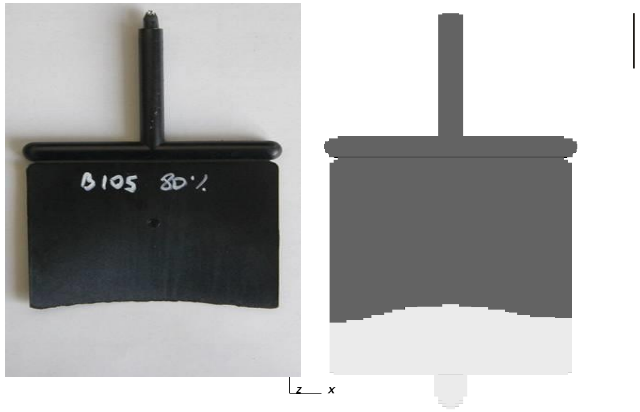
- All solvers can be coupled with all modules through fluid viscosity, friction, stress;
- All solvers can be coupled with GRAIN
- Many input parameters, boundary conditions can be defined in UDF (user defined functions) through functional parameter editor;

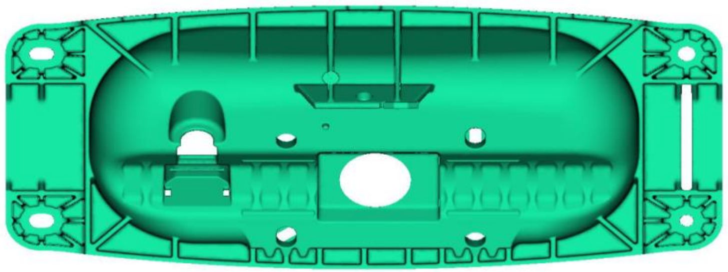


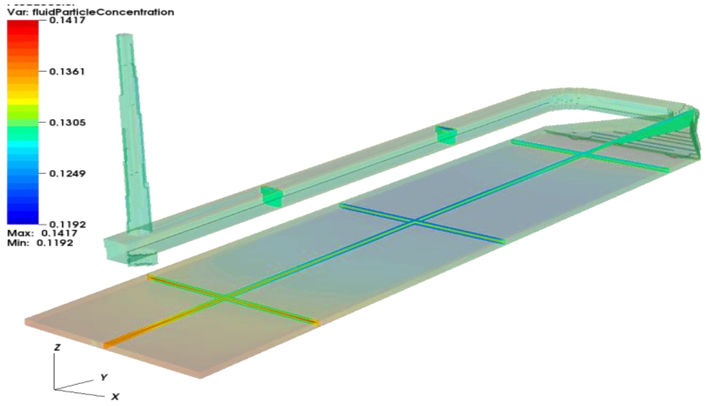


Fiber suspensions: flow and free surface flow (injection molding process).

FLUID injection solver.







FLUID

Generalized Navier-Stokes- Equations

Flow: Incompressible, thermal Navier-Stokes with generalized anisotropic stress

$$\begin{aligned} \nabla \cdot v &= 0, \\ \rho\left(\frac{\partial v}{\partial t} + \nabla \cdot (vv)\right) &= -\nabla p + \nabla \cdot \sigma + \rho g \\ \rho c_p\left(\frac{\partial T}{\partial t} + \nabla \cdot (vT)\right) &= \nabla \cdot (\lambda \nabla T) + \sigma : \kappa \end{aligned}$$

$$\sigma = 2\eta\left(\kappa + N_p(a^{(2)} : \kappa) \cdot a^{(2)}\right), \; \kappa = \frac{1}{2}\left(\nabla v + (\nabla v)^{\mathsf{T}}\right)$$

Modified Folgar-Tucker Equations:

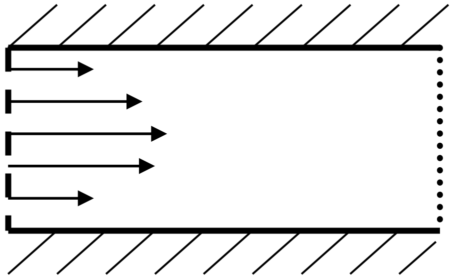
$$\frac{D}{Dt} A^{(2)} = M \cdot A^{(2)} + A^{(2)} \cdot M - 2A^{(4)} : M - 6C_i \dot{\gamma}\left(A^{(2)} - \frac{1}{3} Id\right)$$

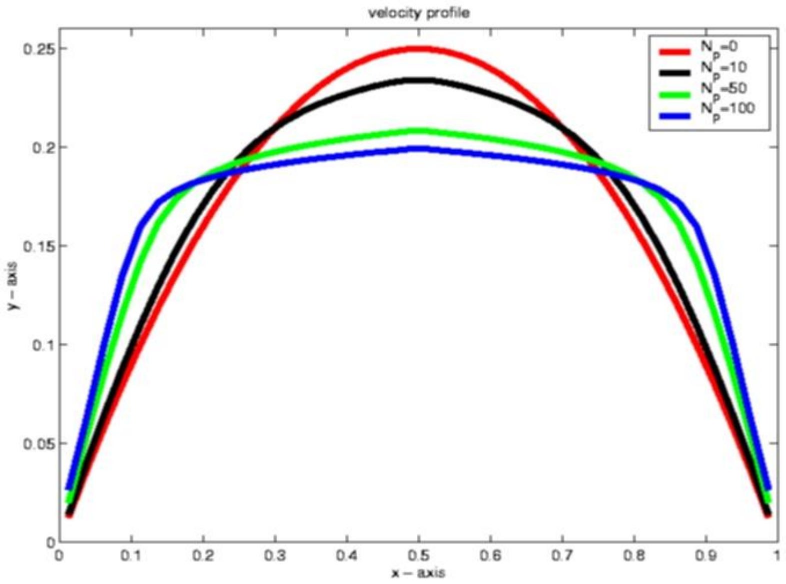
$$M = \frac{\lambda + 1}{2} \nabla v + \frac{\lambda - 1}{2} (\nabla v)^T; \qquad \lambda = \frac{(l/d)^2 - 1}{(l/d)^2 + 1}$$

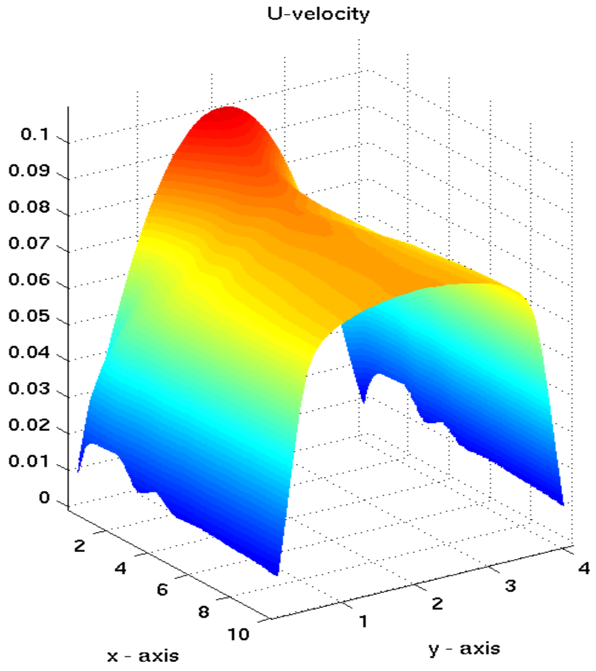
Fiber suspensions.

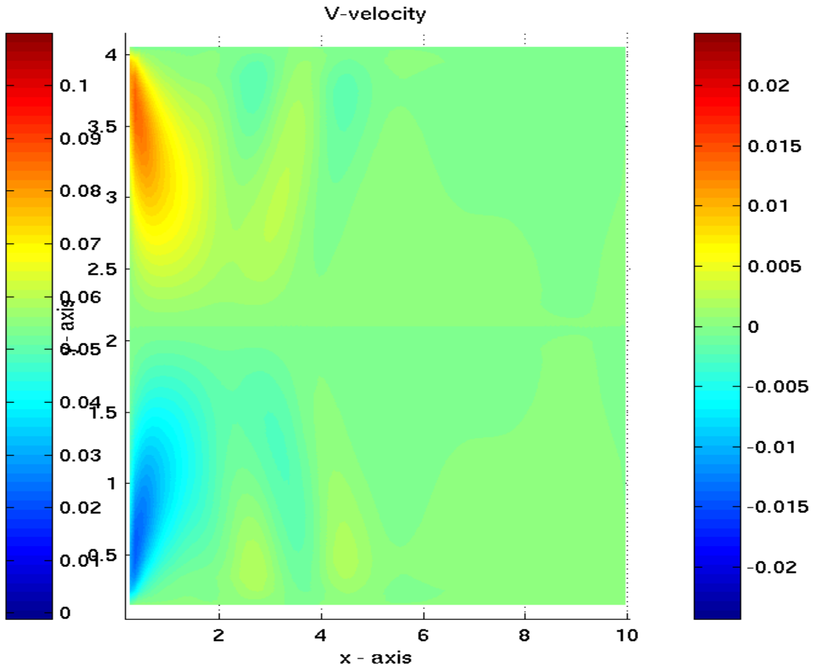
Modeling validation – single phase flow..

Example: Poiselle flow with fiber back coupling







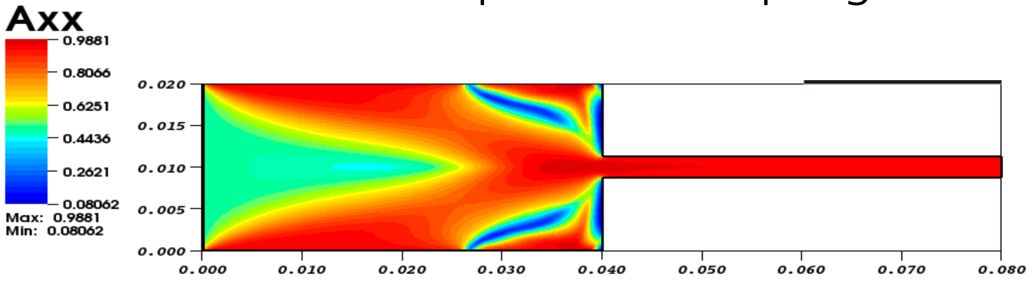


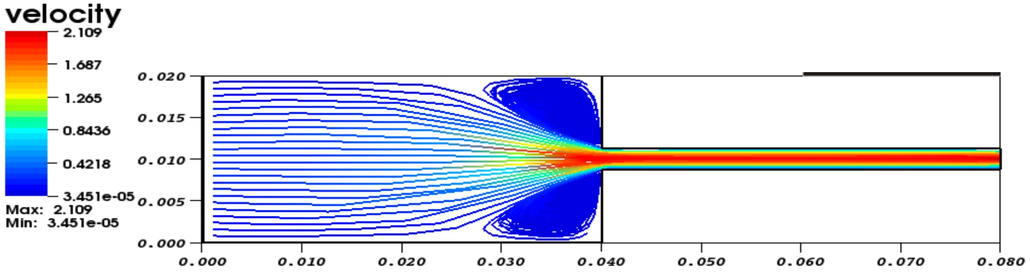
Fiber suspensions.

Modeling validation – single phase flow..

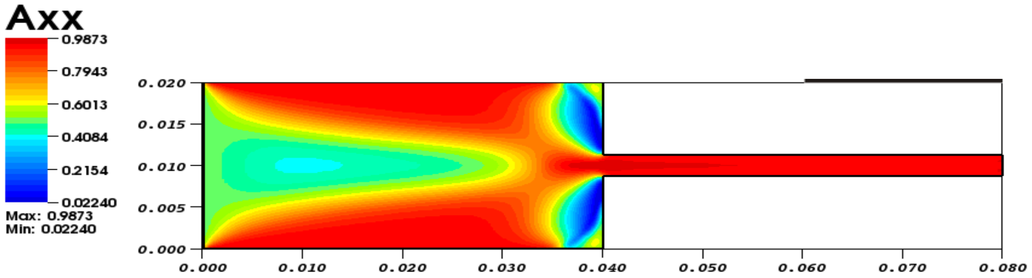
FLUID

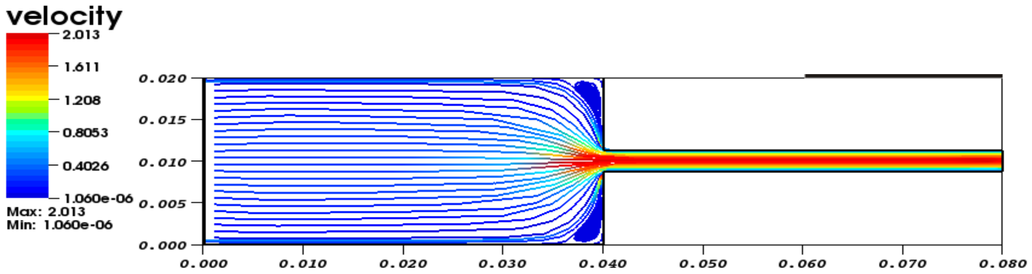
Non-isotropic back coupling model used in ITWM code, Np=10:



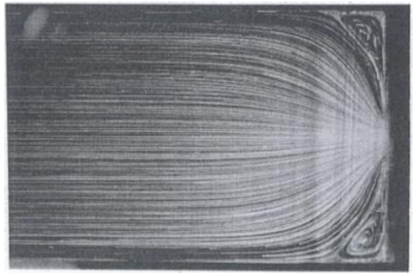


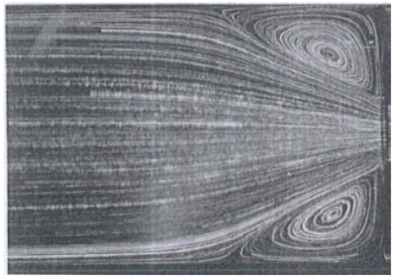
Isotropic back coupling model, Np=10:





Newtonian fluid ->





<- Newtonian fluid with fibers

G.G.Lipscomb et al., Vol.26, p297-325 JNNFM, 1988

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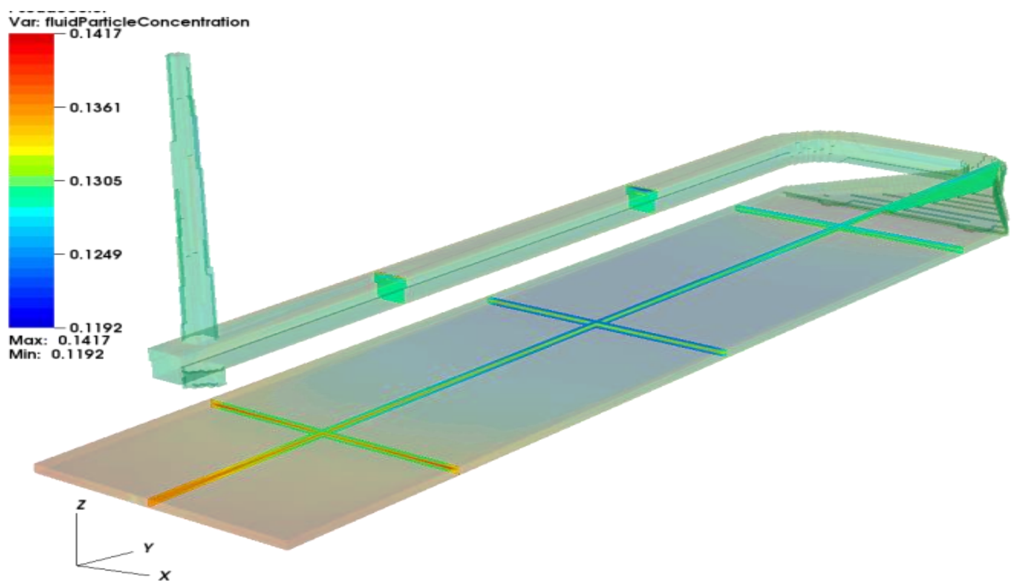
Fiber suspensions.

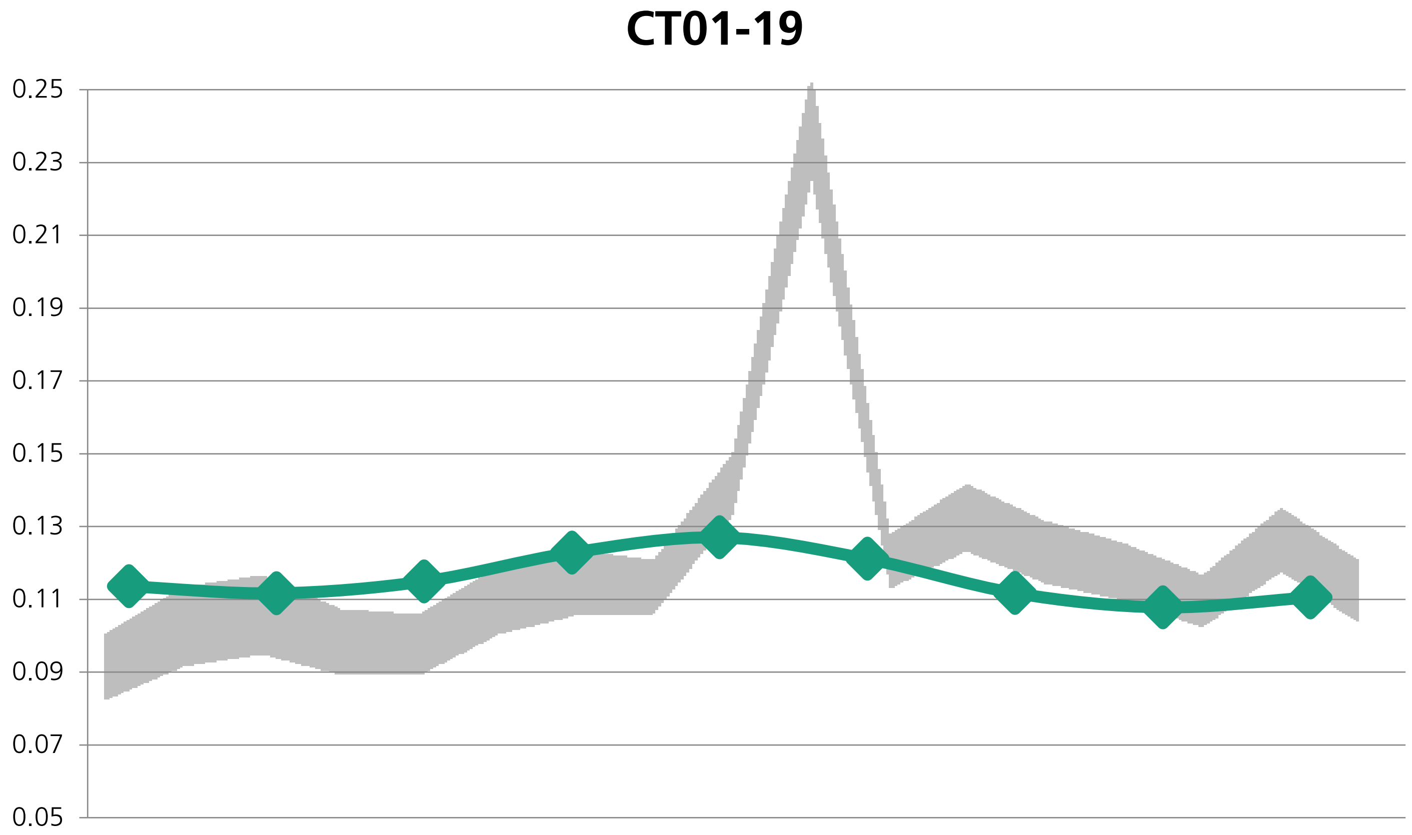
Simulation – long fibers with fiber concentration, 3mm Sabic plate.

- Simulation studies performed for:
  - Closure approximation: smooth orthotropic
  - Diffusion coefficient: $\mathrm{C_i} = 0.0025$
  - Maier-Saupe term: W=7
  - Fiber concentration parameters: $K_{coll} = 0.175$, $K_{visc} = 0.175$



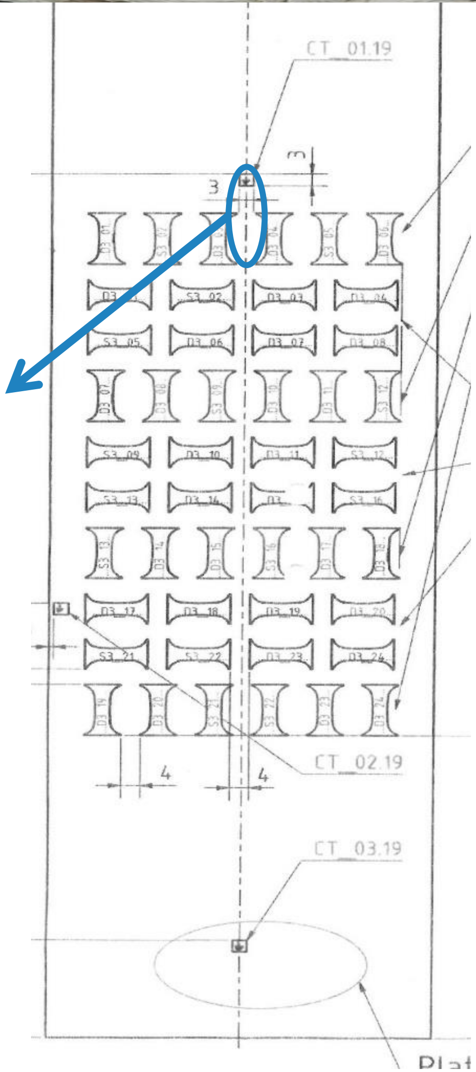
Fiber suspensions.

Simulation validation – fiber volume fraction, 3mm Sabic plate.



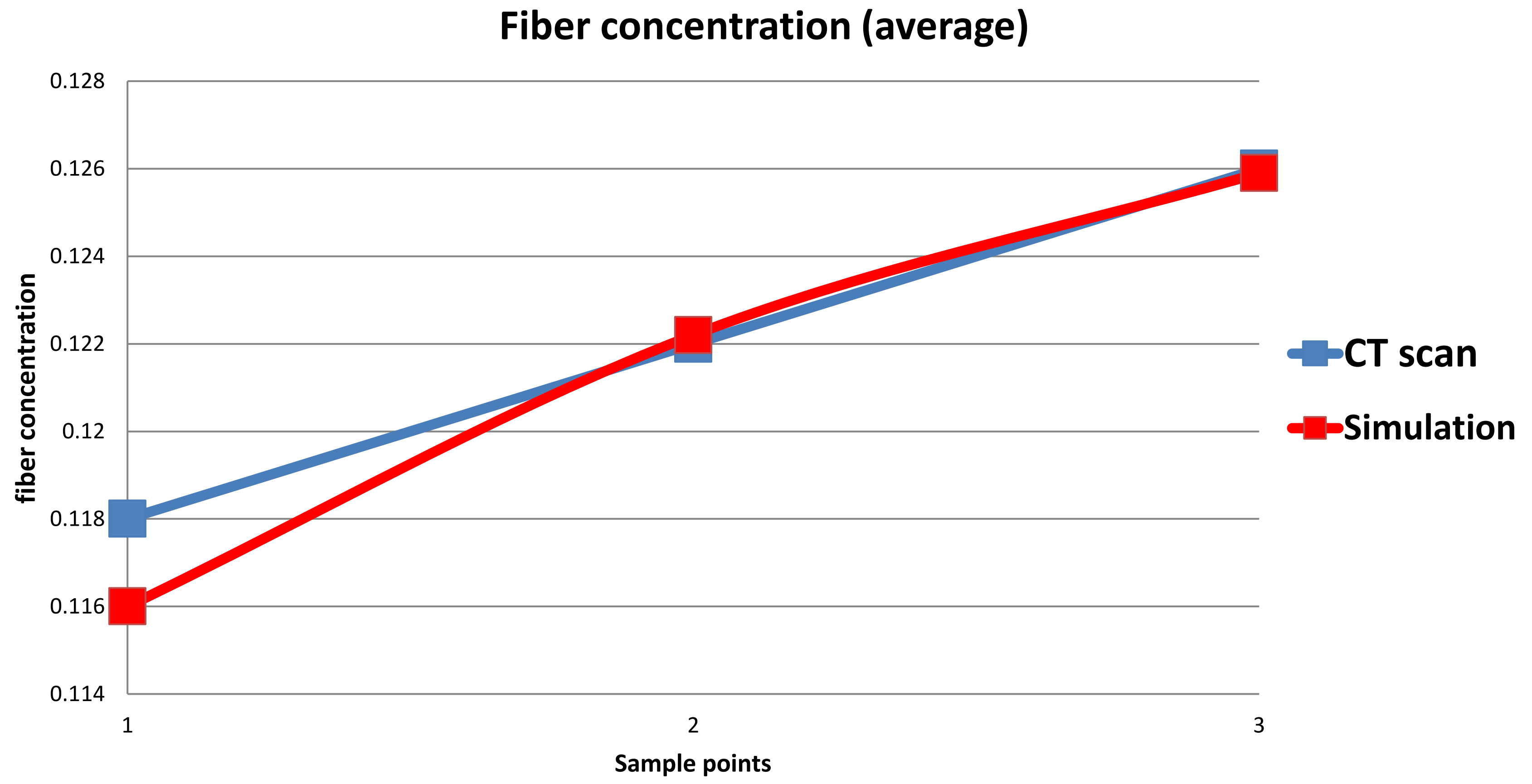
$K_{coll} = 0.175, K_{visc} = 0.175, k = 0.5, C_i = 0.0025, W = 7$

smooth orthotropic closure



Fiber suspensions.

Simulation validation – fiber volume fraction, 3mm Sabic plate.

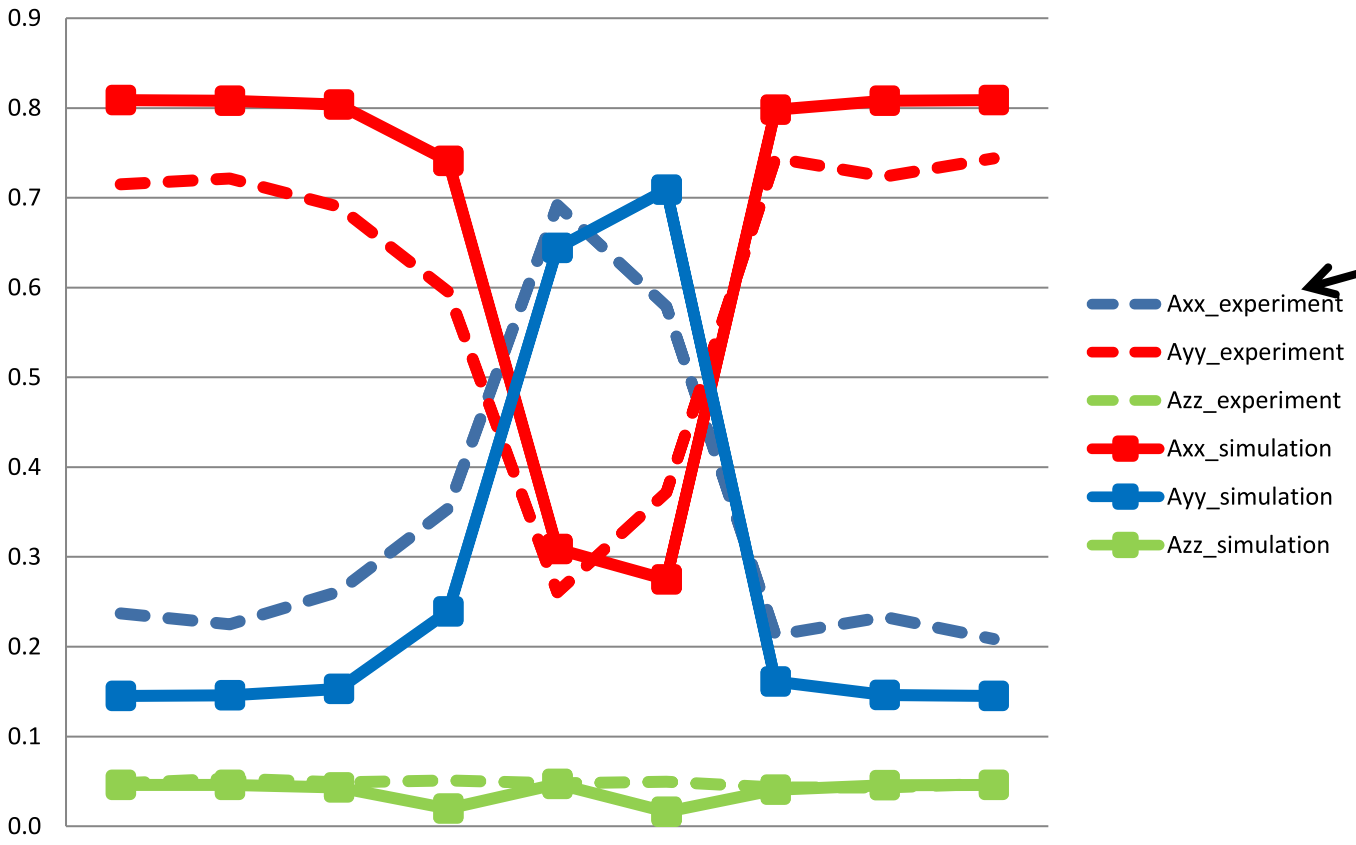


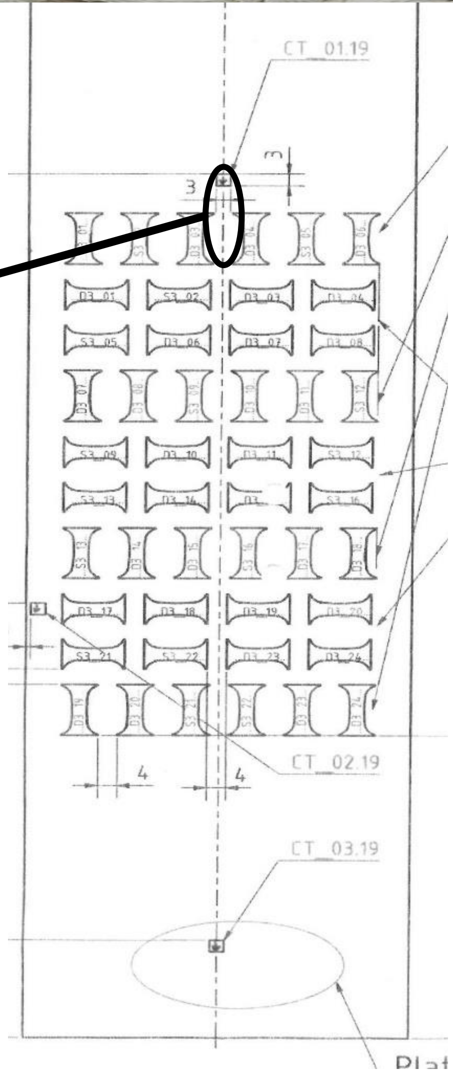
$$K_{coll} = 0.175,\ K_{visc} = 0.175, k = 0.5, C_i = 0.0025, W = 7$$

smooth orthotropic closure

Fiber suspensions.

Simulation validation – fiber orientation, 3mm Sabic plate.





$$K_{coll} = 0.175,\ K_{visc} = 0.175, k = 0.5, C_i = 0.0025, W = 7$$

smooth orthotropic closure

Fiber suspensions.
Simulation validation – fiber orientation, Airbag cavity.

- Simulation studies performed for:
  - Closure approximation: smooth orthotropic
  - Diffusion coefficient: $C_i = 0.0025$
  - Maier-Saupe term: W=7
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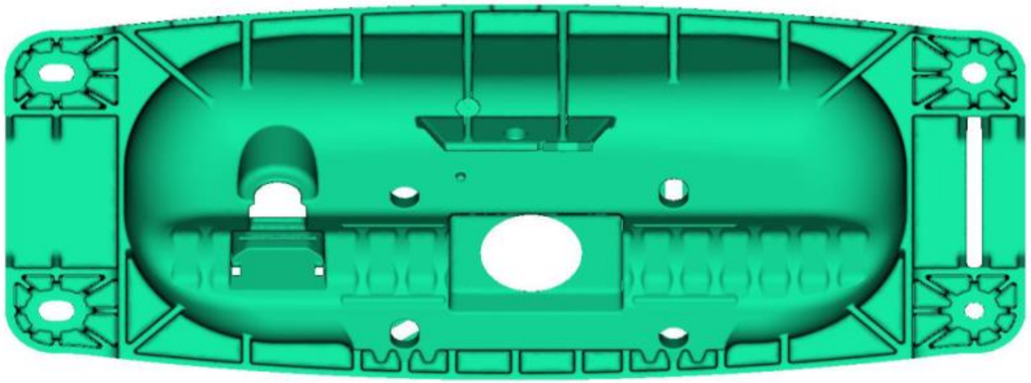
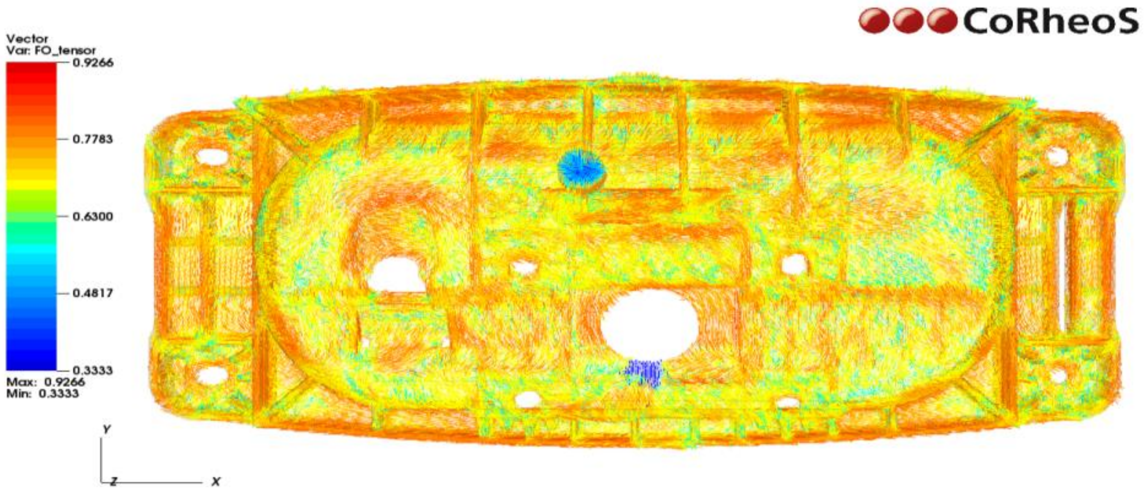
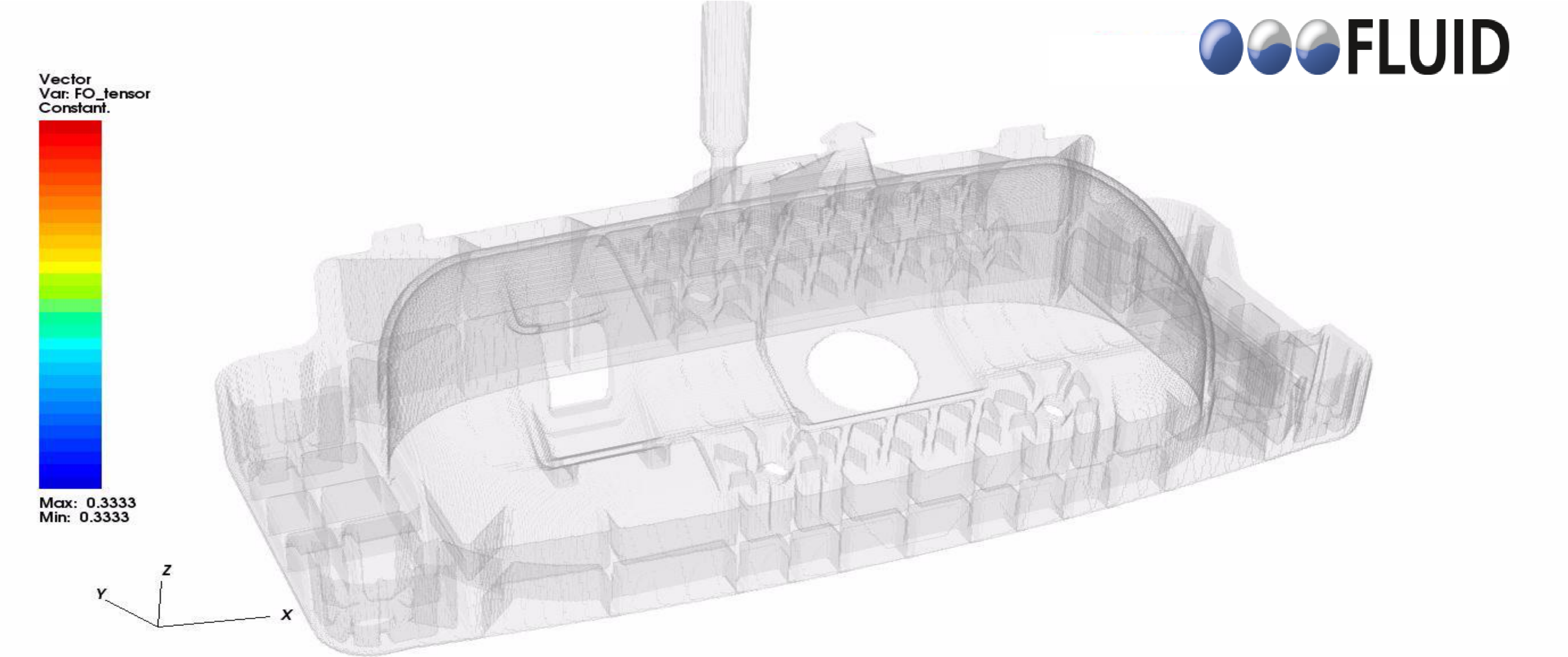




Fiber suspensions.

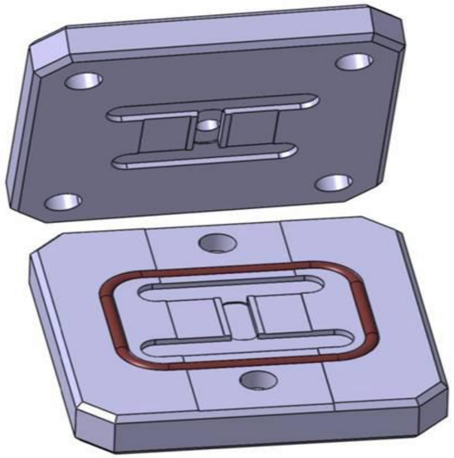
Simulation validation – fiber orientation, Airbag cavity.

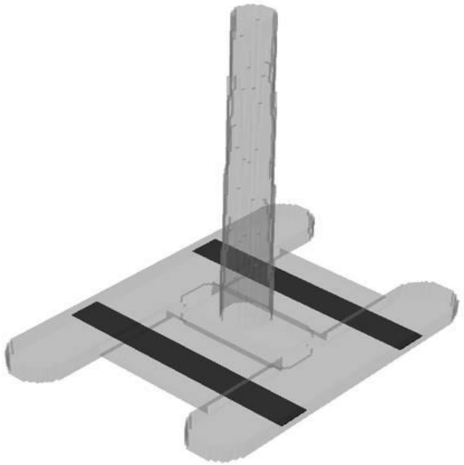


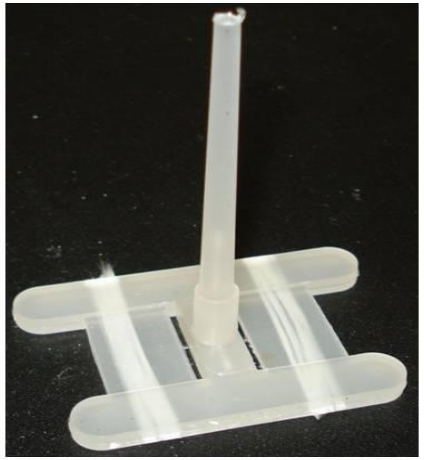
https://www.itwm.fraunhofer.de/de/abteilungen/sms/produkte-und-leistungen/fluid-simulationssoftware-fuer-komplexe-fluide.html

Free surface flow simulations (injection molding process) for parts with integrated textile fiber reinforcement.

FLUID injection solver.







- Fluid flow is governed by Navier-Stokes-Brinkmann equations:

$$\nabla \cdot v = 0$$

$$\frac{\partial \rho v}{\partial t} + \nabla \cdot (\rho v v) = -\nabla p + \nabla \cdot \sigma - \mu \bar{K}^{-1} v,$$

where $\boldsymbol{\rho}$ – density, v – velocity, p – pressure, $\boldsymbol{\sigma}$ – stress, μ – fluid viscosity, $\bar{K}$ - permeability tensor.

$$\bar{K}^{-1} = \begin{cases} 0\,, in\ fluid\ part \\ K^{-1}, in\ porous\ part \end{cases}$$

- Viscosity does not have to be non-constant, permeability tensor might be non-isotropic
- Applications: fluid flow, injection molding (free surface flow), two phase fluids flow

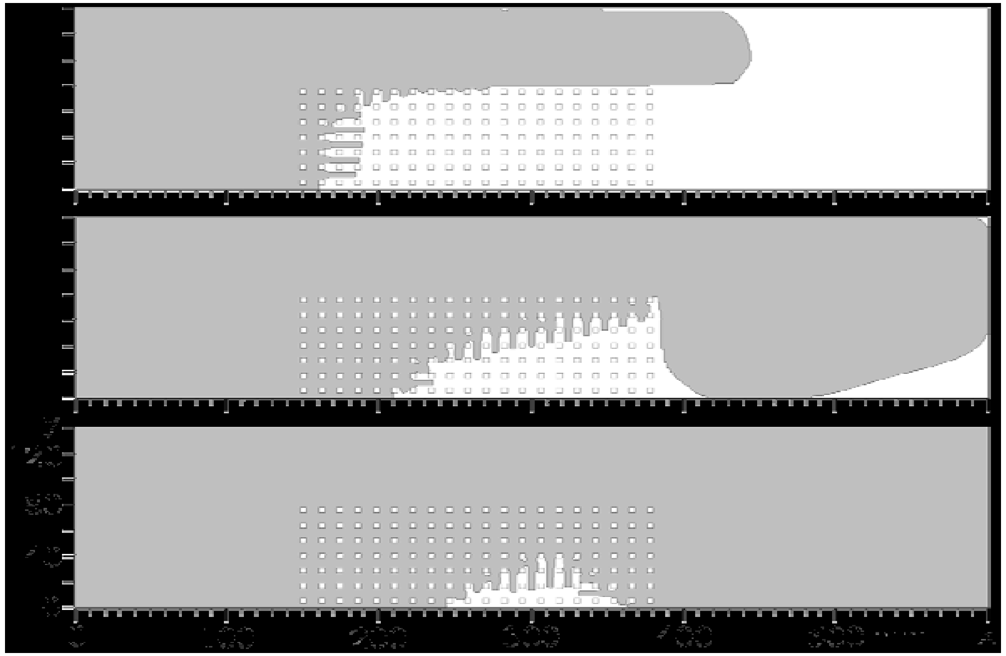
FLUID

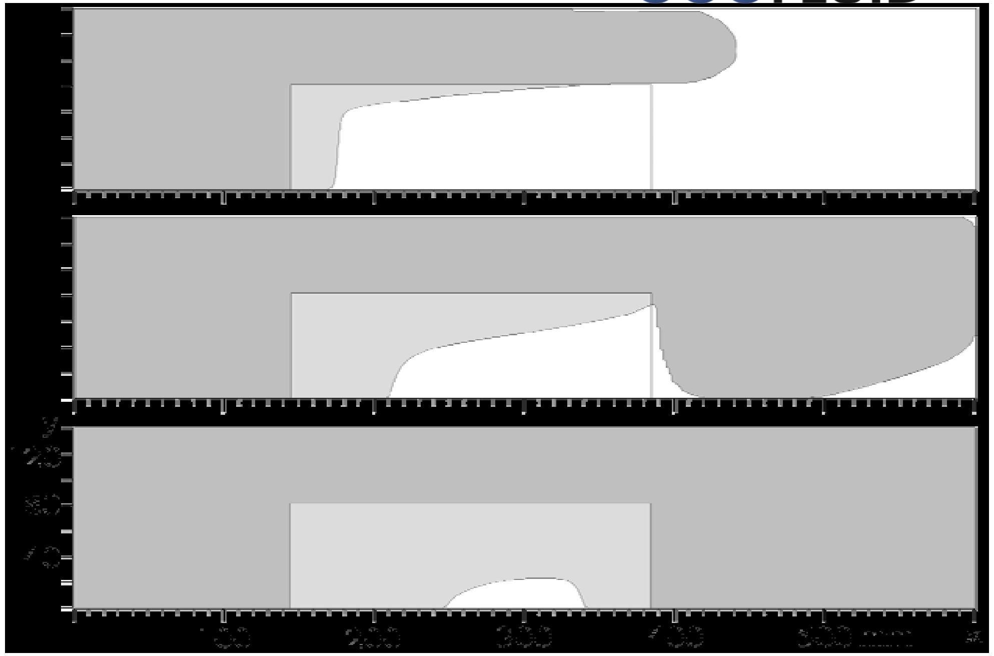
Filling study , 2D test geometry.

Validation of algorithm with porous part:
geometrically resolved porosity (micro case)

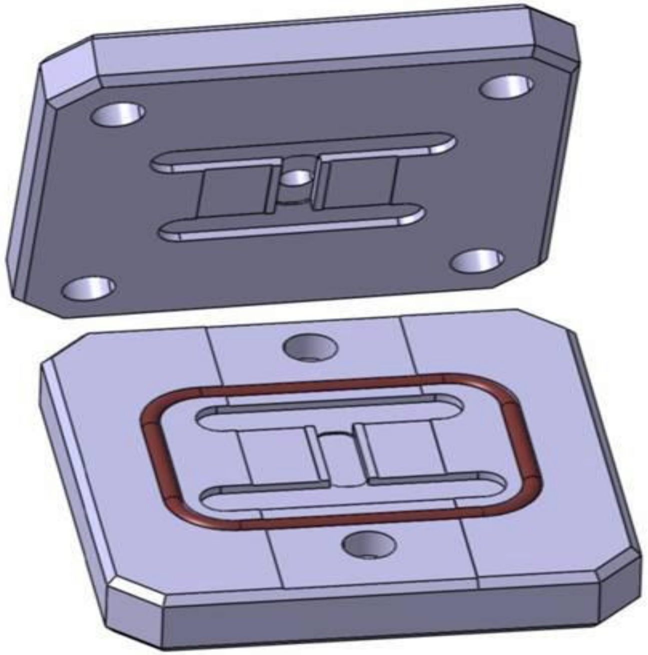
Validation of algorithm with porous part:
porous media described through
permeability tensor K (macro case)

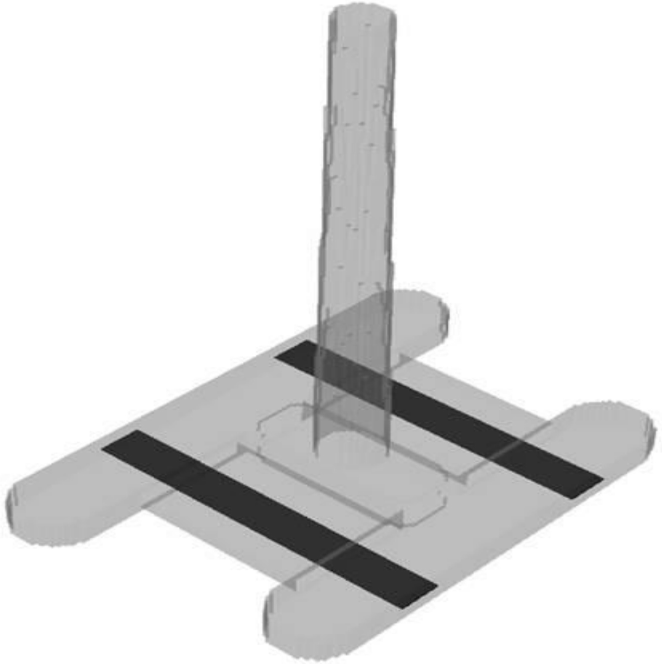
FLUID

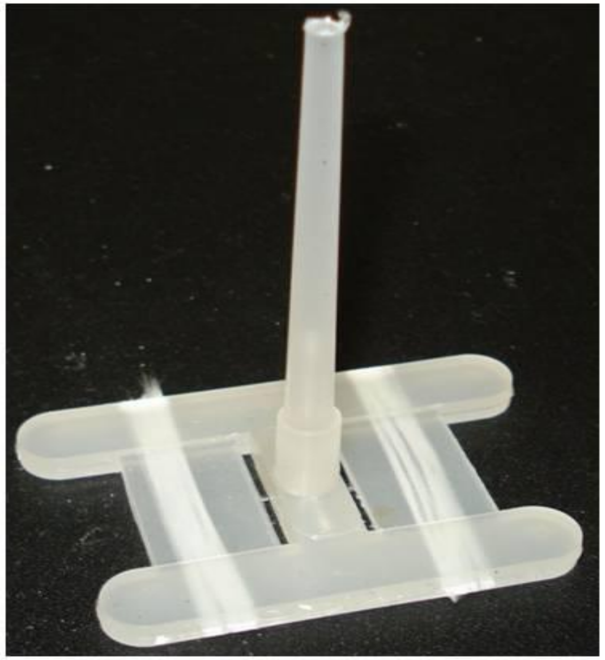




Filling study , 3D mold.



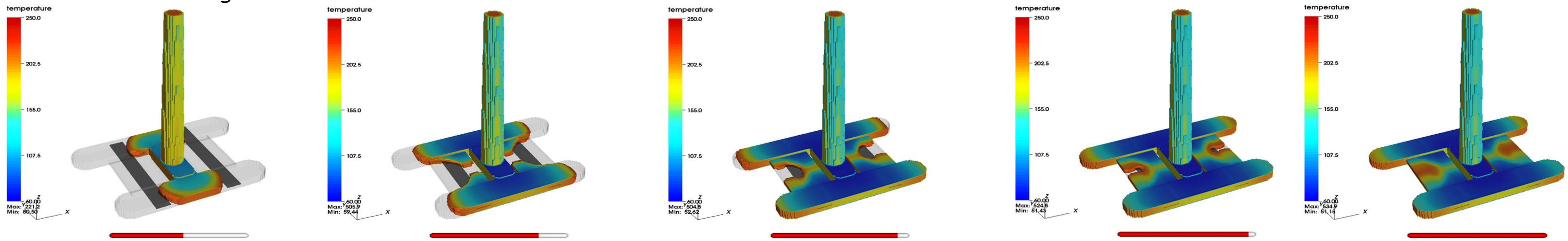




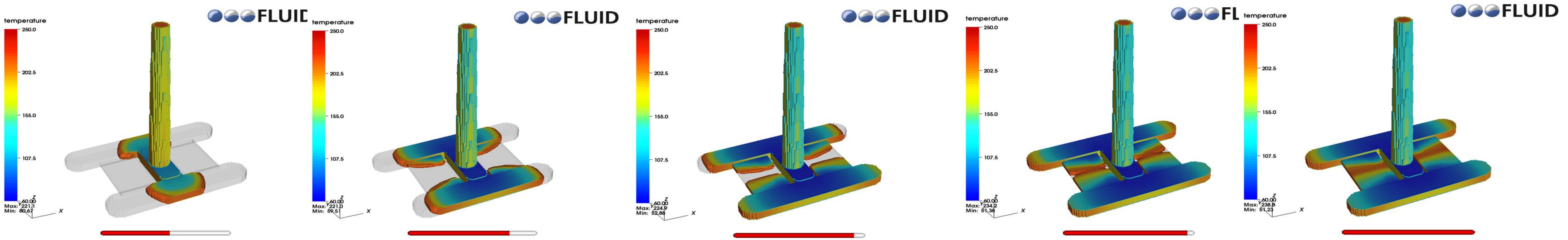
CAD-data of injection mold (left) and part model (middle) and formed part with integrated fiber bundle (right)

Filling study , 3D mold.

Mold with rovings



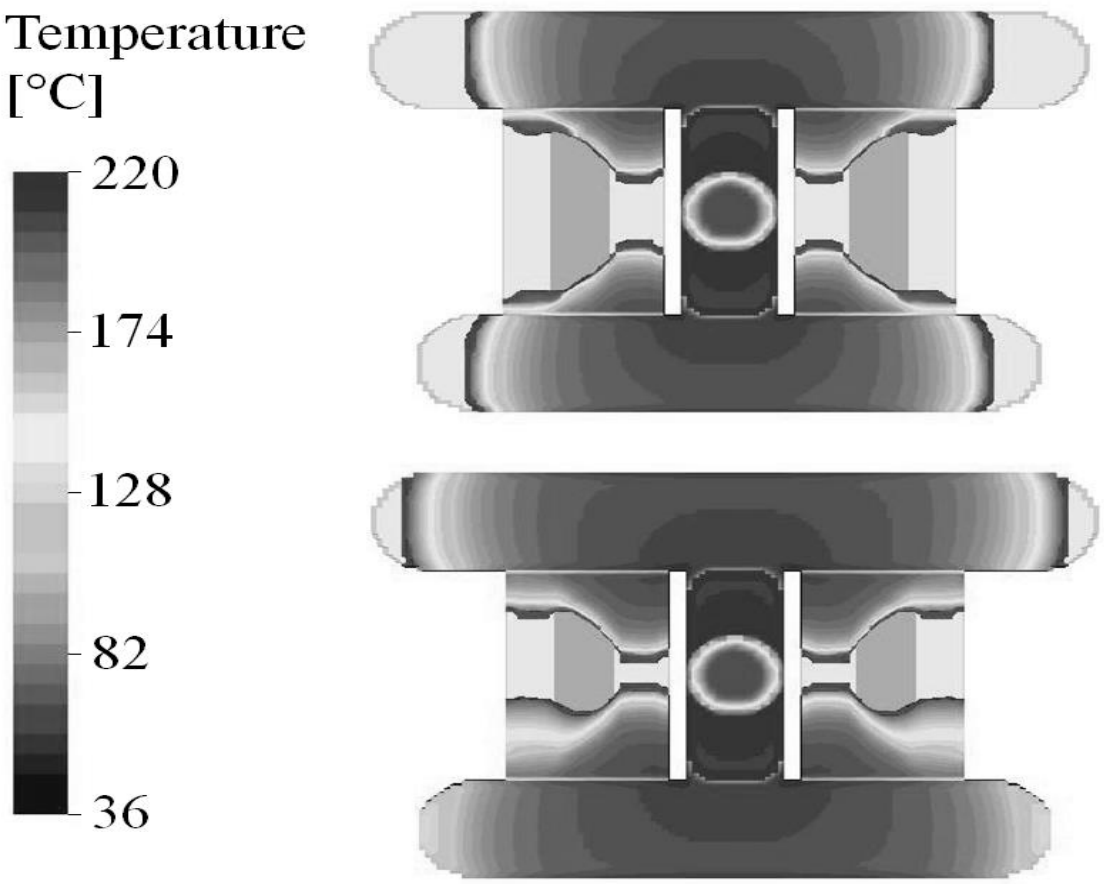
Mold without rovings

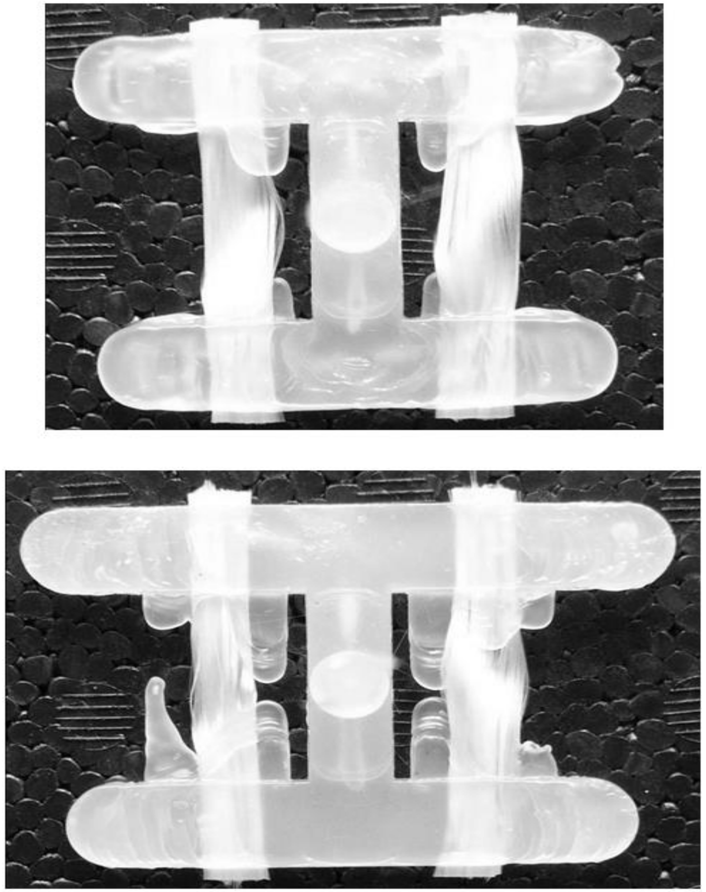


Flow in porous media.

Validation – 3D cavity with fixed rovings.

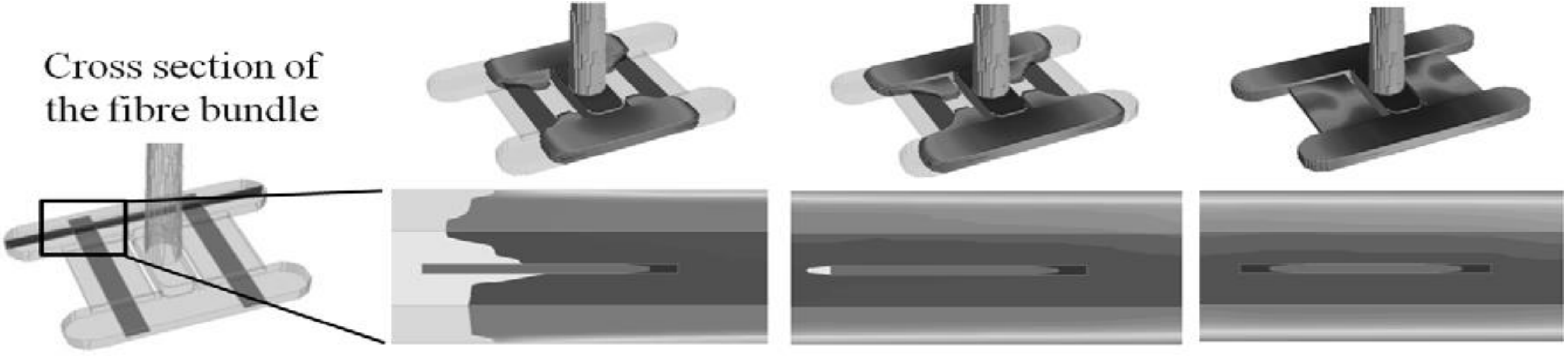
Filling study , 3D mold. Flow front comparison.





Filling study , 3D mold. Flow front comparison.

Simulation: increasing of the impregnation level with duration of melt overflow.

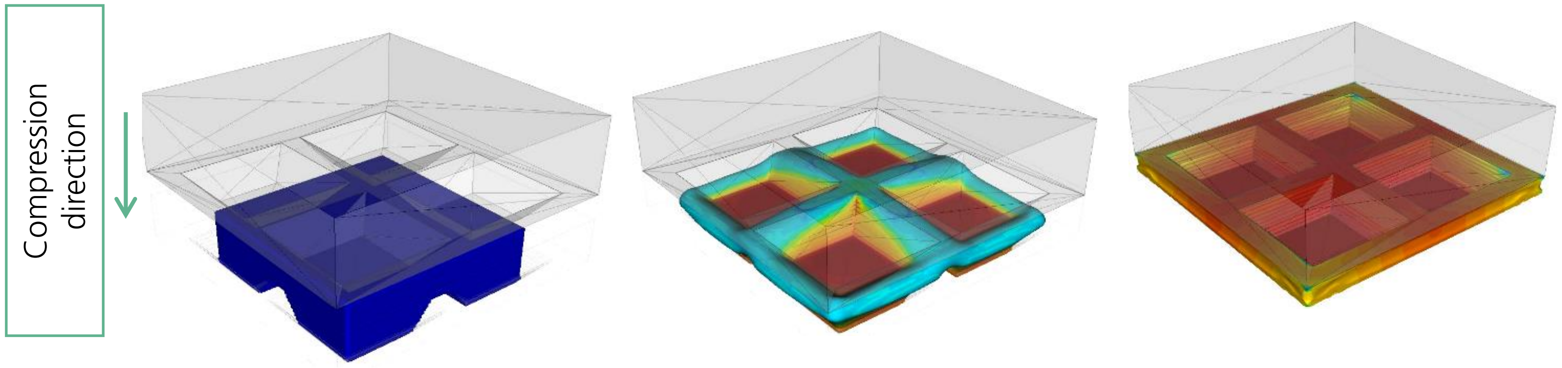


Experiment: Photomicrographs along flow path of embedded fiber bundle.

Simulation indicated regions that could be difficult, or not possible to perforate.

SMC – Sheet mold compression simulations.

FLUIDmultiphase solver.



ALMA

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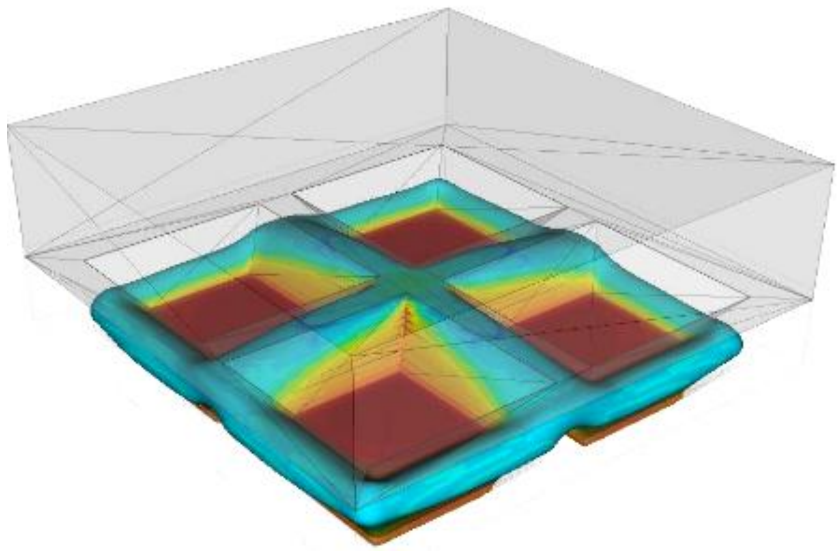
SMC simulations.

Main solver properties.

- SMC process simulated based on fluid mechanics on fixed grids.
- Moving part is modeled via stl file.
- Moving part surface is detected in each time step iteration and moving part velocity is passed to surface grid elements
- Fluid flow is governed by Navier-Stokes, or Navier-Stokes-Brinkmann equations
- Modeling allows to apply all equations used in other applications, like injection molding
    - Temperature
    - Fiber orientation
    - Particle concentration, etc.



- Many SMC materials consist of fiber bundles and matrix material.
- In the modeling we want to add option for the matrix material to partially overflow fibrous skeleton.
- We assume that velocity is decomposed into (Perez et.al. 2019):

$$\begin{cases} v = v_s + v_d \\ v_s = \alpha \cdot v \\ v_d = (1-\alpha) \cdot v \end{cases}$$

- where in dilute regime $\boldsymbol{\alpha}\approx\mathbf{1}$. Then we have two pressure gradient contributions:

$$\begin{cases} \nabla p_s = \nabla \cdot (\mu \nabla v_s + 2\mu N_p (D_s : a) a) \\ \nabla p_d = -\mu \bar{K}^{-1} v_d \end{cases}$$

- Where $\boldsymbol{a}$ denotes fiber orientation tensor and $\boldsymbol{D_s}$ fluid rate-of-deformation tensor. Combining pressure gradients, we get

$$\nabla p = \nabla p_s + \nabla p_d$$

FLUID

- In the modeling we have option for the matrix material to partially overflow fibrous skeleton
- Fluid flow is governed by Navier-Stokes-Brinkmann equations:

$$\nabla \cdot v = 0$$

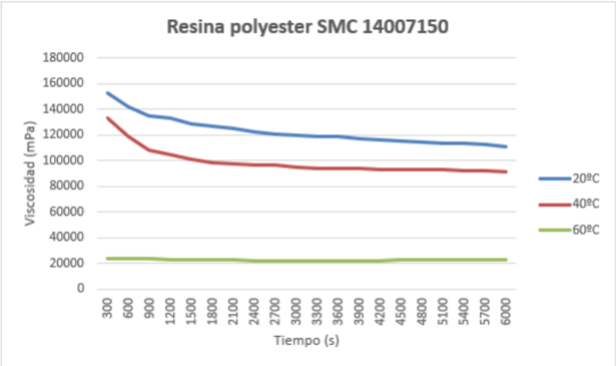
$$\frac{\partial \rho v}{\partial t} + \nabla \cdot (\rho v v) = -\nabla p + \nabla \cdot (\alpha \mu \nabla v) - (1-\alpha)\mu \bar{K}^{-1} v,$$

- where ρ – density, v – velocity, p – pressure, $\boldsymbol{\sigma}$ – stress, μ – fluid viscosity, $\bar{K}$ - permeability tensor

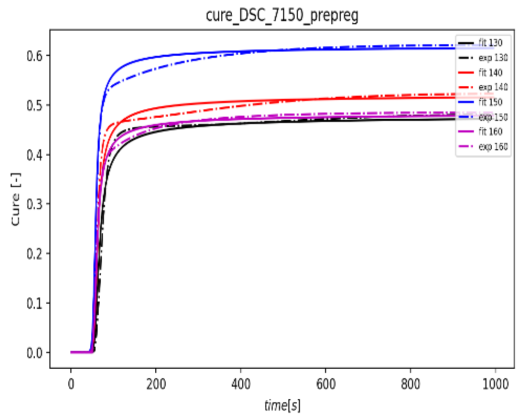
$$\bar{K}^{-1} = \begin{cases} 0, \mathit{outside\ SMC} \\ K^{-1}, \mathit{inside\ SMC} \end{cases}$$

- Parameter α describes fiber-fiber (skeleton), fiber-fluid interaction. It defines how much fluid overflows fibrous skeleton. For $\alpha \approx 1$ fibers flow with fluid (matrix) material. For smaller α more flow through porous-like fibrous skeleton occurs.
- Permeability should depend on fiber orientation tensor a and fiber concentration ϕ.
- In addition, fiber orientation, temperature, curing equations are solved.

Viscosity measurements



DSC curing measurements



- Fibers flow with velocity $v_s = \alpha \cdot v$. We solve additional equation

$$\frac{\partial \varphi}{\partial t} + \alpha v \cdot \nabla \varphi = 0$$

- where $\varphi \in [0,1]$ and represents fiber position for $\varphi = 1$.
- Position of SMC material follows:

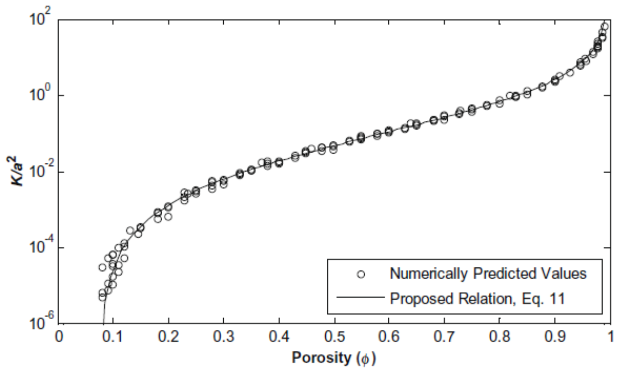
$$\frac{\partial f}{\partial t} + v \cdot \nabla f = 0$$

- where $f \in [0,1]$ and represents SMC position for $f = 1$.
- Since we assume incompressibility, fiber volume concentration can be obtained from simple re-scaling

$$\phi = \phi_{init} \frac{\sum_{f>0} f_{cv}}{\sum_{\varphi>0} \varphi_{cv}}$$

- for permeability Gebart's relation could be used (Nabovati et.al. 2009), permeability depends on porosity $\theta = 1 - \phi$:

$$K(\theta) = K_0 C_1 \left(\sqrt{\frac{1-\theta_c}{1-\theta}} - 1 \right)^{C_2}$$

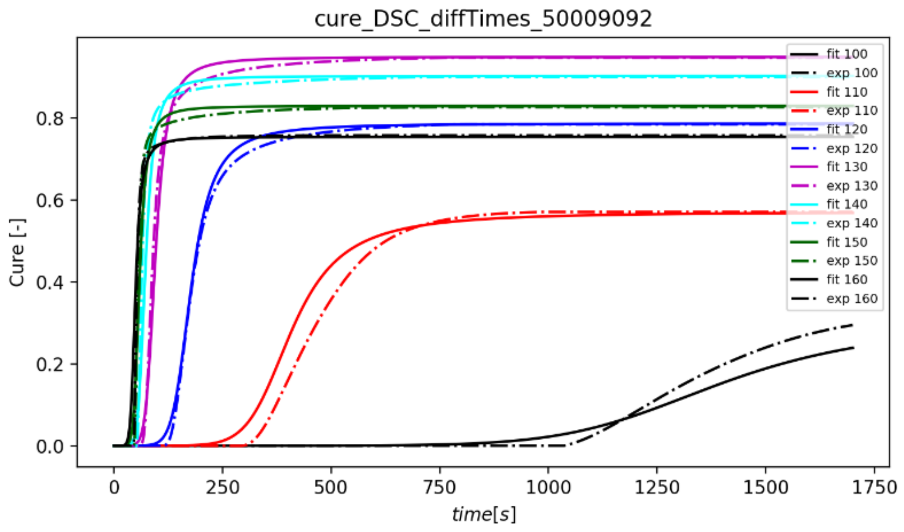


- Curing model based on Rao.et.al. (2017):

$$\frac{D\xi}{Dt} = k(b + \xi^m)(\xi_{max} - \xi)^n$$

$$k = \left[(0.5 - B)\left(1 + \tanh\left(D\left(t - t_s^{\xi}\right)\right)\right) + 2B\right]\frac{1}{(1 + \omega\alpha_T)^{\beta}} k_0 e^{-\frac{E_{\xi}}{RT}}$$

$$\log_{10}\alpha_T = \frac{-C_1\left(T - T_g\right)}{C_2 + T - T_g}, \qquad T_g = \frac{T_{g0}(1 - \xi) + A\xi T_{g\infty}}{1 - \xi + A\xi}$$



- Temperature:

$$\rho C_p\left(\frac{\partial T}{\partial t} + \mathbf{v}\cdot\nabla T\right) = \nabla\cdot(k\nabla T) + \frac{1}{2}(\eta_m \mathbf{D} : \mathbf{D}) + \rho C_p H_R \frac{d\xi}{dt}$$

- Viscosity contribution:

$$\mu = \mu \cdot \left(\frac{\zeta}{\zeta - \zeta_{max}}\right)^{A+B\zeta}$$

Formula for SMC permeability $\overline{K}$

- In formulas below fiber orientation $\boldsymbol{\lambda_x} > \boldsymbol{\lambda_y} > \boldsymbol{\lambda_z}$ denote fiber orientation tensor eigenvalues

Value for K_x and K_y :

$$K_x(\lambda_x, \lambda_z, \theta_{cluster}) = 10^{-9} \times (4{,}27 + 4{,}62\,\lambda_x - 6{,}75\,\lambda_z) \times \left(\sqrt{\frac{1-0{,}0743}{\theta_{cluster}}} - 1\right)^{2{,}31}$$

$$K_y = K_x(\lambda_y, \lambda_z, \theta_{cluster}) = K_x(1 - \lambda_x - \lambda_z, \lambda_z, \theta_{cluster})$$

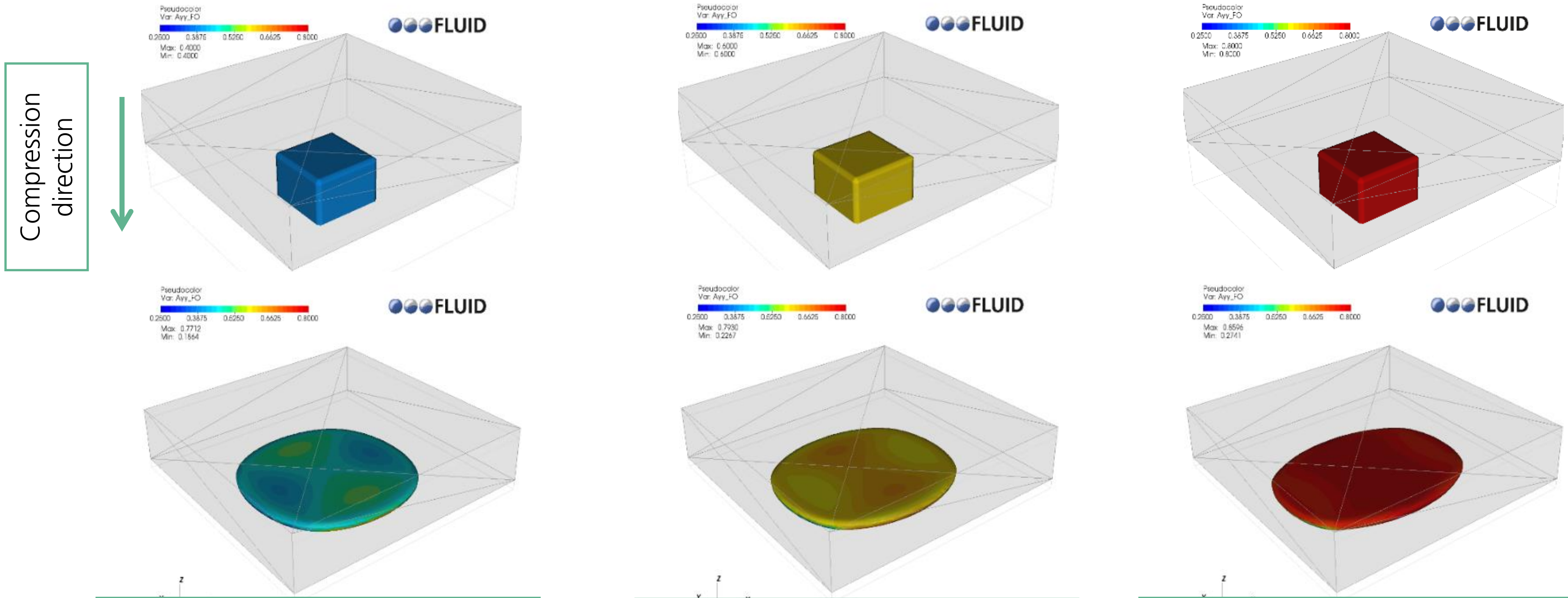
Value for K_z (here, $\lambda_x \geq \lambda_y$):

$$K_z(\lambda_x, \lambda_z, \theta_{cluster}) = 10^{-9} \times (1{,}432 - 0{,}723\,\lambda_x + 1{,}3\,\lambda_z) \times \left(\sqrt{\frac{1-0{,}0743}{\theta_{cluster}}} - 1\right)^{2{,}31}$$

SMC simulations.

Validation – simple example.

- FLUID SMC solver test examples, cuboid initial material shape, flat press, flat bottom
- Arbitrary model and fibre orientation input data.
- Test of back coupling of fibre orientation on the flow.



Initial fiber orientation (0.4,0.4,0.2)

Initial fiber orientation (0.3,0.6,0.1)

Initial fiber orientation (0.1,0.8,0.1)

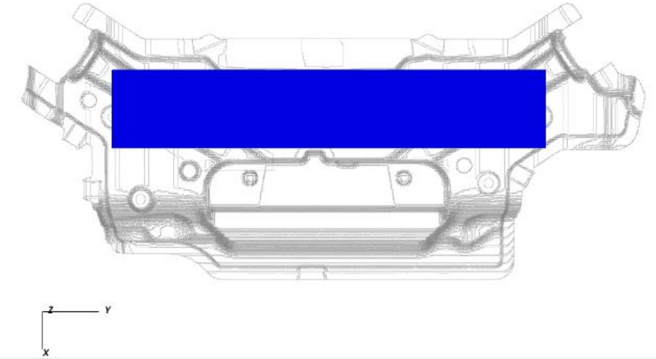
SMC simulations.

Validation – Cowl panel.

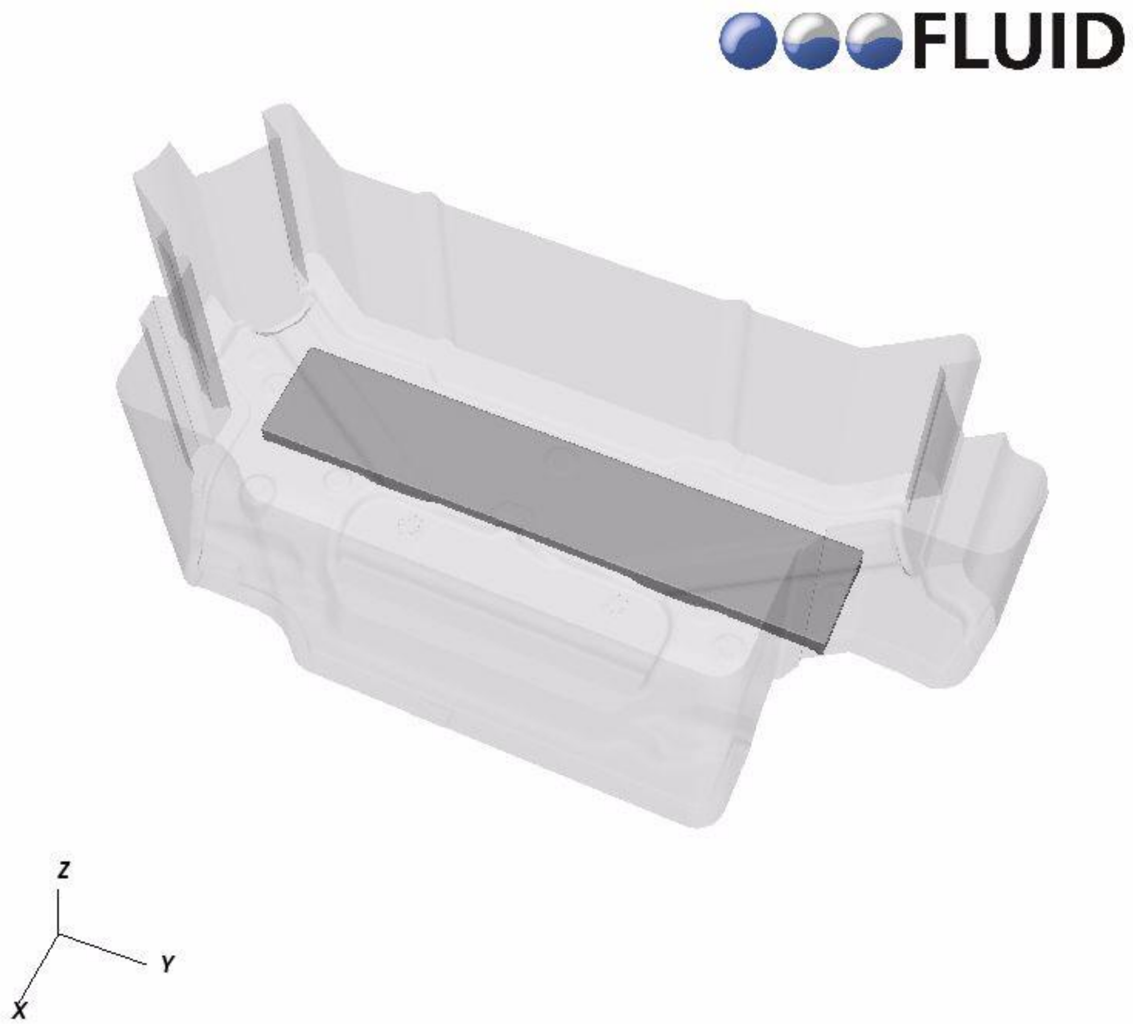
- Cowl Panel
  - Initial prepreg position consists of 6 blanks placed on top of each other
  - Front flow studies are preformed.
  - The experimental data were obtained by stopping the pressing process at different closing heights of +2mm, +1.4mm, +1.0mm, +0.4mm from the final closure.
  - Cure data are evaluated

Process conditions

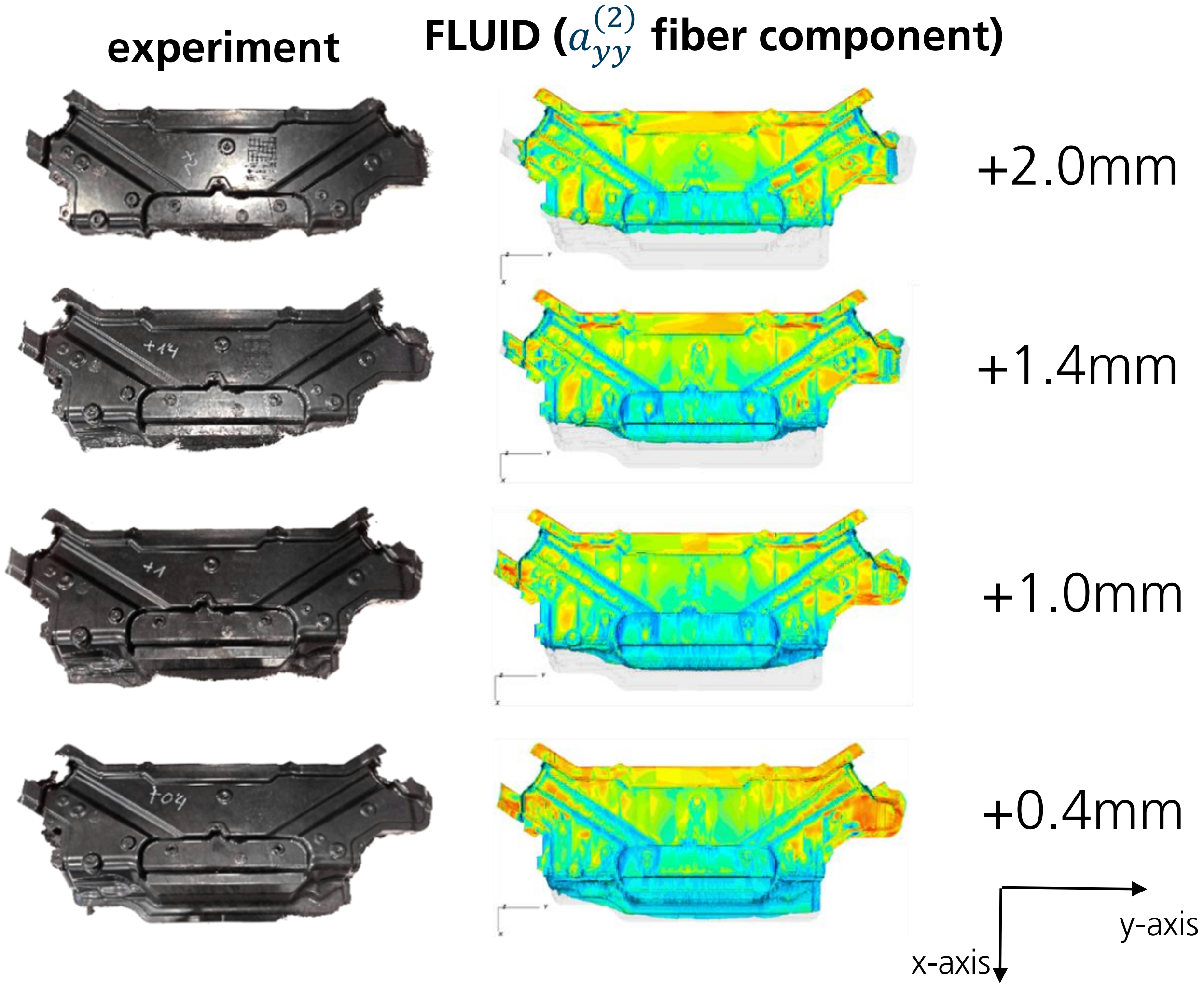
Applied tonnage	Pressing speed	Tool Temperature	Blank size	Curing time
680Tn	20mm/sg	150°C /153°C	6 blanks of 120x500mm	35sg



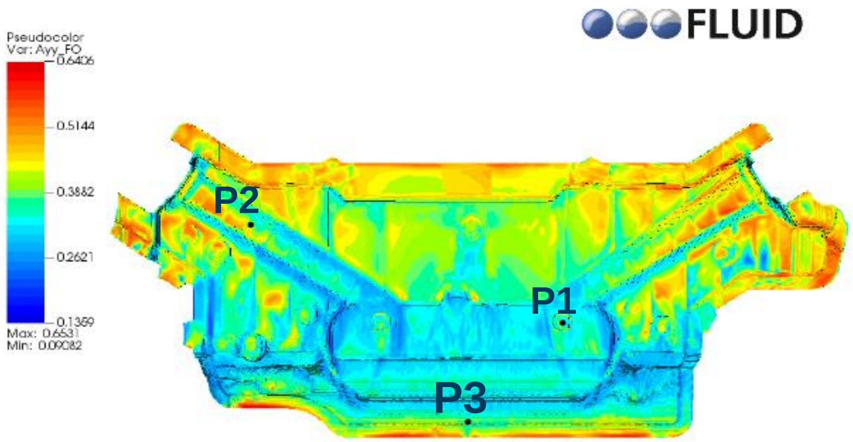
- Cowl Panel front flow propagation.

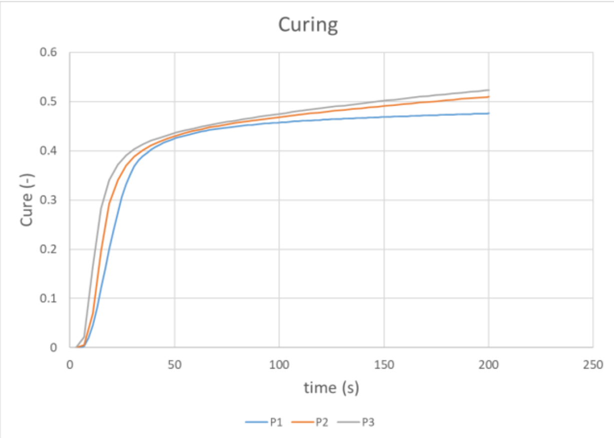


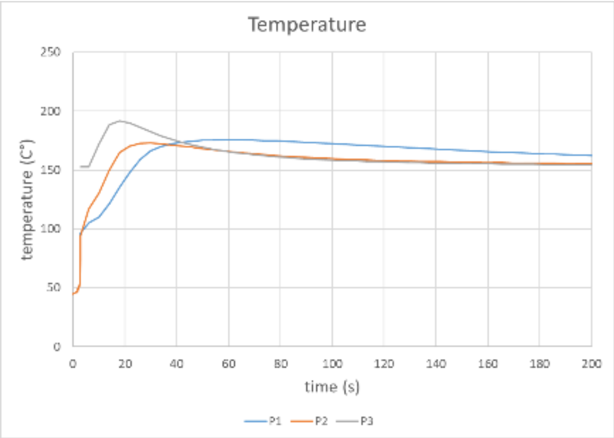
- Cowl Panel front flow comparison.
  - FLUID: good agreement, material tends to flow sideways (in the y-axis direction) at first. Afterwards, the front spreads downward (in the positive x-axis direction)



- Cowl Panel curing comparison.
  - The real cycle time is about 35 seconds.
  - FLUID simulation predicts more than 79% of cure at about 34 seconds for all sample point, where solid state should be already expected







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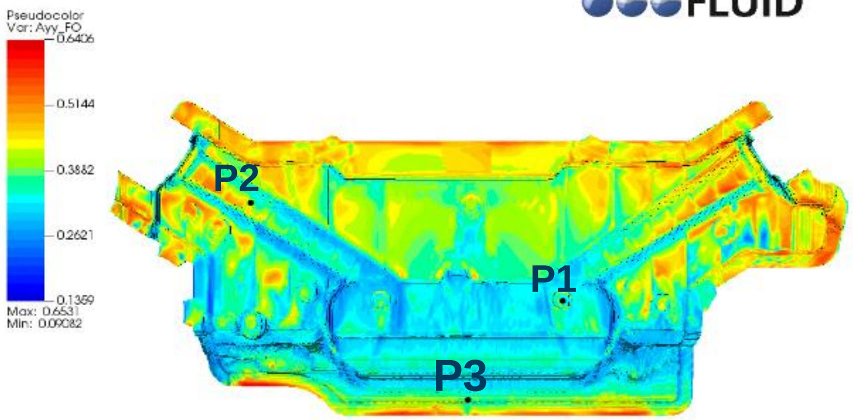

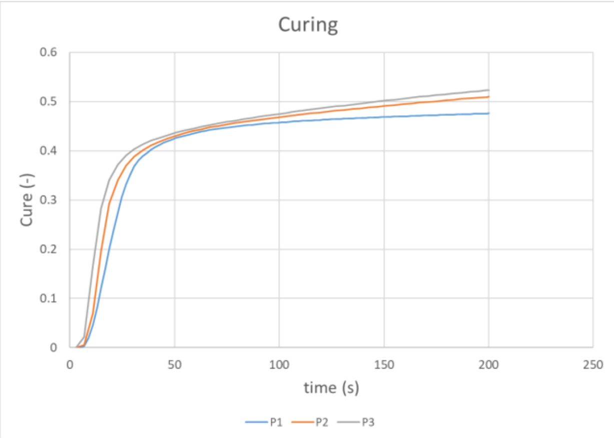

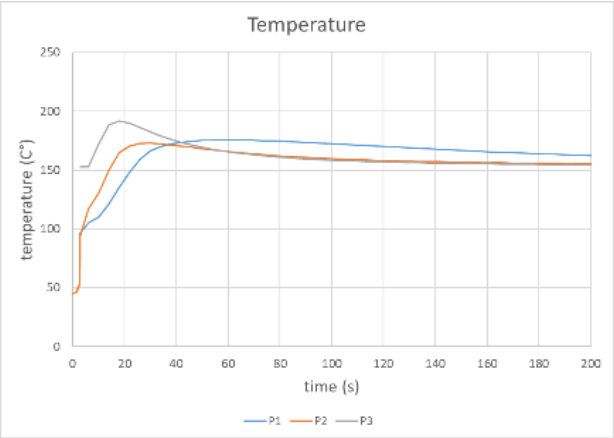

Summary CoRheoS framework and FLUID

Framework for Solver Kernel development

Linear and nonlinear PDE Systems

Object oriented system description

Automatic discretization

Input of Solver Kernels

STL Surface Mesh

CIF (XML CoRheoS Input Format)

Output of Solver Kernels

VTK

User defined integral data and history

Numerics available to Solver Kernels

Finite Volume Discretization

Parallel linear and nonlinear algebra

Newton Methods with AMG linear solver

Available Solver Kernels

Compressible and incompressible fluid flow

Coupling with Granular Flow (Dilute, Dense)

Potting simulations.

Injection molding, sheet mold compression

Electrochemistry (Li-Ion Batteries)

Polymer flow

Fiber orientation

Advanced CFD features

Moving parts/boundaries interaction (experimental)

Free surface flow

Two phase immiscible fluid flow.

User-defined functions.

Summary and outlook.

- We presented some aspects of computational fluid dynamics.
- We discussed several examples of industrial applications.
- Do not be afraid of CFD ! It is not trivial, but all efforts are compensated when simulation predicts experiments and shows what we can observe experimentally.
- Next lecture:
  - Presentation of FOAM software
  - FOAM – simulation software for expanding foams (chemical, physical blown)

Vielen Dank für Ihre Aufmerksamkeit

Fraunhofer ITWM