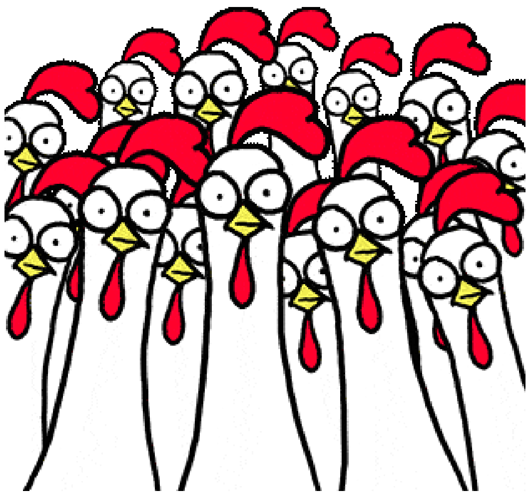
Mathematical Modeling: An Industrial Perspective

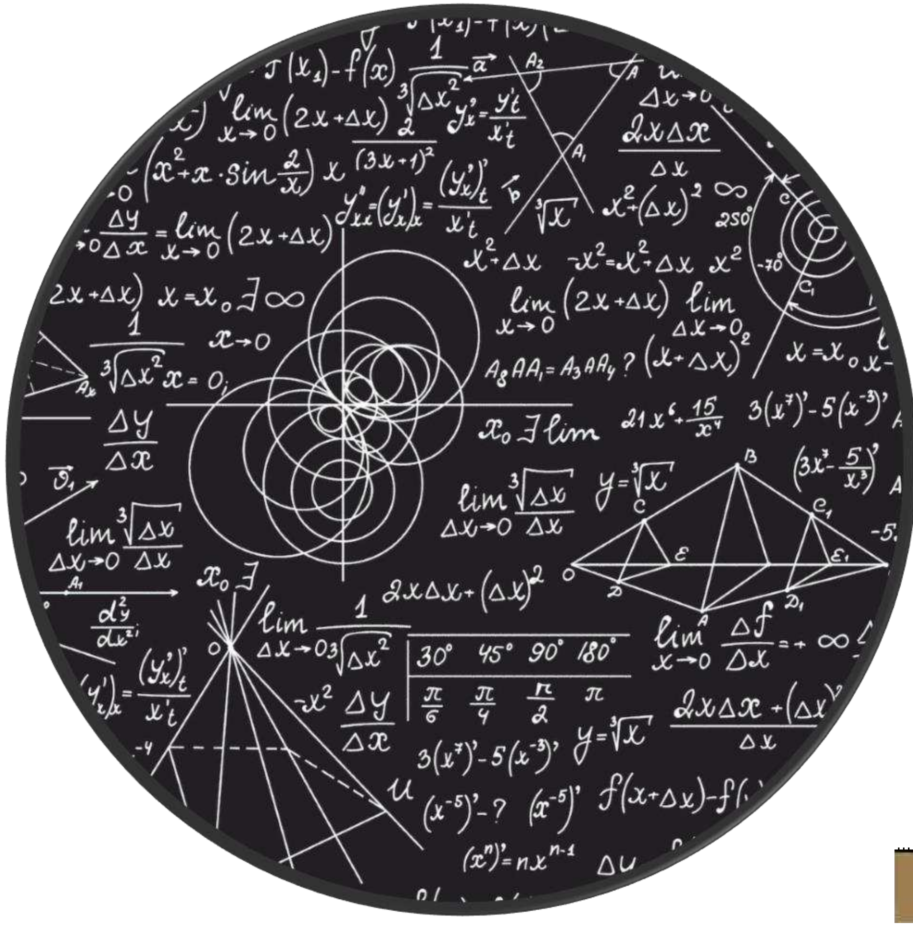
Ikenna Ireka *(Ph.D.)*

International Conference and Advanced Workshop on Modelling and Simulation of Complex Systems, May 2024, Obafemi Awolowo University Ile-Ife, Nigeria

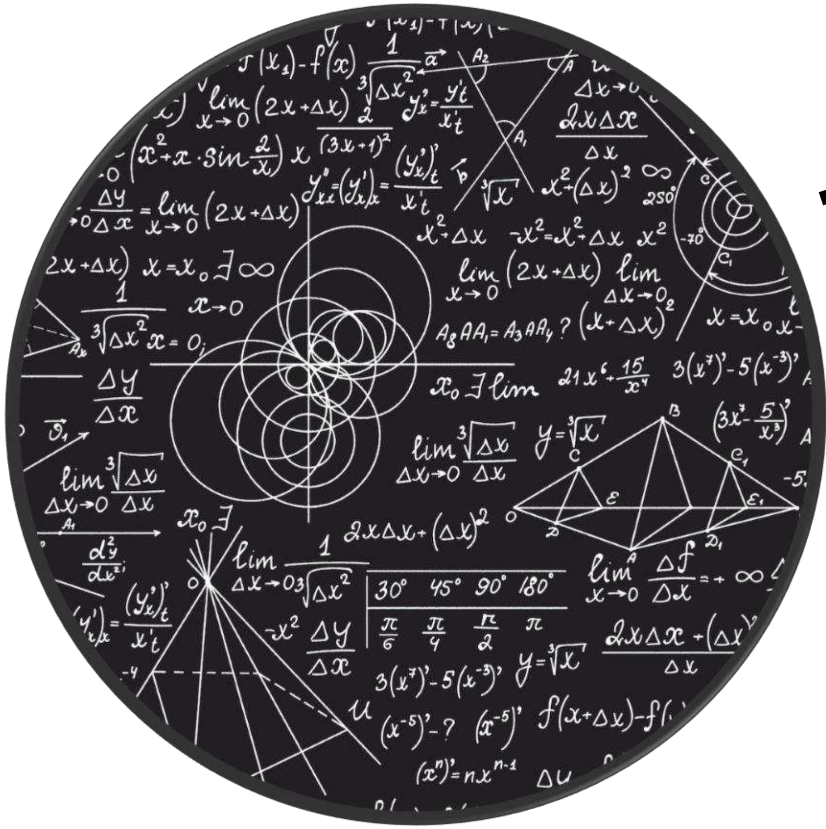
Journey of most STEM students

Freshmen / Jambites





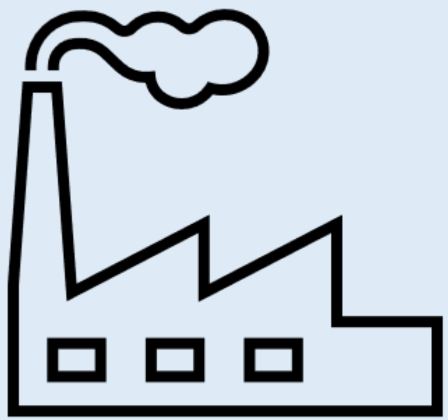
Toolbox



INDUSTRIAL CHALLENGES AN OPPORTUNITY FOR APPLYING MATHEMATICAL TOOLS

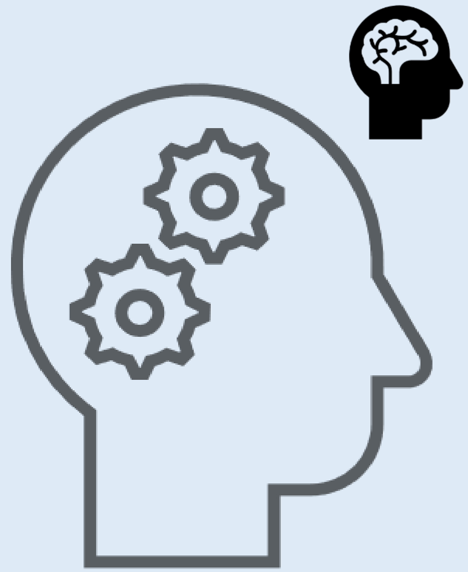
Some Challenges in the Industrial

- Optimize processes at minimal cost
- Remain Competitive at minimal cost
- Minimize experimental cost
- Optimize time to market
- Understand processing behavior of products
- Create/Design new products for competitive advantage
- …



Resolving industrial challenges Mathematically

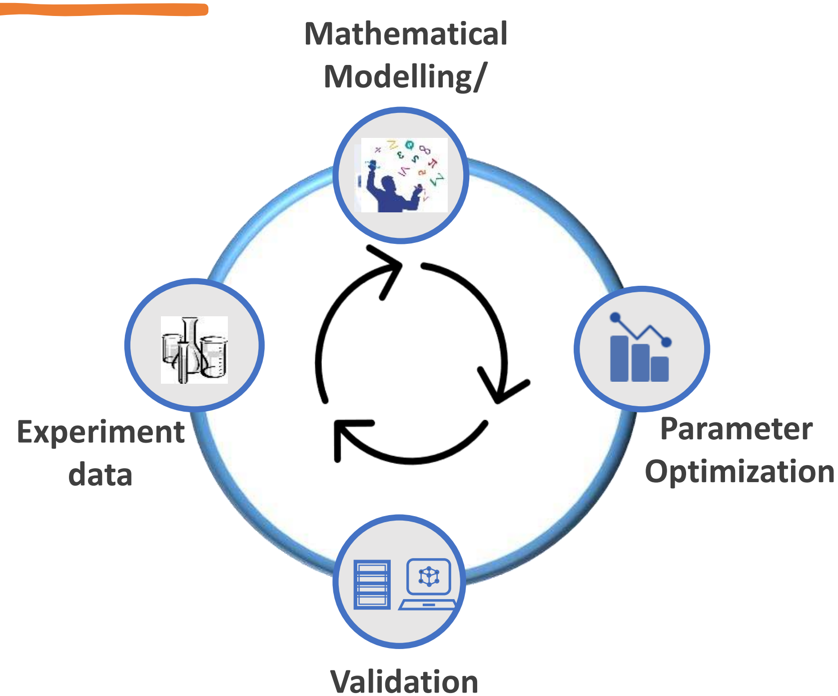
- Deterministic approach (known inputs)
  - Mathematical Modeling via physical laws (Differentia-Algebraic equations)
  - Numerical techniques
- Stochastic approach (randomness)
  - Data driven techniques
    - Machine Learning models
  - Forecasting (probabilistic models)
- Hybrid approach
  - Artificial Intelligence
  - AI-augmented simulations



Modeling Industrial Problems

Problem Definition

Mathematical Description



Virtual Experimentation

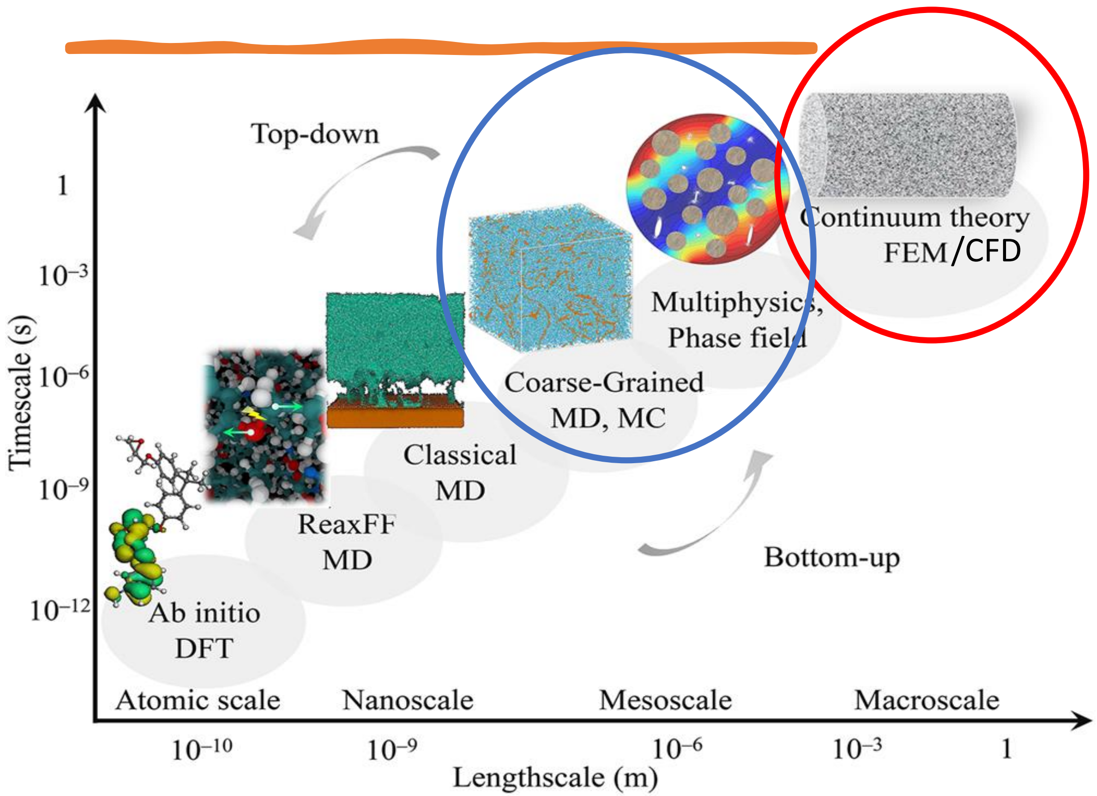
Virtual prototype

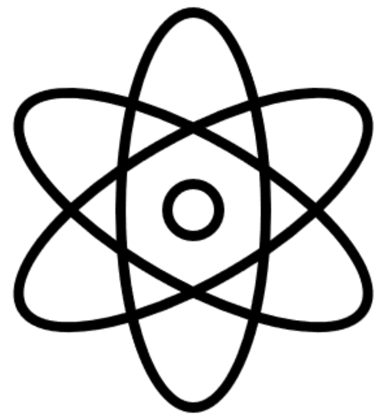
Conceptualization phase

Digital Twin

USE CASE
POLYMER INDUSTRY
(SIMULATION SCALE)

Multiscale system



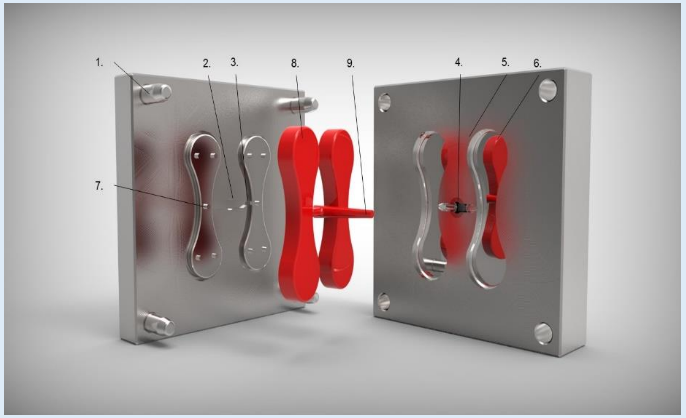


[Multiscale mechanics and molecular dynamics simulations of the durability of fiber-reinforced polymer composites | Communications Materials (nature.com)]

USE CASES:
MATHEMATICAL METHODS IN POLYMER INDUSTRY
(MACRO-SCALE SIMULATIONS)

Case 1: Some Questions in Polymer Injection molding

- How can we
  - understand the mold filling behavior in closed molds?
  - optimize process conditions and cycle time per molding process?
  - minimize defects in finished parts?
  - understand the material that is optimal for the mold of interest?
  - Efficiently design and maintain mold tooling to minimize failure?



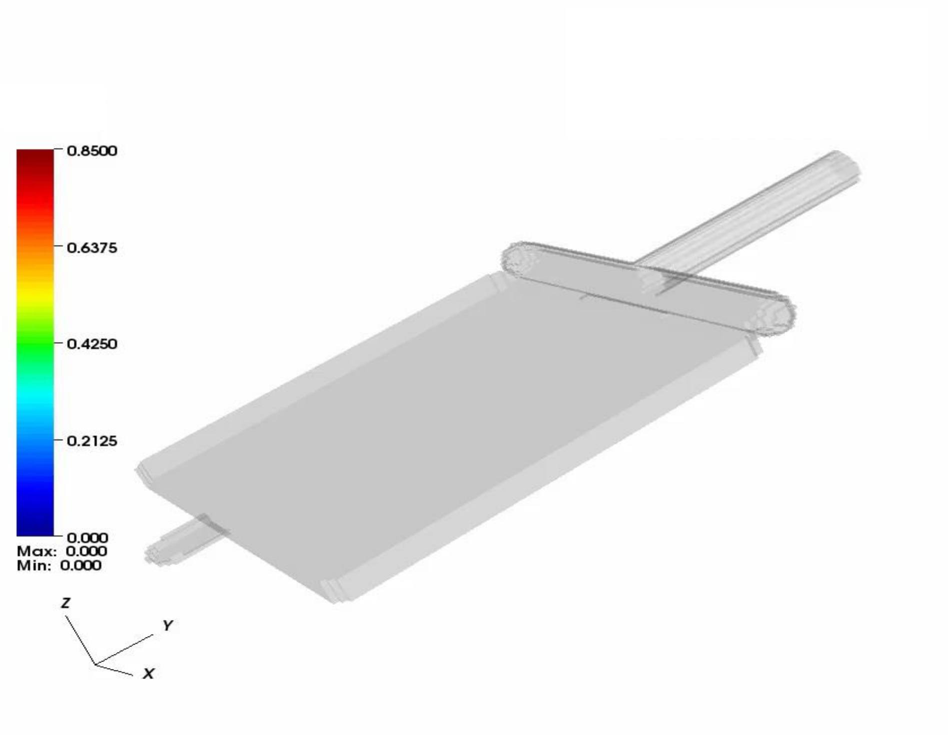
Plastics Injection Mould Tool | Rutland Plastics

Modeling Injection molding

The **Navier-Stokes Equations** subject to appropriate boundary conditions

- **Conservation of mass** $$\nabla \cdot \vec{v} = -\frac{1}{\rho}\left(\frac{\partial \rho}{\partial t} + \vec{v} \cdot \nabla \rho\right) = 0 \text{ (incompressibility)}$$
- **Conservation of linear momentum** $$\frac{\partial \rho \vec{v}}{\partial t} + \nabla \cdot (\rho \vec{v}\vec{v}) = -\nabla p + \nabla \cdot \boldsymbol{\sigma} + \rho g$$
- **Conservation of energy:** $$\rho C_p \left(\frac{\partial T}{\partial t} + \vec{v} \cdot \nabla T\right) = \nabla \cdot (\boldsymbol{\kappa} \nabla T) + \frac{1}{2}(\mu_{mix} \mathrm{D} : \mathrm{D})$$

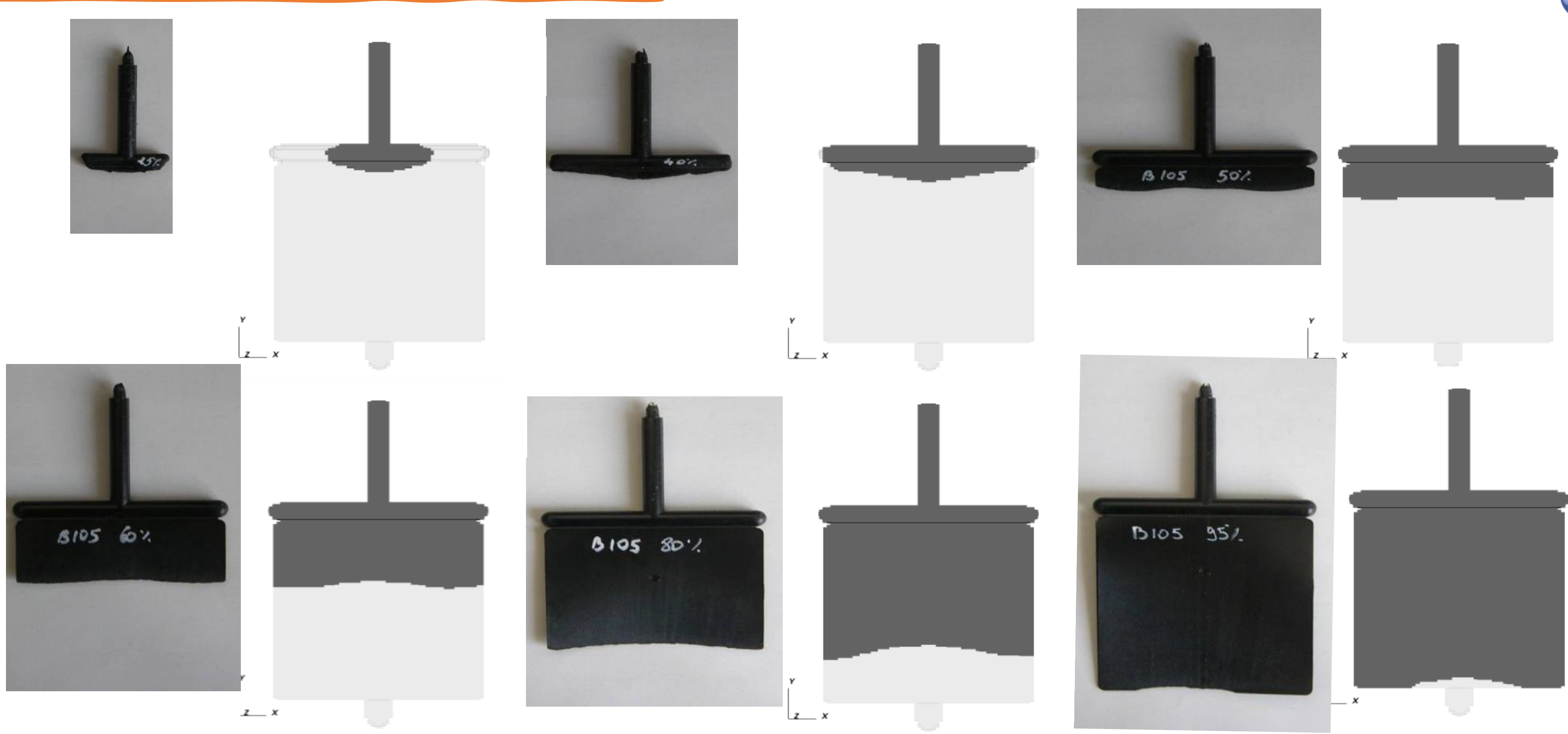
Case 1: Results
Injection molding



Case 1: Results & Validation
Injection molding (3mm thickness)

FLUID

Fraunhofer ITWM



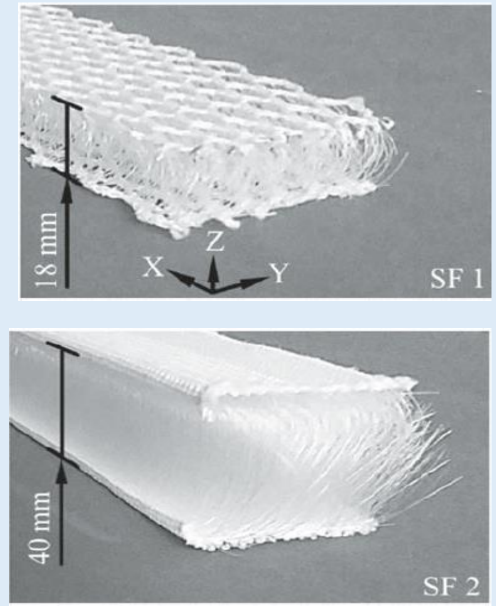
Case 1: Results & Validation
Injection molding (5mm thickness)

FLUID

Fraunhofer ITWM

Case 2:
Some Questions in Polymer Reinforced Injection molding

- What
  - is the effect of the reinforcing structure on the flow pattern?
  - regions of the structure will not be impregnated (wetted/dry) in the mold?
  - would be the optimal processing condition for such composite structure?
  - is the orientation of reinforcing chopped fiber glass in the formed part?



Sample Spacer fabrics used as inserts in the molding tools

K Schäfer et al: Eng. Res. Express 3 (2021) 025027

Governing equations: Structural / chopped fiber Reinforced Injection molding

The **Navier-Stokes-Brinkman Equations** with appropriate boundary conditions

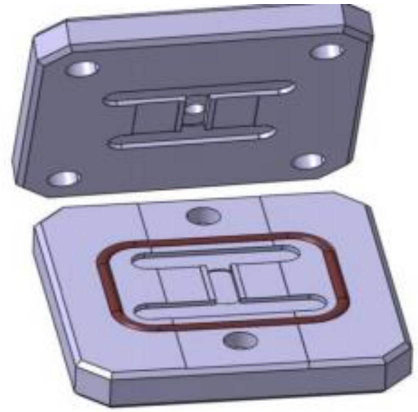
- **Conservation of linear momentum** $\frac{\partial \rho \vec{v}}{\partial t} + \nabla \cdot (\rho \vec{v}\vec{v}) = -\nabla p + \nabla \cdot \boldsymbol{\sigma} + \rho g - \mu_p \widehat{\boldsymbol{K}}^{-1} \vec{v}$

$$\widehat{\boldsymbol{K}}^{-1} \begin{cases} \boldsymbol{K}^{-1}, & \text{porous region} \\ 0, & \text{non} - \text{porous region} \end{cases}$$

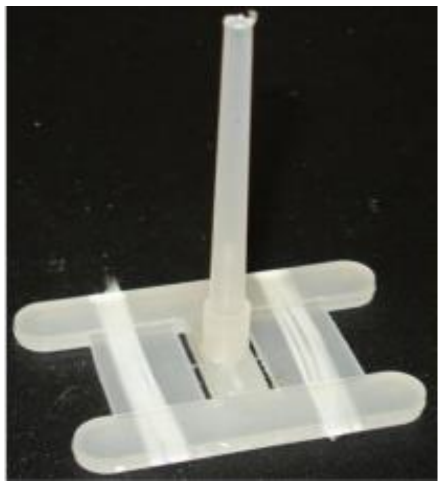
The **Navier-Stokes-equations + Folgar-Tucker equations** with appropriate boundary conditions

- **Orientation tensor** $\frac{dA}{dt} = \boldsymbol{W} \cdot \boldsymbol{A} - \boldsymbol{A} \cdot \boldsymbol{W} + \varepsilon\left(D \cdot \boldsymbol{A} + \boldsymbol{A} \cdot D \ - 2\mathbf{A}^{(4)} : D\right)\text{-} +2D_r(\mathbf{I} - 3\mathbf{A})$

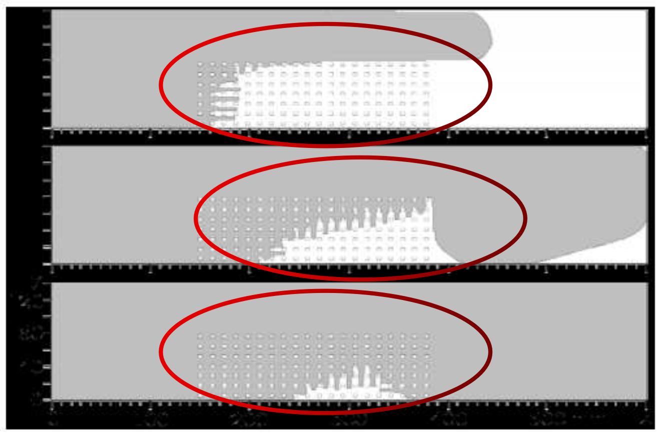
Case 2: Result, structural Reinforced Injection molding



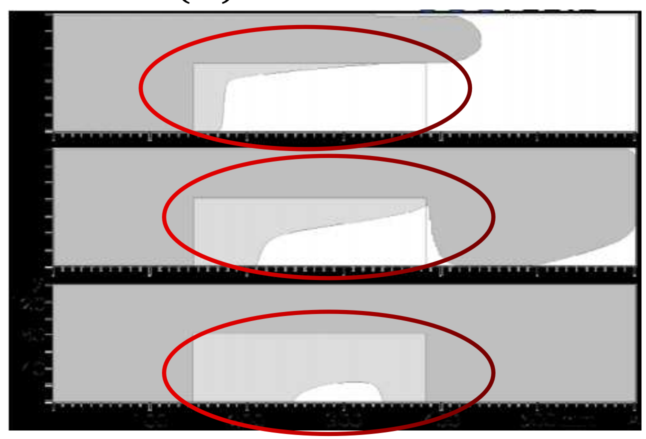
Finished Part



2D Micro pore simulation

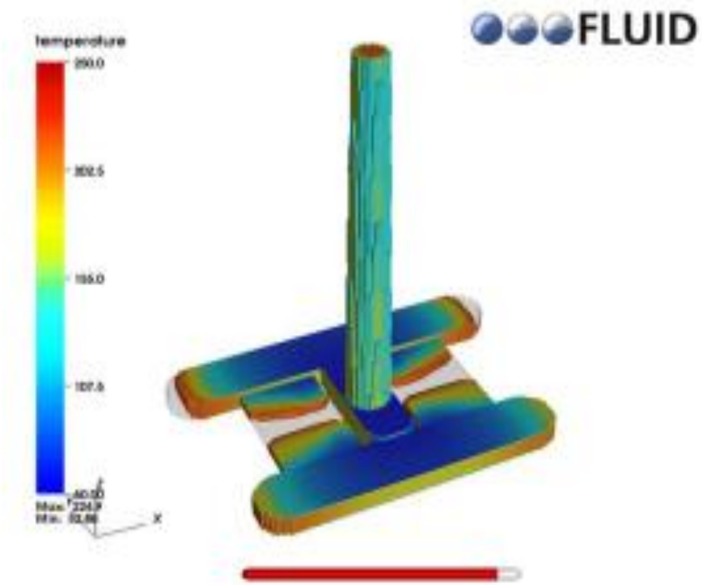


2D Simulation with permeability tensor $(\boldsymbol{K})$

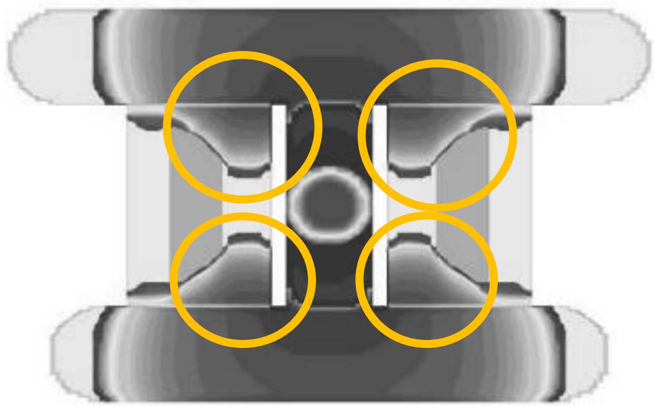


Fraunhofer ITWM

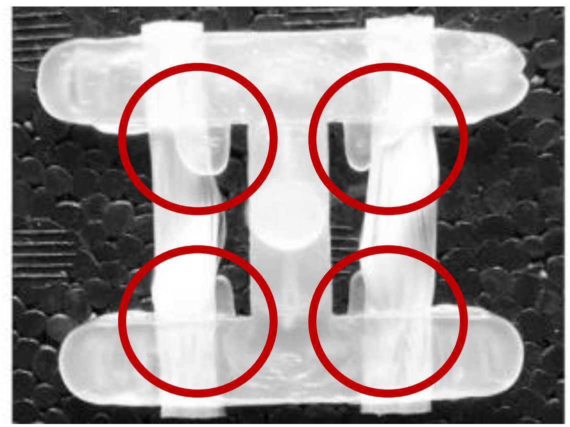
Case 2: Result, structural Reinforced Injection molding



Simulation

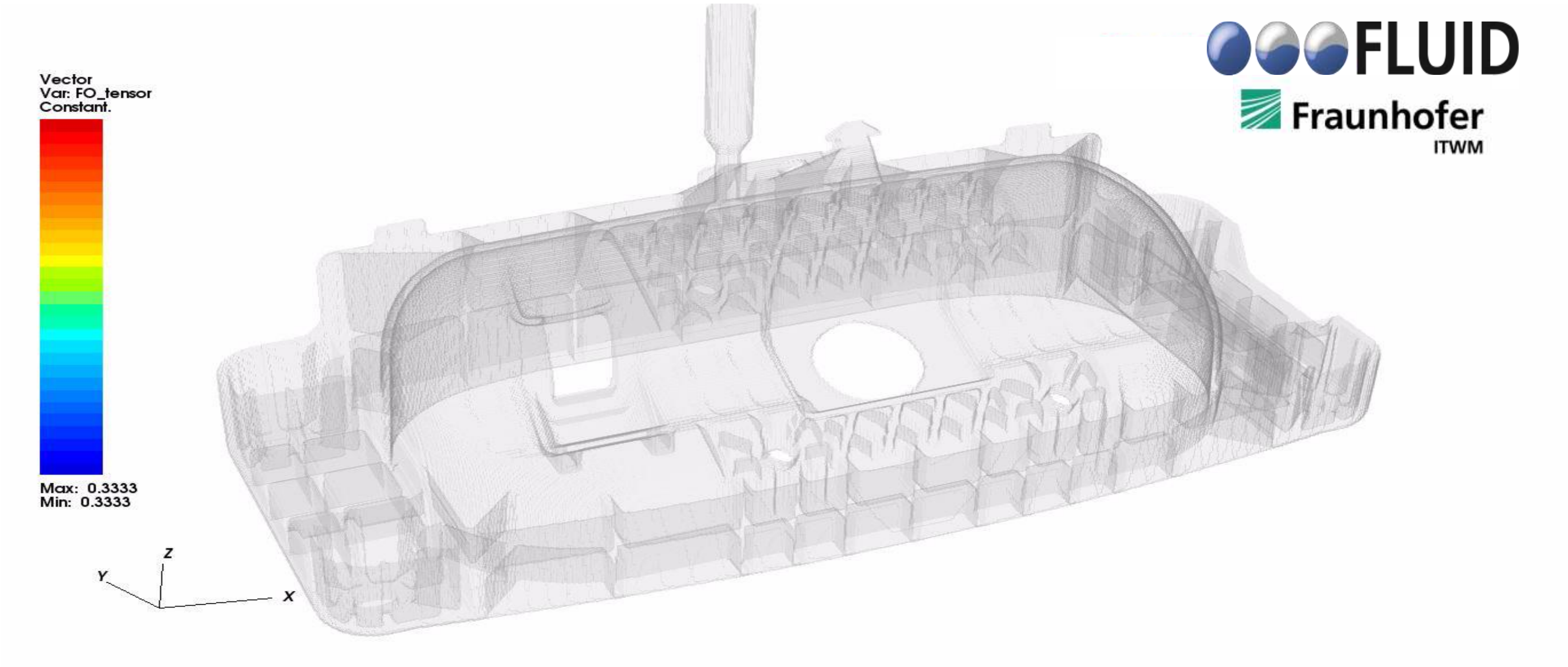


Experiment



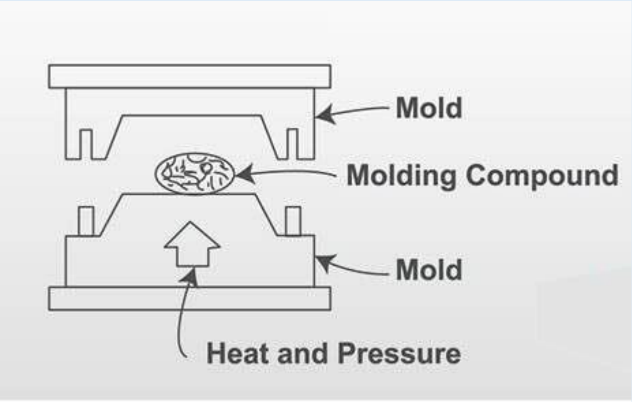
Fraunhofer
ITWM

Case 2: Results
Orientation tensor of chopped fiber in reinforced Injection Molding



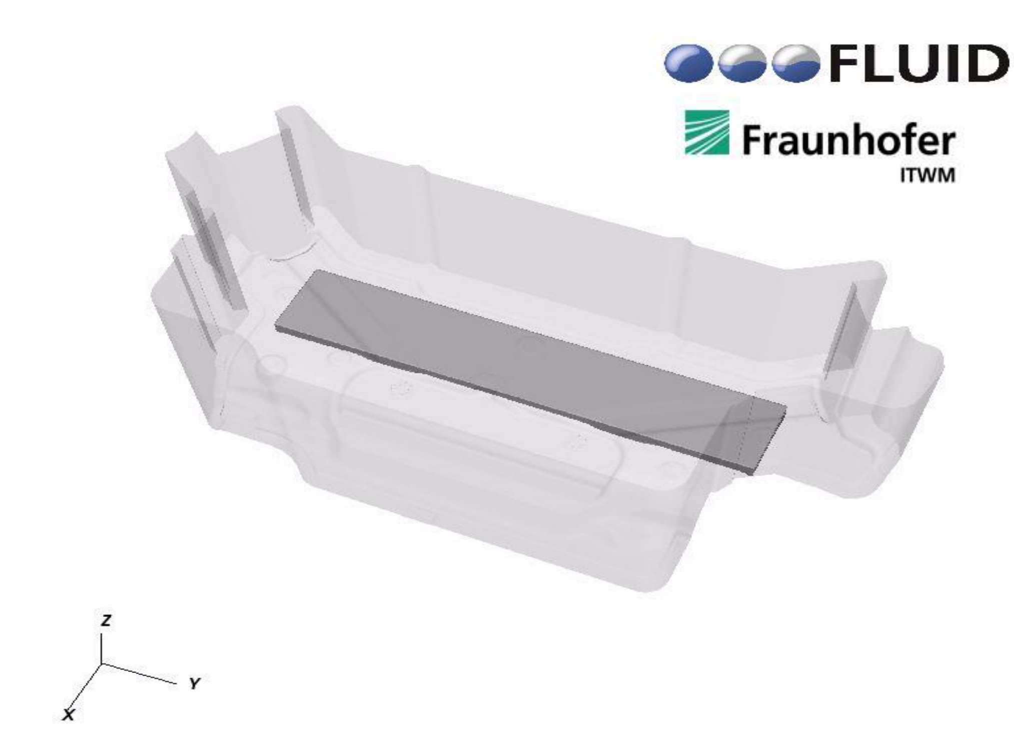
Case 3:
Some questions in
Sheet Compression Molding (SMC)

- What amount of lumped polymer should put in the mold,
- Where should the initial material (lump polymer be placed in the mold for optimal distribution.
- What is the solidification time, i.e. how long do I need to wait for before opening the mold?
- What is the orientation of reinforcing chopped fiber glass?
- What is the distribution of the fiber in the finished part



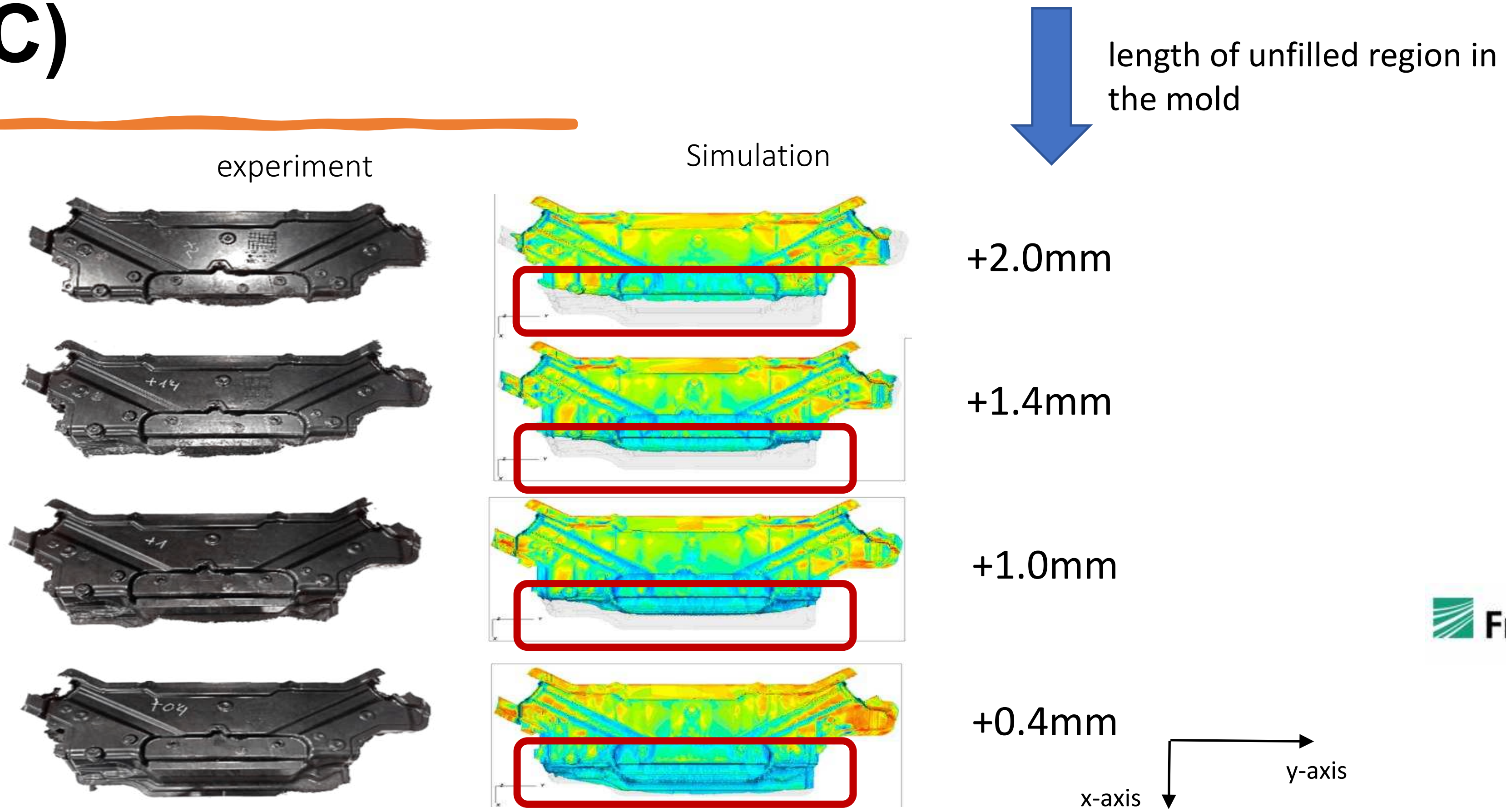
The Complete Guide to Compression Molding - MDC Mould (zjmdc.com)

Case 3: Results, Compression molding



ALMA

Case 3: Results, Sheet Compression molding (SMC)



Case 4:
Reaction Injection Molding of Polyurethane (PUR) or Polyisocyanurate (PIR) foams

How can one

- minimize number of experimental trials
- enhance product development time
- understand the complex dynamics of expanding PUR foams in closed molds
- optimize processing (venting plan in automotive dashboard, optimal process temperature...)
- optimize mold design
- ...

Application of reaction Injection molding of Polyurethane foams

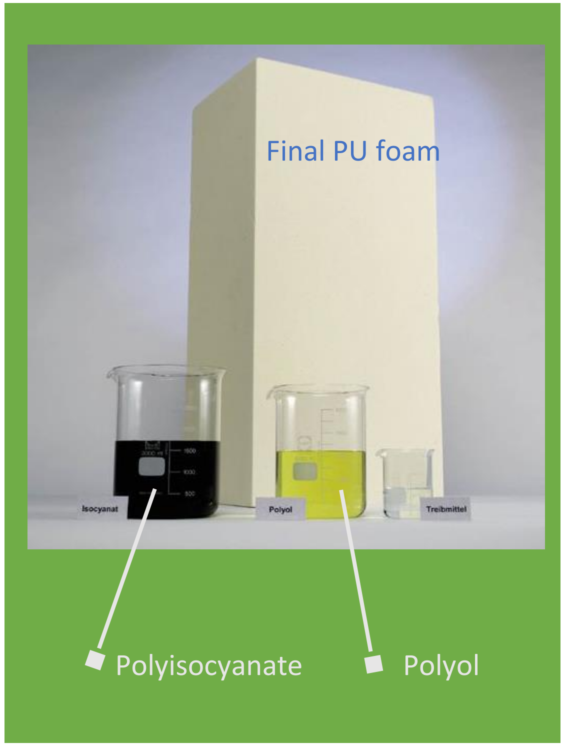
Automotive

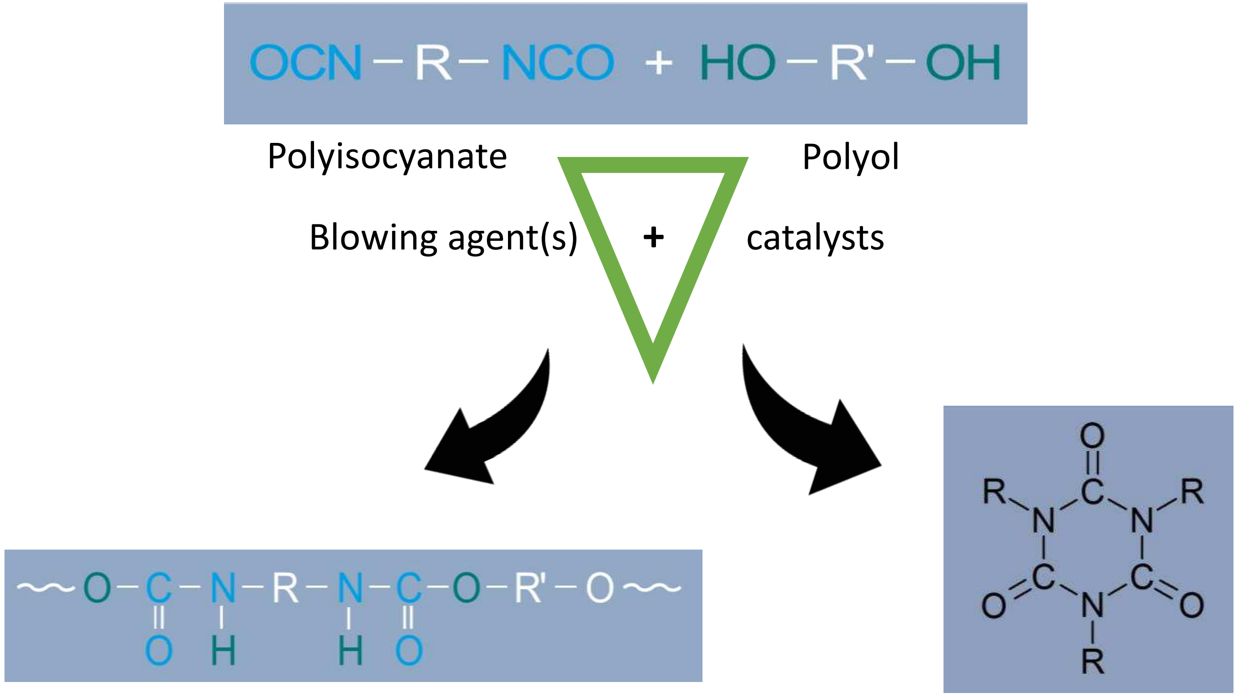
Housing

Appliances

Comfort

Quick overview:
Chemistry of PUR/PIR foams

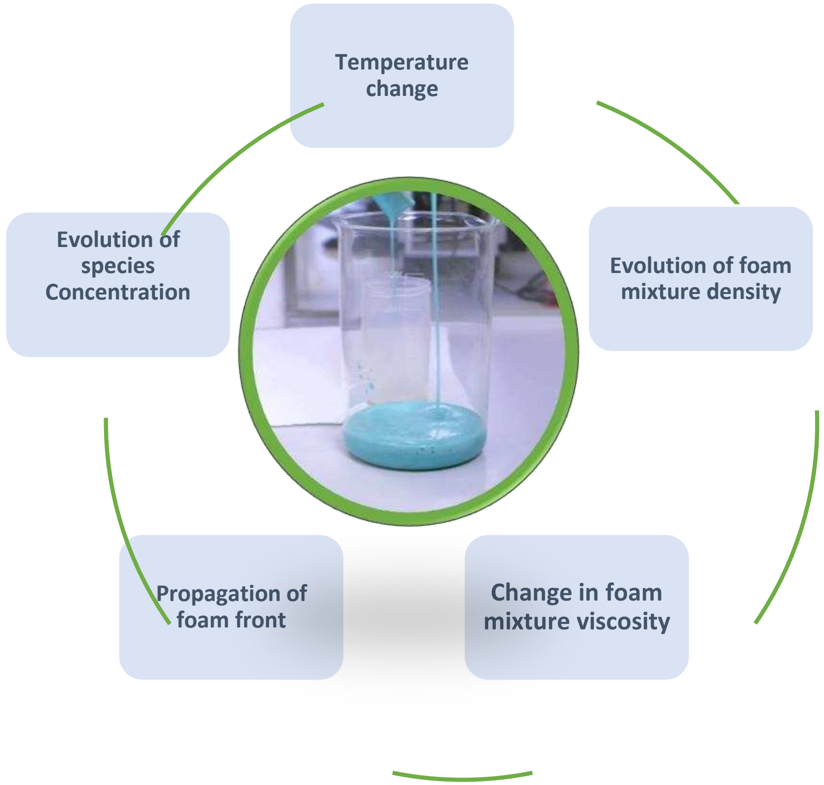




Polyurethane foams

Polyisocyanurate foam

PUR Foam expansion experiment: Observed Physics



Modeling Reaction Injection Molding of Polyurethane (PUR)foams

The **Navier-Stokes Equations** + additional equations for specie transport

- **Conservation of energy:**

$$\rho C_p \left(\frac{\partial T}{\partial t} + v \cdot \nabla T\right) = \nabla \cdot (\boldsymbol{\kappa} \nabla T) + \frac{1}{2}(\mu_{mix} \mathrm{D} : \mathrm{D}) + S_R$$

$$(-\Delta H_{OH}, -\Delta H_w, \Delta H_{PIR}) \cdot \left(\frac{dC_{OH}}{dt}, \frac{dC_w}{dt}, \frac{dC_{PIR}}{dt}\right)^T$$

- **Equation for Concentration of CO_2:**

$$\frac{\partial C_{CO_2}}{\partial t} + \nabla \cdot (v C_{CO_2}) = K_w C_{NCO} C_w ,$$

- **Equation for Water and Polyol concentrations:**

$$\frac{\partial C_i}{\partial t} + \nabla \cdot (v C_i) = -K_i C_i C_{NCO}$$

$$K_i = A_i e^{-\frac{E_i}{RT}} \quad and \quad i = \mathrm{OH}, w$$

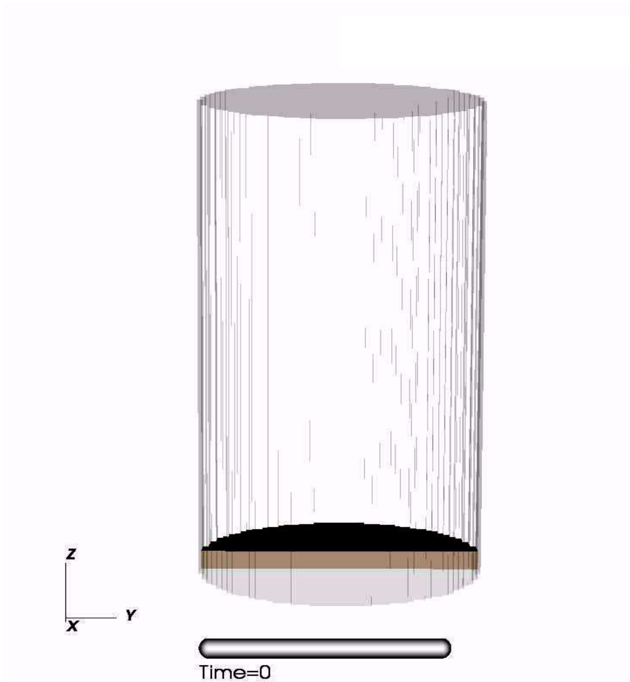
- **Equation for NCO Concentration**

$$\frac{\partial C_{NCO}}{\partial t} + \nabla \cdot (v C_{NCO}) = -(K_w C_w + K_{OH} C_{OH}) * C_{NCO}$$

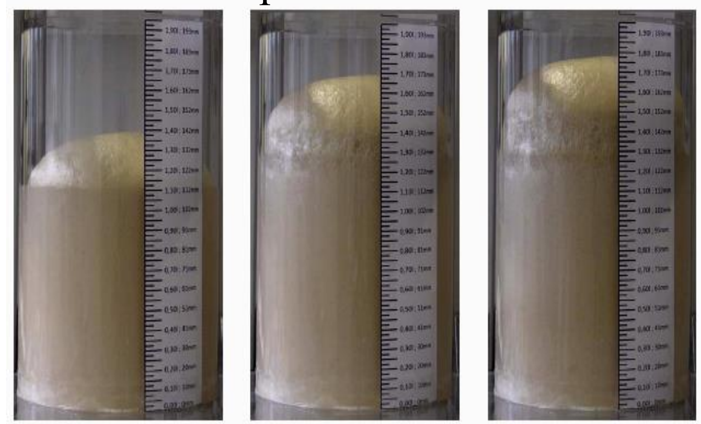
Case 2: Result & Validation, PUR Foam expansion

FOAM

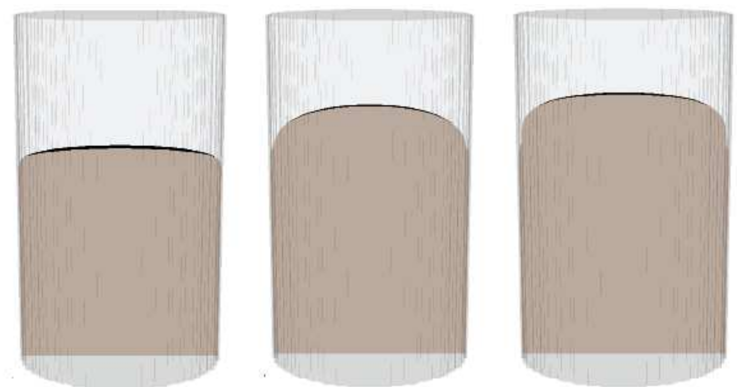
Fraunhofer ITWM



Experiment



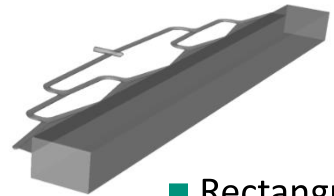
(d) t=150secs (e) t=200secs (f) t=250secs



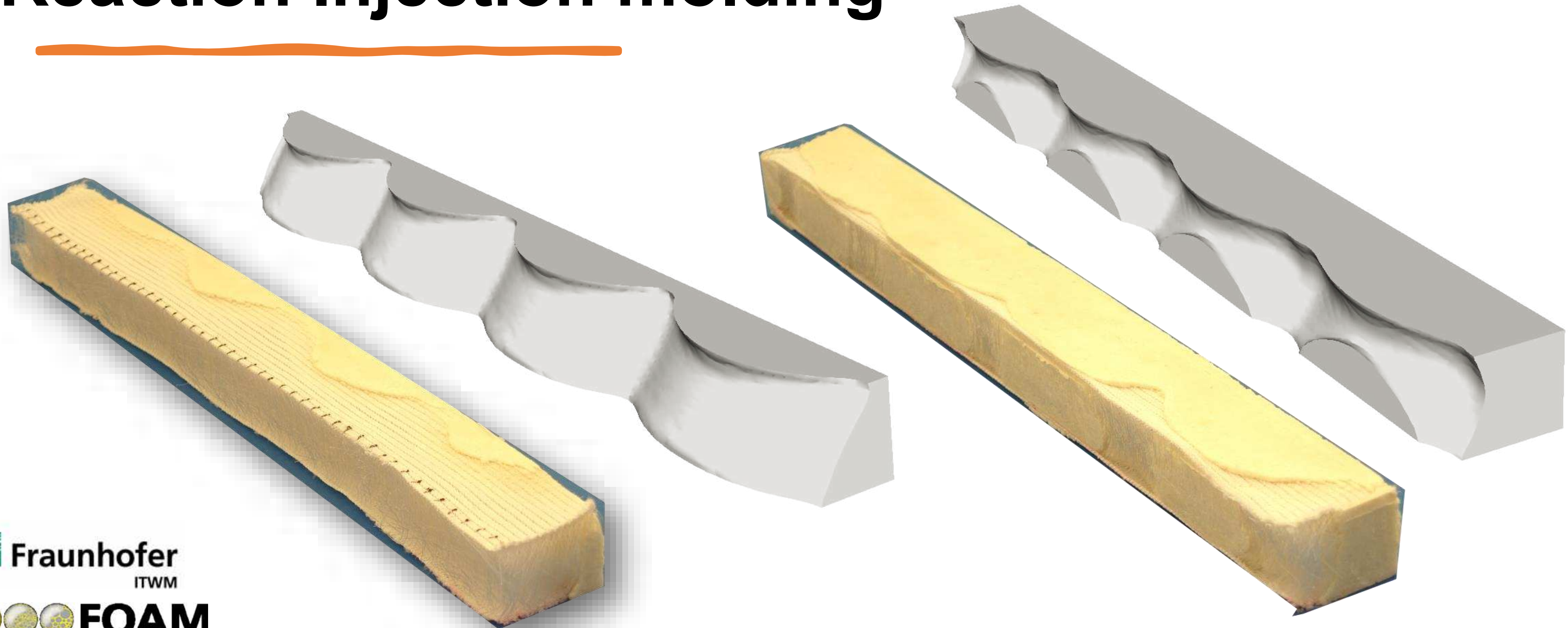
(a) t=150secs (b) t=200secs (c) t=250secs

Simulation

Case 2: Result, PUR foam Structural Reinforced Reaction Injection molding



- Rectangular geometry:



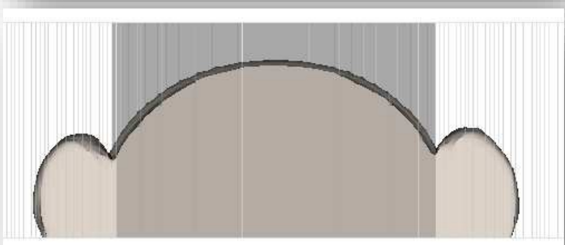
Fraunhofer ITWM

FOAM

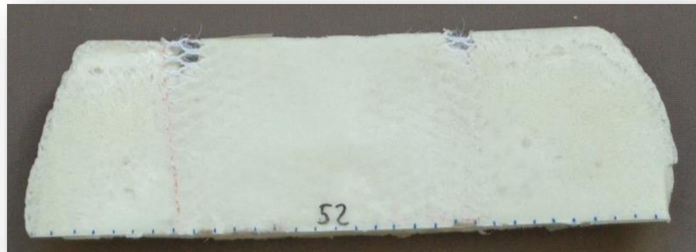
Case 2: Result, PUR foam Structural Reinforced Reaction Injection molding

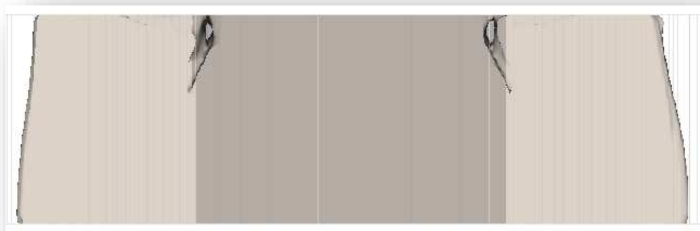
■ Wave geometry:

20 g



30 g



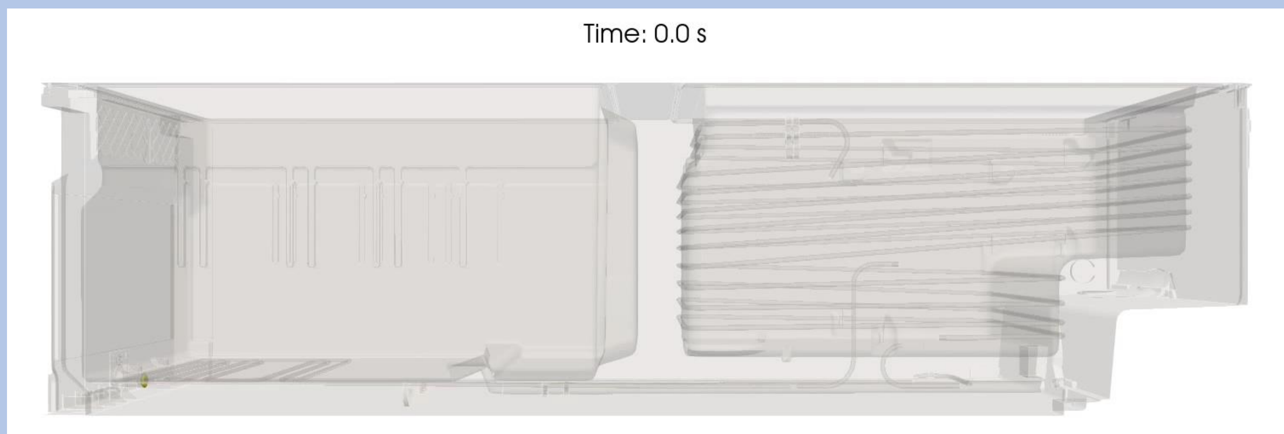


Fraunhofer ITWM

FOAM

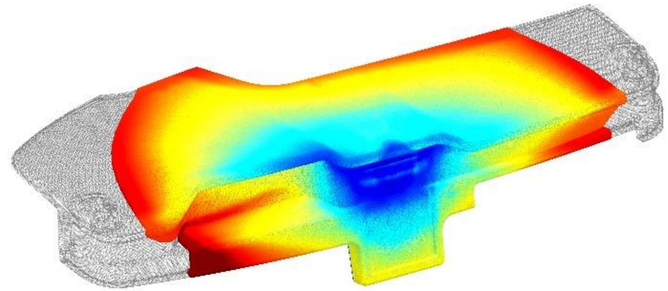
Foaming Simulation of Refrigerator cabinet

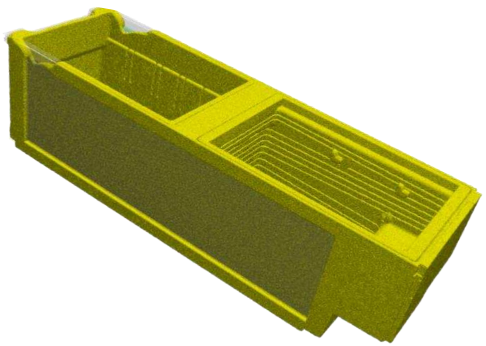
Validation with experiment

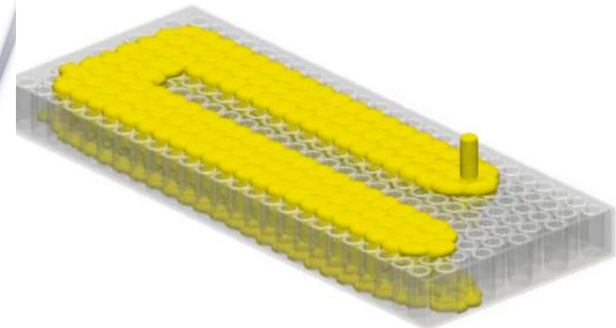


Simulation aided prototyping

Conclusion







Conclusion

Industrial virtual material prototyping via Mathematical concepts

- Interaction with domain experts
- Experimentation
- Model development
- Parameter optimization
- Model validation (numerical simulations simple cases)
- Simulation of real industrial case
- Virtual prototype & experimentation for process optimization (Digital twin)

THANK YOU
FOR YOUR ATTENTION

Introduction to Complex Fluids

Ikenna Ireka *(Ph.D.)*

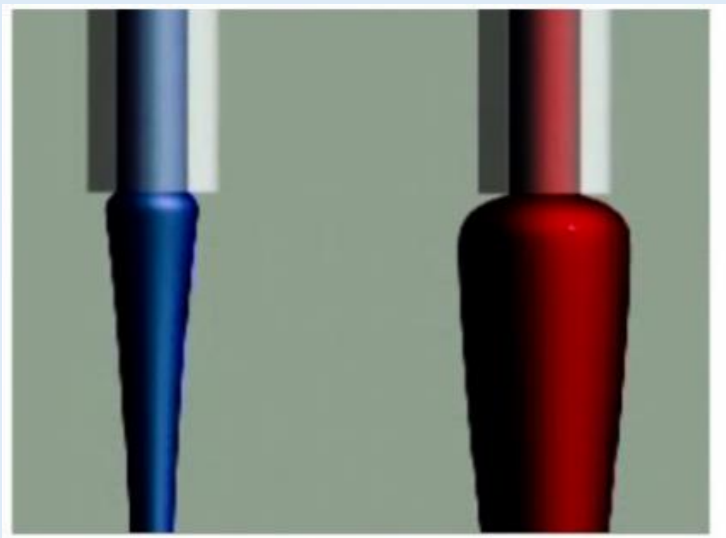
Overview

- Newtonian vs Non-Newtonian (complex) fluids
    - Complex rheological models
        - Generalized Newtonian fluids
        - Viscoelastic fluids
        - Chemorheological fluids (Polyurethane foams)
- The Navier Stokes Equation
- The Navier-Stokes Brinkman Equations

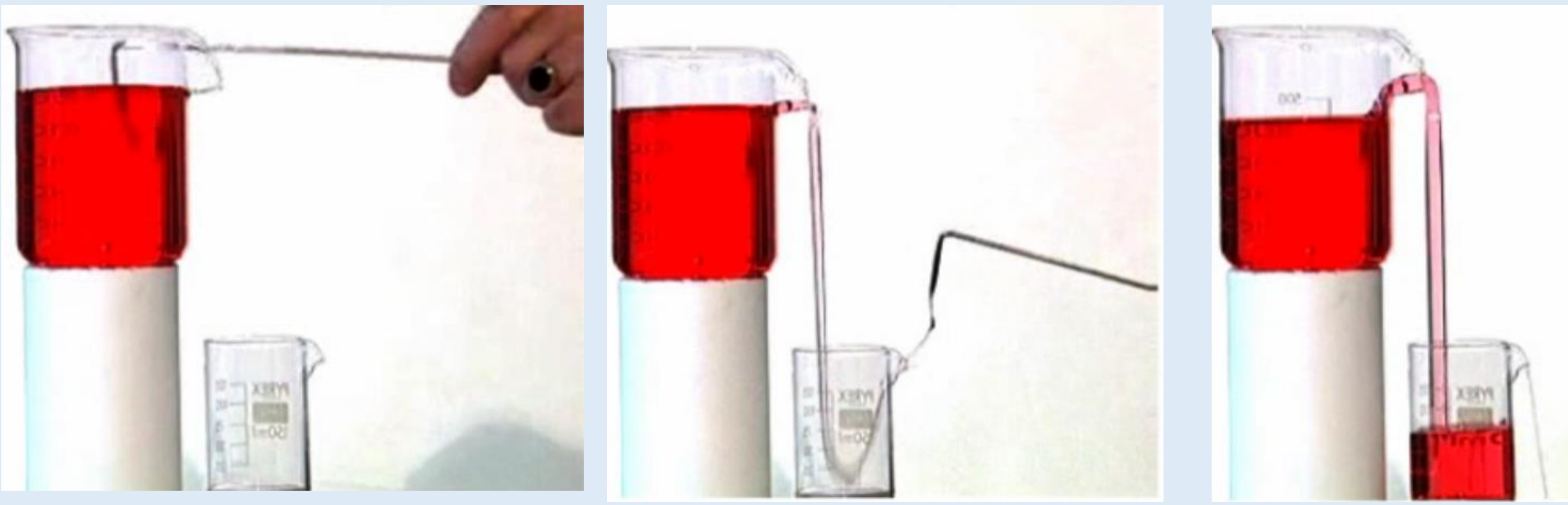
Simple Fluids

https://www.nicepng.com/ourpic/u2q8i1t4u2w7r5y3_water-pouring-png-cup-of-water-png/

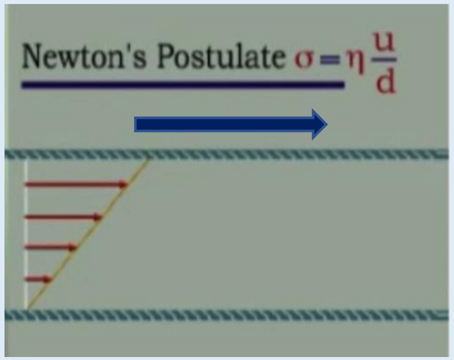
Simple vs Complex Fluids



Complex Fluids



Newtonian Fluids



σ is the shear stress

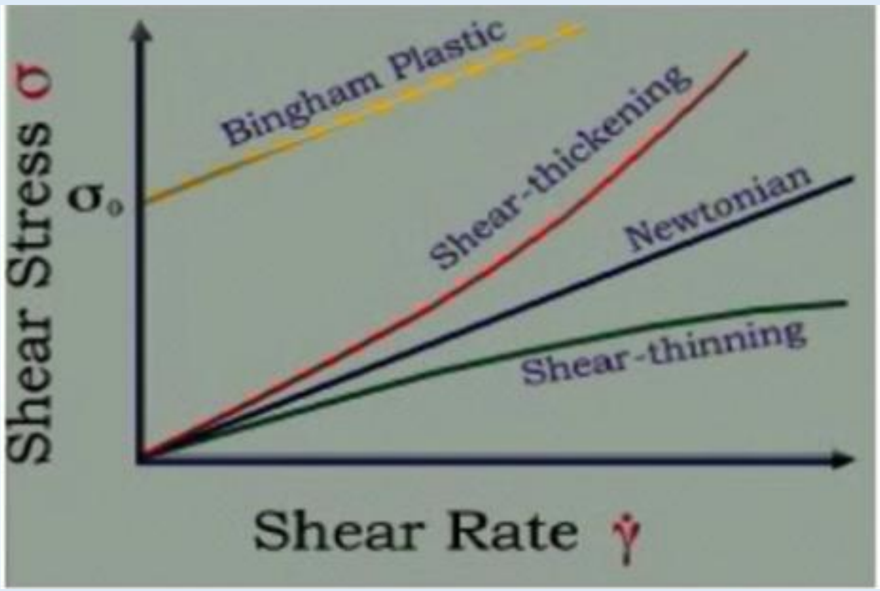
u/d is the velocity gradient

η is the coefficient of viscosity

Table 1.1: Temperature dependent viscosity models

Reynold's model	$\eta(T) = \eta_0 \exp(-BT)$
Vogel's model	$\eta(T) = \eta_0 \exp\left(\frac{B}{T-T_0}\right)$
Arrhenius model	$\eta(T) = \eta_0 \exp(E/RT)$
Nahme model	$\eta(T) = \eta_0 \exp\left(\frac{T-T_0}{T_0}\right)$
William-Landel-Ferry (WLF) model	$\eta(T) = \eta_0 \exp\left(\frac{-C_1(T-T_0)}{C_2+T-T_0}\right)$
Fulcher model	$log_{10}(\eta(T)) = -A + \frac{B\times10^3}{T-T_0}$

Stress strain Curves: Simple vs Complex Fluids



- Viscoelasticity
- Variable Viscosity
- Normal Stresses
- Extensional Viscosity
- Thixotropy and Anti-Thixotropy
- Other Effects

The Navier-Stokes Equations

The **Navier-Stokes Equations** subject to appropriate boundary conditions

- **Conservation of mass** $$\nabla \cdot \vec{v} = -\frac{1}{\rho}\left(\frac{\partial \rho}{\partial t} + \vec{v} \cdot \nabla \rho\right)$$
- **Conservation of linear momentum** $$\frac{\partial \rho \vec{v}}{\partial t} + \nabla \cdot (\rho \vec{v}\vec{v}) = -\nabla p + \nabla \cdot \boldsymbol{T} + \boldsymbol{F}$$
- **Conservation of energy:** $$\rho C_p \left(\frac{\partial T}{\partial t} + \vec{v} \cdot \nabla T\right) = \nabla \cdot (\boldsymbol{\kappa} \nabla T) + \frac{1}{2}(\mu_{mix} \boldsymbol{D} : \boldsymbol{D})$$

Constitutive relations

- Newtonian $$\boldsymbol{T} = 2\eta \boldsymbol{D}, \quad \text{with,} \quad \boldsymbol{D} = \frac{1}{2}\left[\nabla \boldsymbol{v} + (\nabla \boldsymbol{v})^T\right].$$
- **Generalized Newtonian** $$\boldsymbol{T} = 2\eta(\dot{\gamma})\,\boldsymbol{D}.$$
  - Power law Model $$\eta = K\dot{\gamma}^{n-1},$$
    if $n < 1$ $\quad \lim_{\dot{\gamma}\to 0} \eta(\dot{\gamma}) = \infty \quad \lim_{\dot{\gamma}\to\infty} \eta(\dot{\gamma}) = 0,$
    if $n > 1$ $\quad \lim_{\dot{\gamma}\to 0} \eta(\dot{\gamma}) = 0 \quad \lim_{\dot{\gamma}\to\infty} \eta(\dot{\gamma}) = \infty.$
  - Prandtl-Eyring $$\eta = \eta_0 \frac{\sinh^{-1}(\lambda\dot{\gamma})}{\lambda\dot{\gamma}}, \quad \lim_{\dot{\gamma}\to 0} \eta(\dot{\gamma}) = \eta_0, \quad \lim_{\dot{\gamma}\to\infty} \eta(\dot{\gamma}) = 0.$$

More generalized Newtonian fluids

- Powell-Eyring model $\eta = \eta_\infty + (\eta_0 - \eta_\infty)\frac{\sinh^{-1}(\lambda\dot\gamma)}{\lambda\dot\gamma}$. $\frac{\eta - \eta_\infty}{\eta_0 - \eta_\infty} = \frac{\sinh^{-1}(\lambda\dot\gamma)}{\lambda\dot\gamma}$. $\lim_{\dot\gamma\to 0} \eta = \eta_0$ and $\lim_{\dot\gamma\to\infty} \eta = \eta_\infty$.
- Cross model

$$\frac{\eta - \eta_\infty}{\eta_0 - \eta_\infty} = \frac{1}{1 + (\lambda\dot\gamma)^m}, \quad \text{if } m < 1 \quad \lim_{\dot\gamma\to 0} \eta(\dot\gamma) = \eta_0 \quad \lim_{\dot\gamma\to\infty} \eta(\dot\gamma) = \eta_\infty,$$

$$\frac{\eta_0 - \eta}{\eta - \eta_\infty} = (\lambda\dot\gamma)^m. \quad \text{if } m > 1 \quad \lim_{\dot\gamma\to 0} \eta(\dot\gamma) = \eta_\infty \quad \lim_{\dot\gamma\to\infty} \eta(\dot\gamma) = \eta_0,$$

- Sisko model $\eta = \eta_\infty + K\dot\gamma^{n-1}$.
- Carreau-Yasuda model $\frac{\eta - \eta_\infty}{\eta_0 - \eta_\infty} = [1 + (\lambda'\dot\gamma)^c]^{(n-1)/c}$. c = 2 (Carreau Model)