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Rheology modeling of a Multiphase Detergent Processing

Vincenzo Guida

P&G Pomezia F&HC R&D

ACE

ARIEL

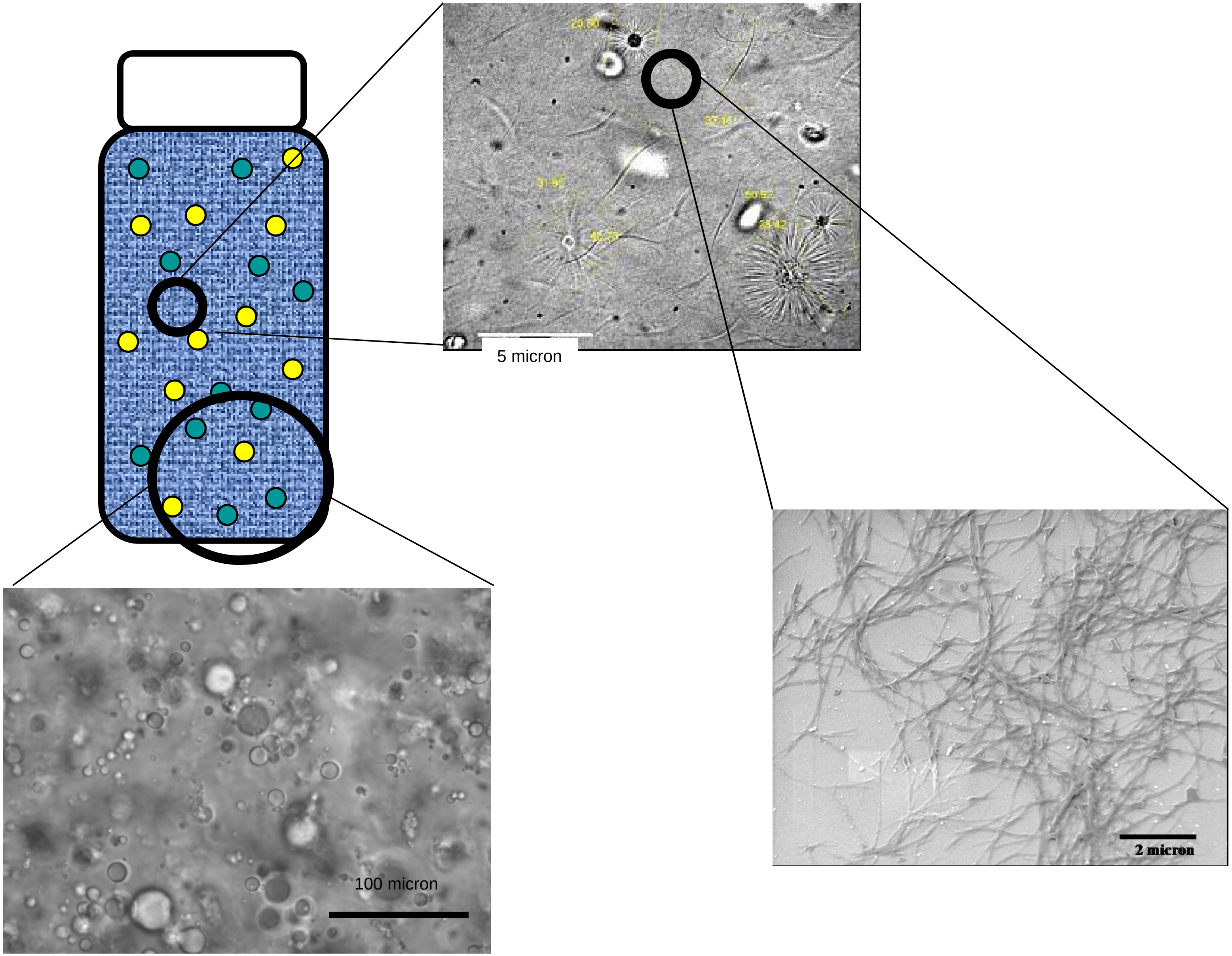
Tide

Downy

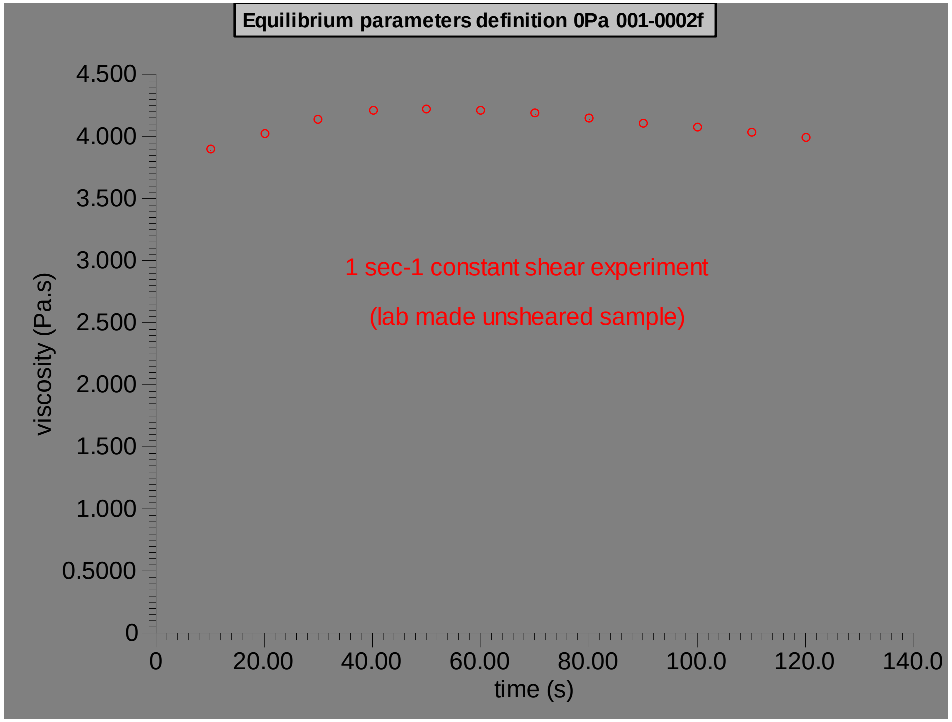
Bold

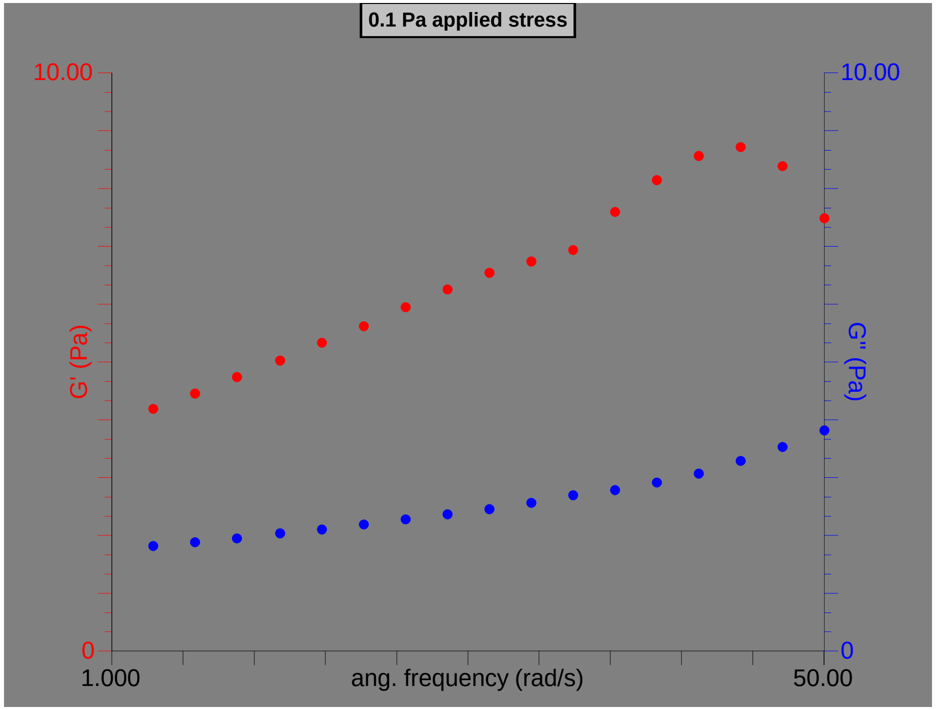
Lenor

Background



Rheology of FP

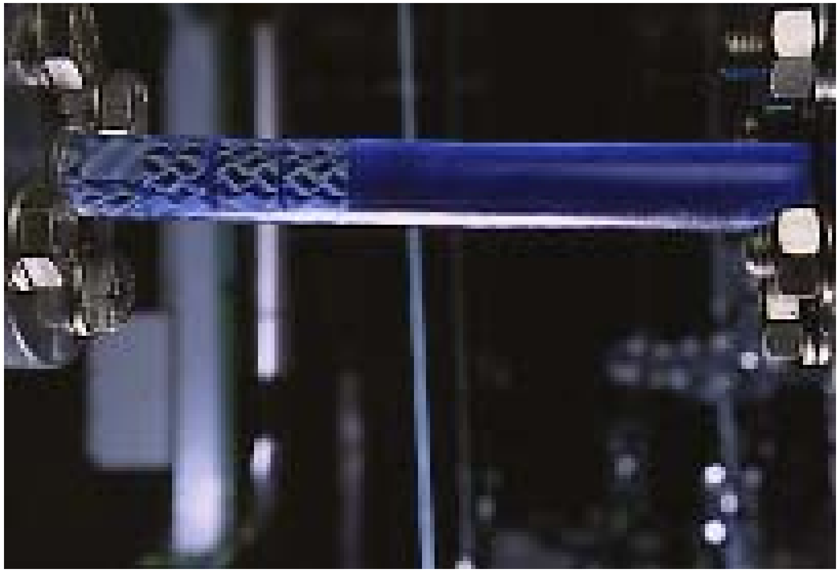


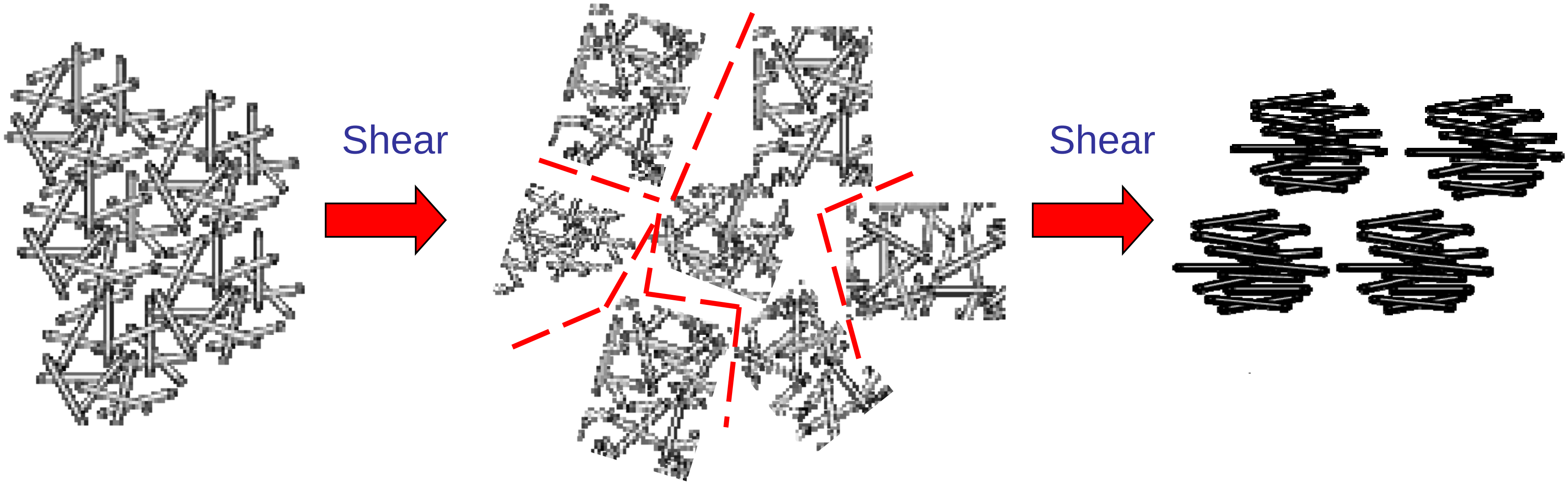


Thixotropic Material
Under flow

Weak elastic gel at rest

Detergent processing



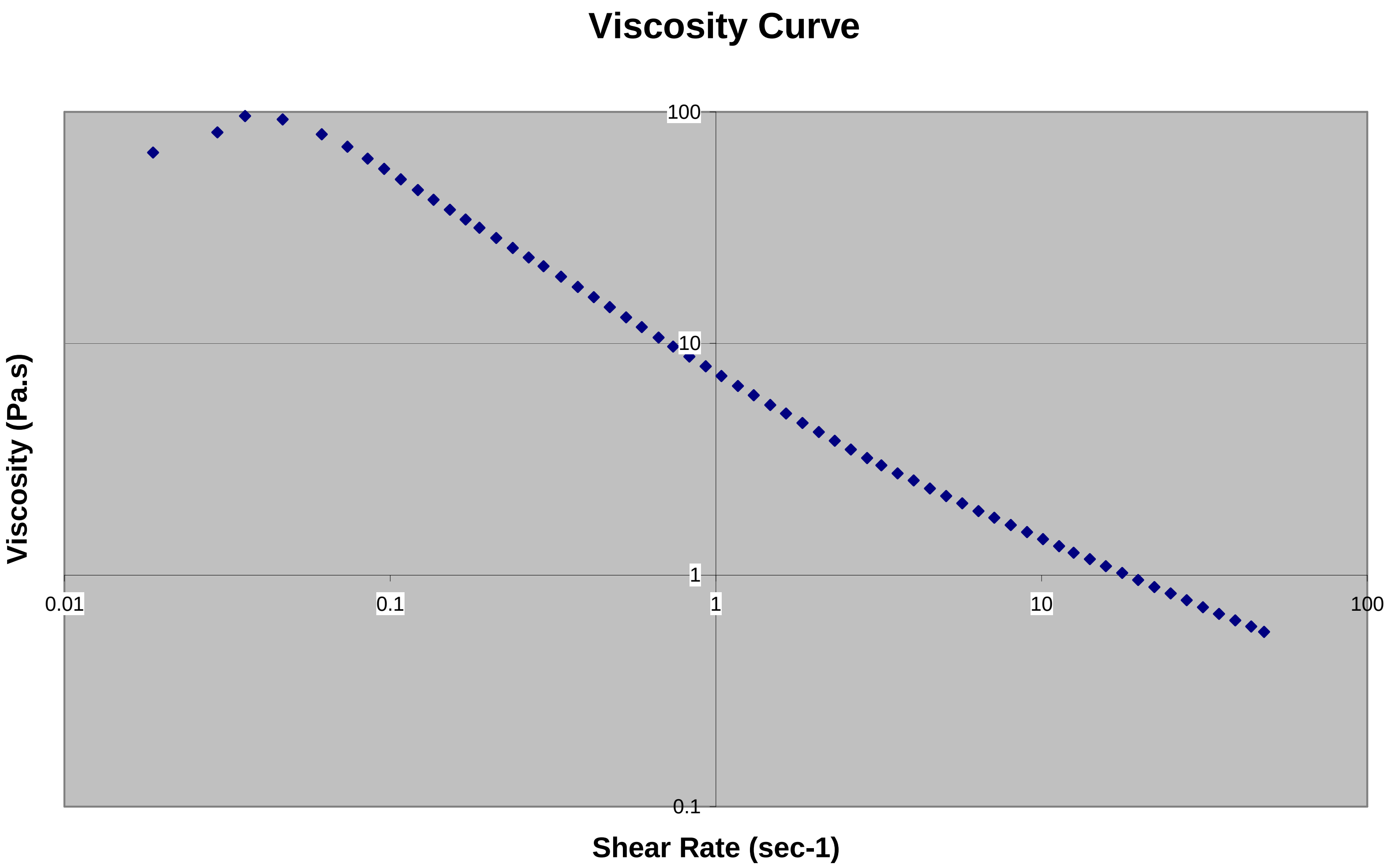


Industrial problems for detergents manufacturing

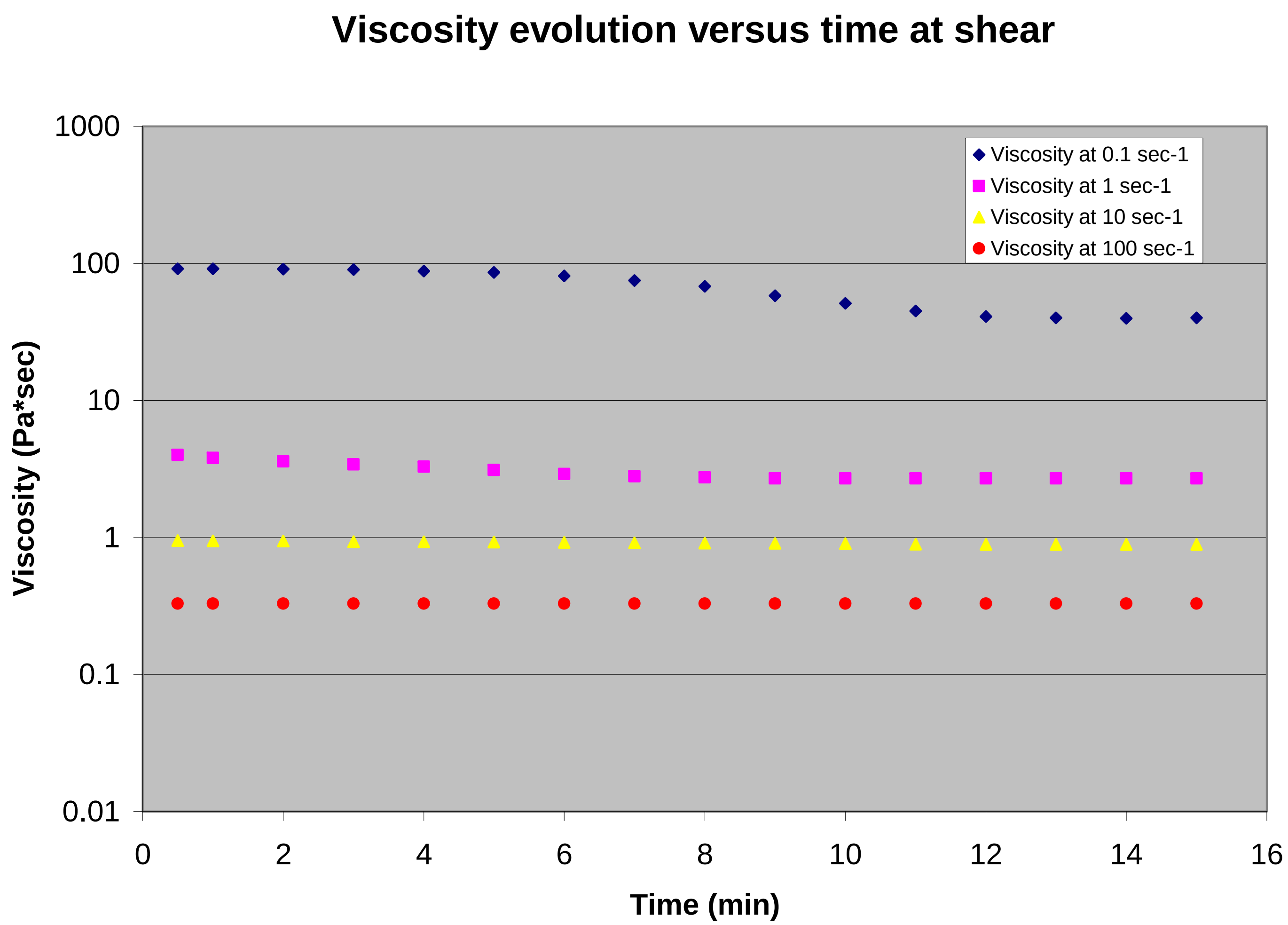
- Predict flow of detergents
  - Size pumps and pipelines
  - Calculate pressure drop in mixing devices, packing nozzles, manifold etc…
- Predict finished product properties
  - Achieve a determined microstructure
  - Predict rheology, stability, apperance

Flow problem: modeling thixotropy

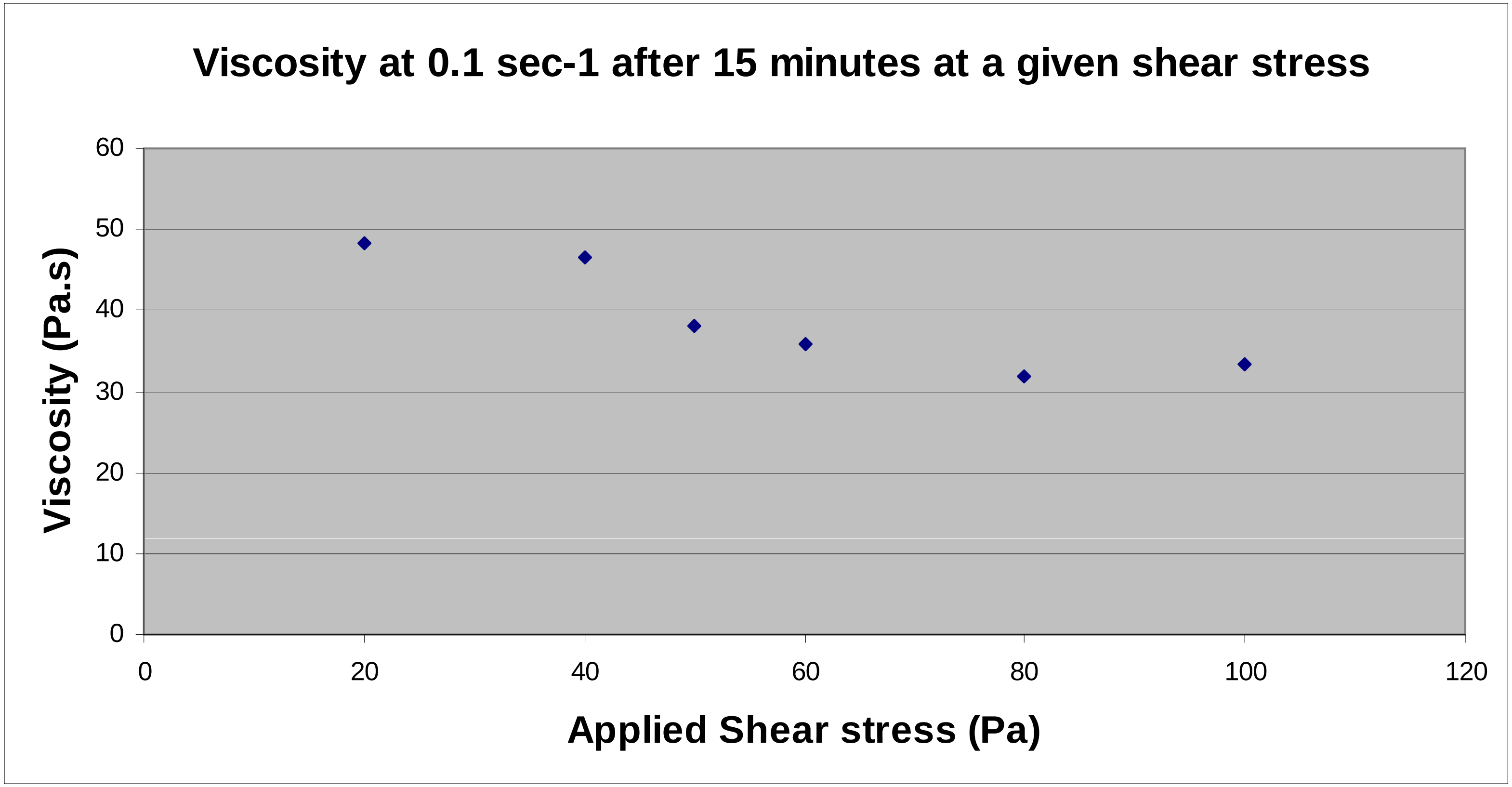
Product rheology



Thixotropy

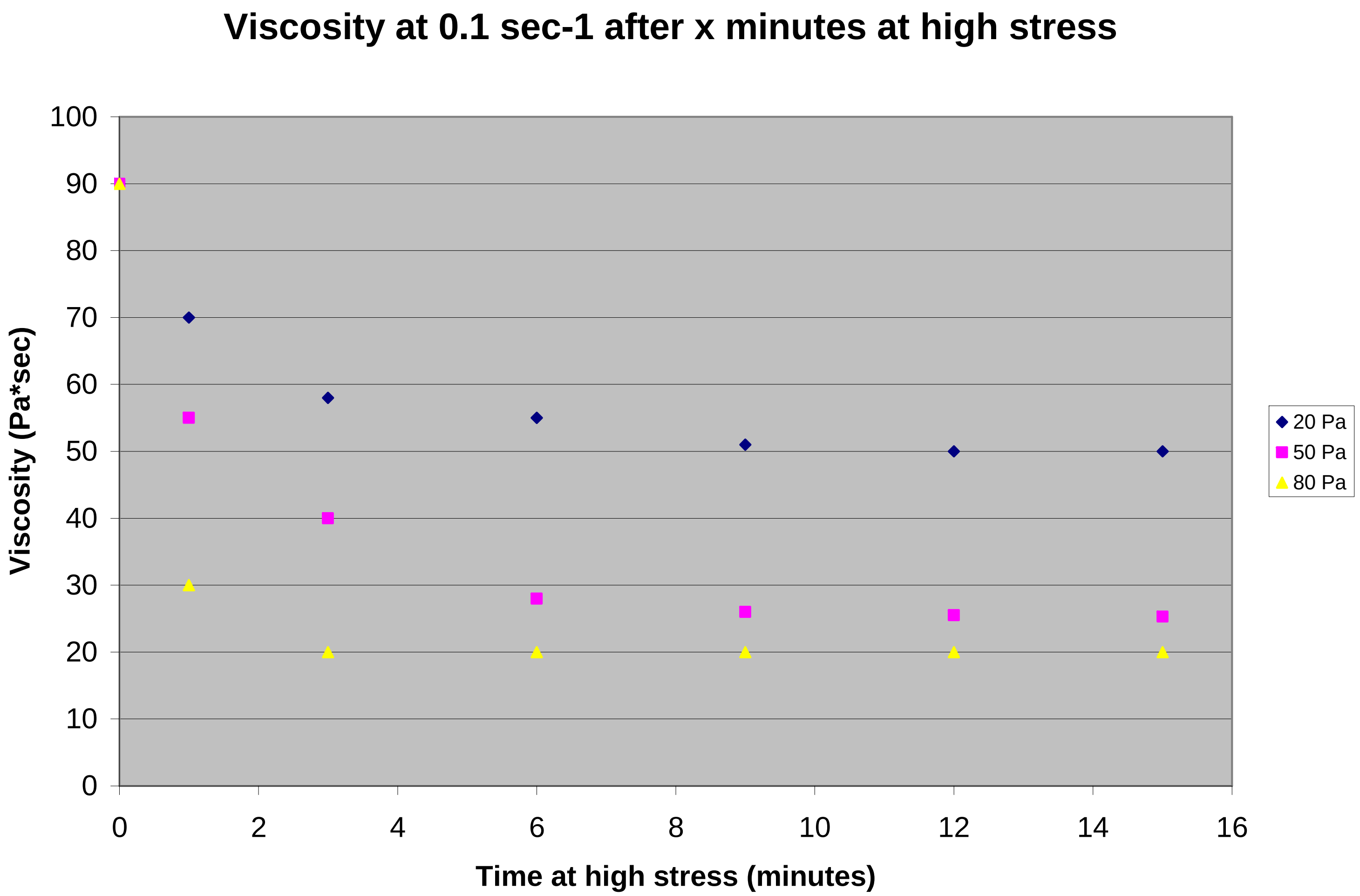

Viscosity evolution versus time at shear
Viscosity (Pa*sec)
1000
100
10
1
0.1
0.01
0
2
4
6
8
10
12
14
16
Time (min)
Viscosity at 0.1 sec-1
Viscosity at 1 sec-1
Viscosity at 10 sec-1
Viscosity at 100 sec-1

Thixotropy experimental investigation



$$\frac{\eta - \eta_\infty}{\eta_0 - \eta_\infty} = c_{eq} = \frac{1}{1 + \left(\frac{\tau}{\tau_{critic}}\right)^{\alpha}}$$

Thixotropy experimental investigation



Rheology model

$$\begin{cases} \eta = K \cdot \dot{\gamma}^{n} \\ \dfrac{K - K_\infty}{K_0 - K_\infty} = c \\ \dfrac{dc}{dt} = -(a + b \cdot \tau) \cdot \eta \cdot \dot{\gamma} \cdot \left[c - c_{eq}(\tau)\right] \\ c_{eq}(\tau) = \dfrac{1}{1 + \left(\dfrac{\tau}{\tau_{crit}}\right)^{n}} \end{cases}$$

Modification of Moore’s model

3D implementation in Comsol

Equations

$$\rho(\mathbf{u}\cdot\nabla)\mathbf{u} = \nabla\cdot[-p\mathbf{I} + \eta(\nabla\mathbf{u} + (\nabla\mathbf{u})^T)] + \mathbf{F}$$

$$\nabla\cdot\mathbf{u} = 0$$

Momentum balance

$$\eta = m\gamma'^{n-1}$$

Rheology constitutive equation

Equation

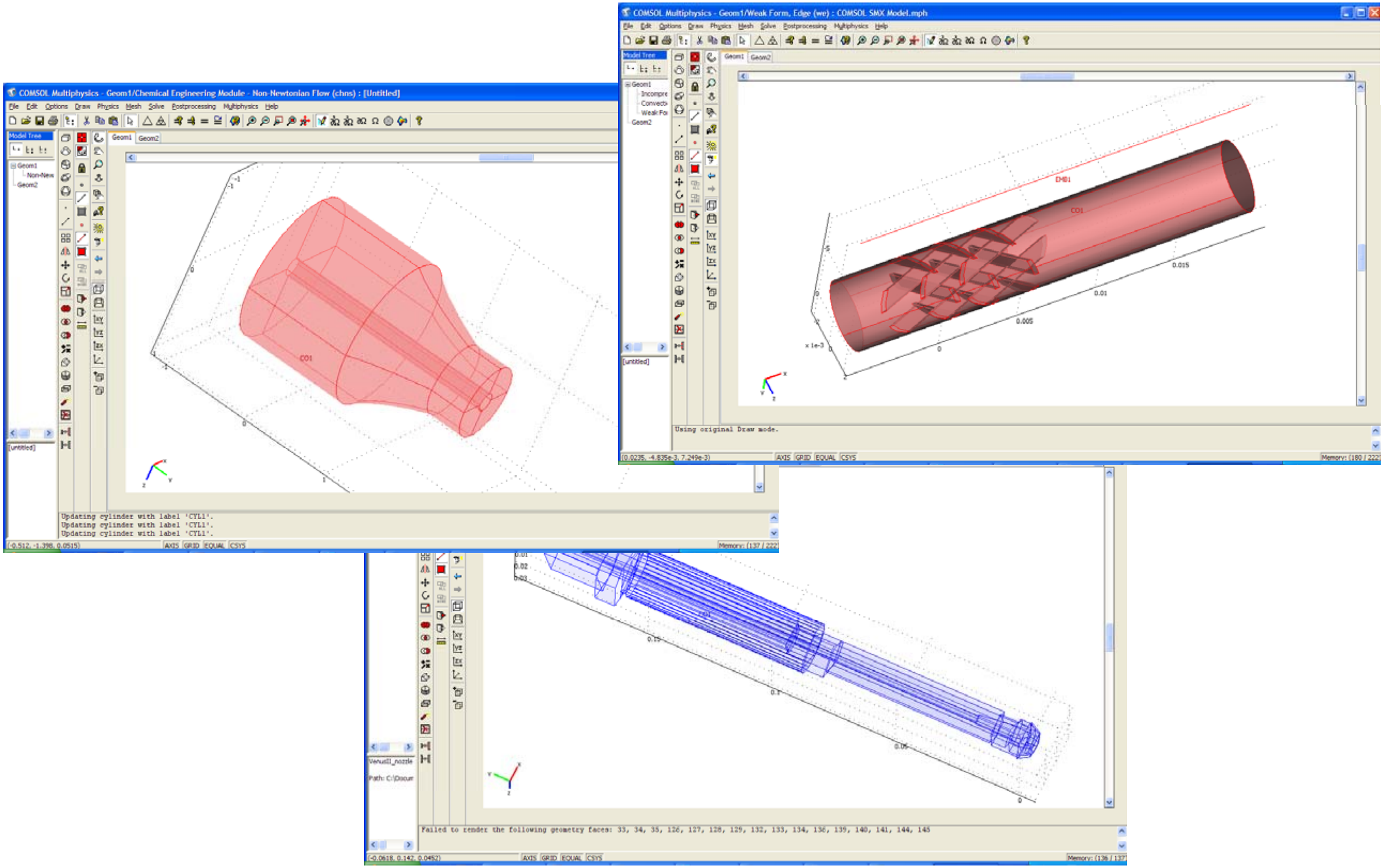
$$\nabla\cdot(-D\nabla c) = R - \mathbf{u}\cdot\nabla c, \ c = \text{concentration}$$

Conservation law for connectivity

$$\dot{\gamma} = k\cdot\left(\sqrt{\frac{1}{2}\left(4u_x^2 + 4v_y^2 + 4w_z^2\right) + 2\left(u_y + v_x\right)^2 + 2\left(u_z + w_x\right)^2 + 2\left(v_z + w_y\right)^2}\right)^n$$

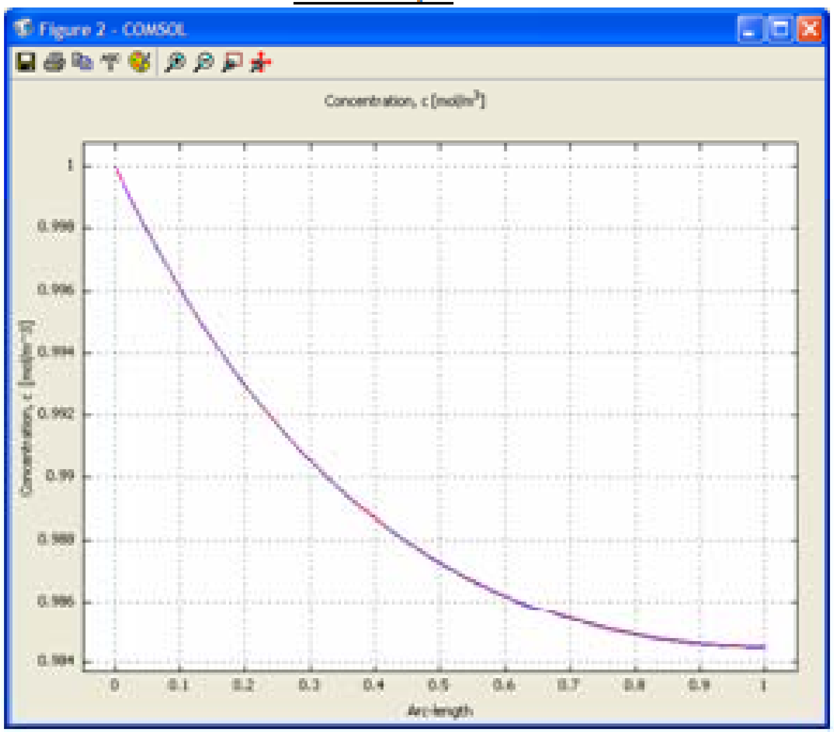
$$R = -(a + b\cdot\tau)\cdot\eta\cdot\dot{\gamma}\cdot\left[c - c_{eq}(\tau)\right]$$

Fluid dynamics simulation

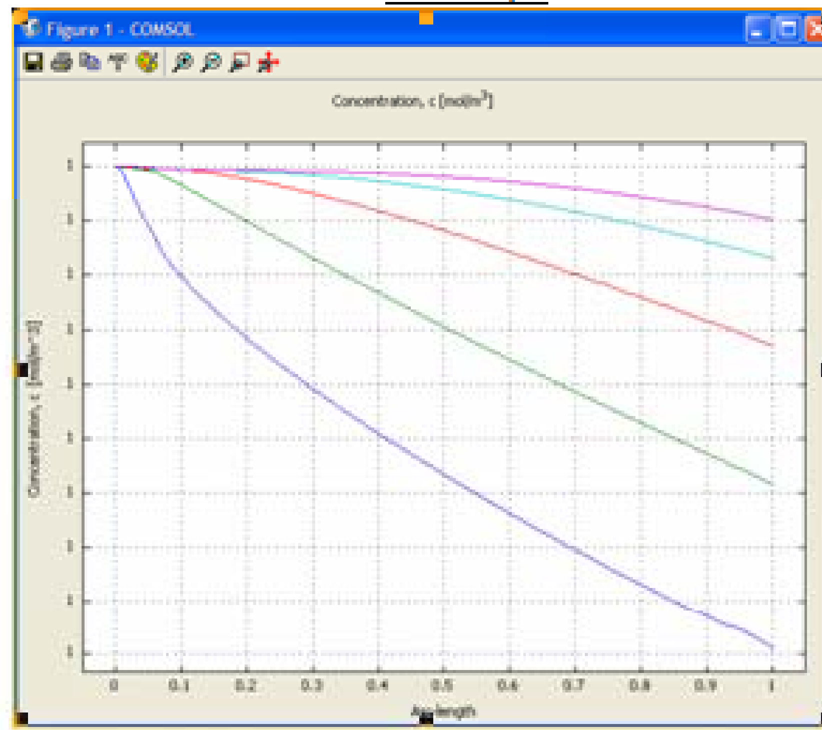


Simulation Results

Geometry 1

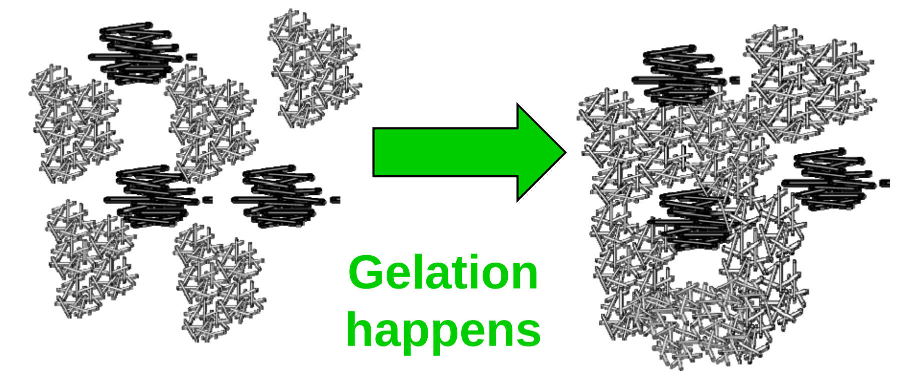


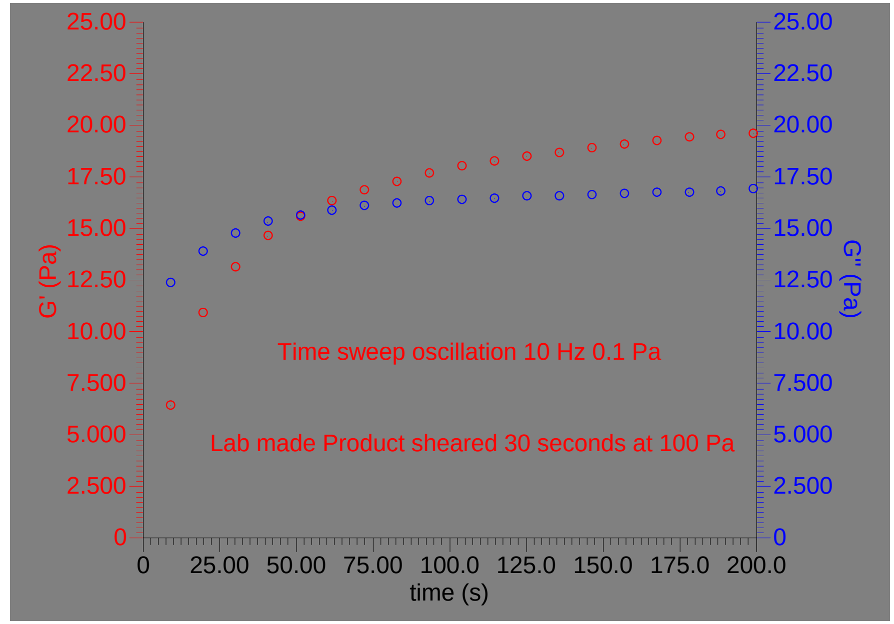
Geometry 2

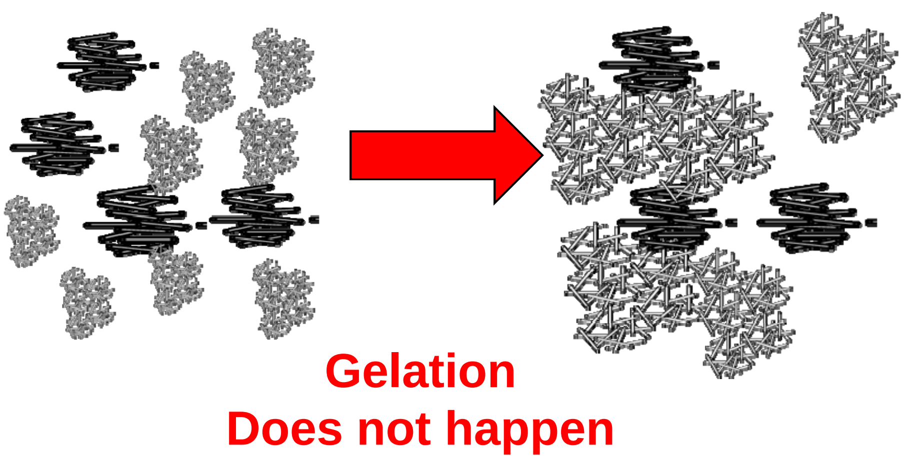


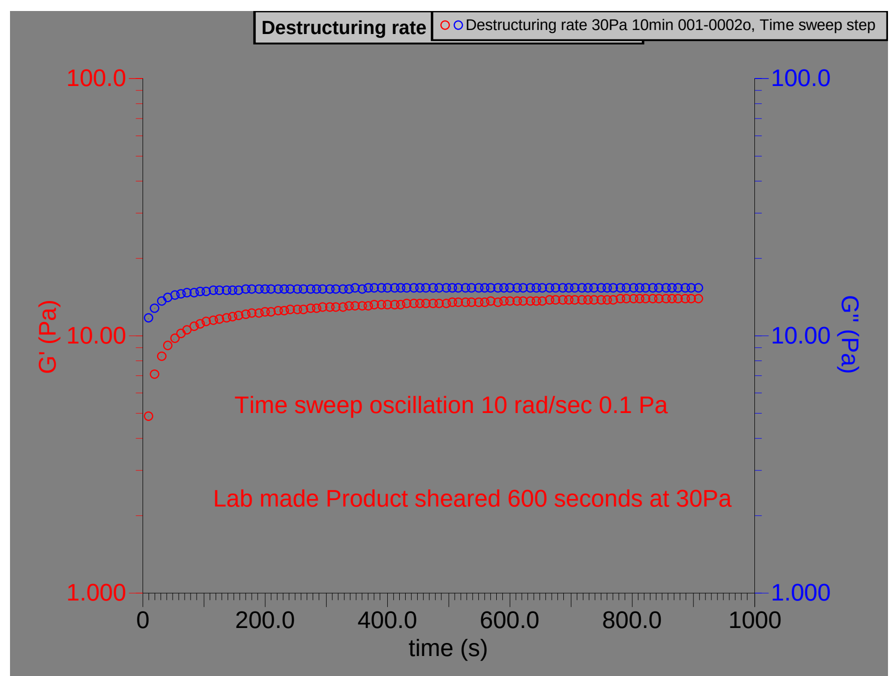
Microstructure problem: modeling gelation

After Processing

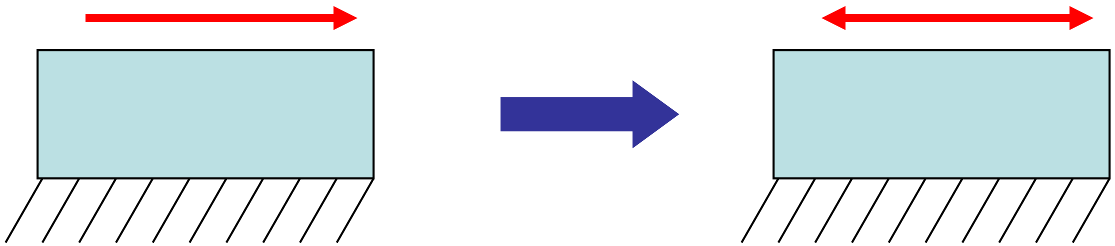








Rheological Characterization

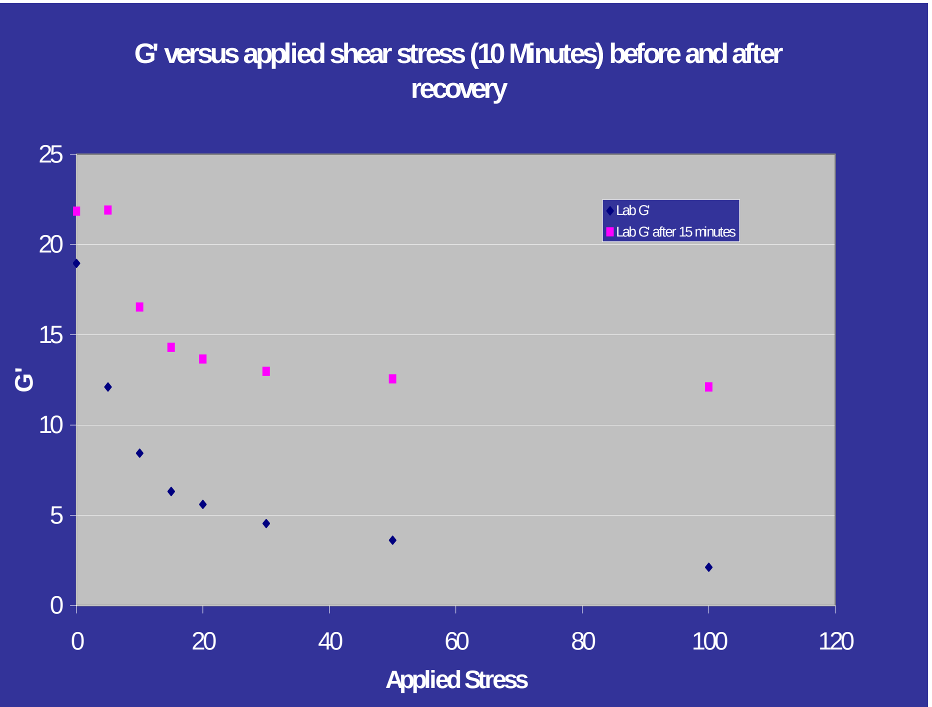


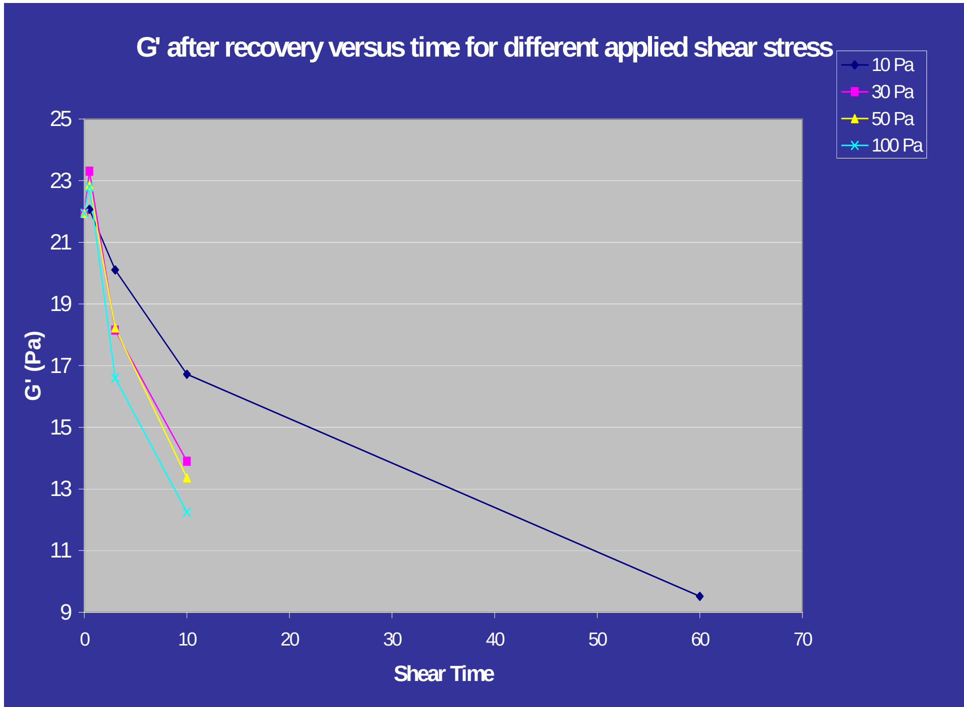
Constant Stress Flow

τ = 5, 10, 30. 50 100 Pa
t =, 30, 60, 180, 600 sec

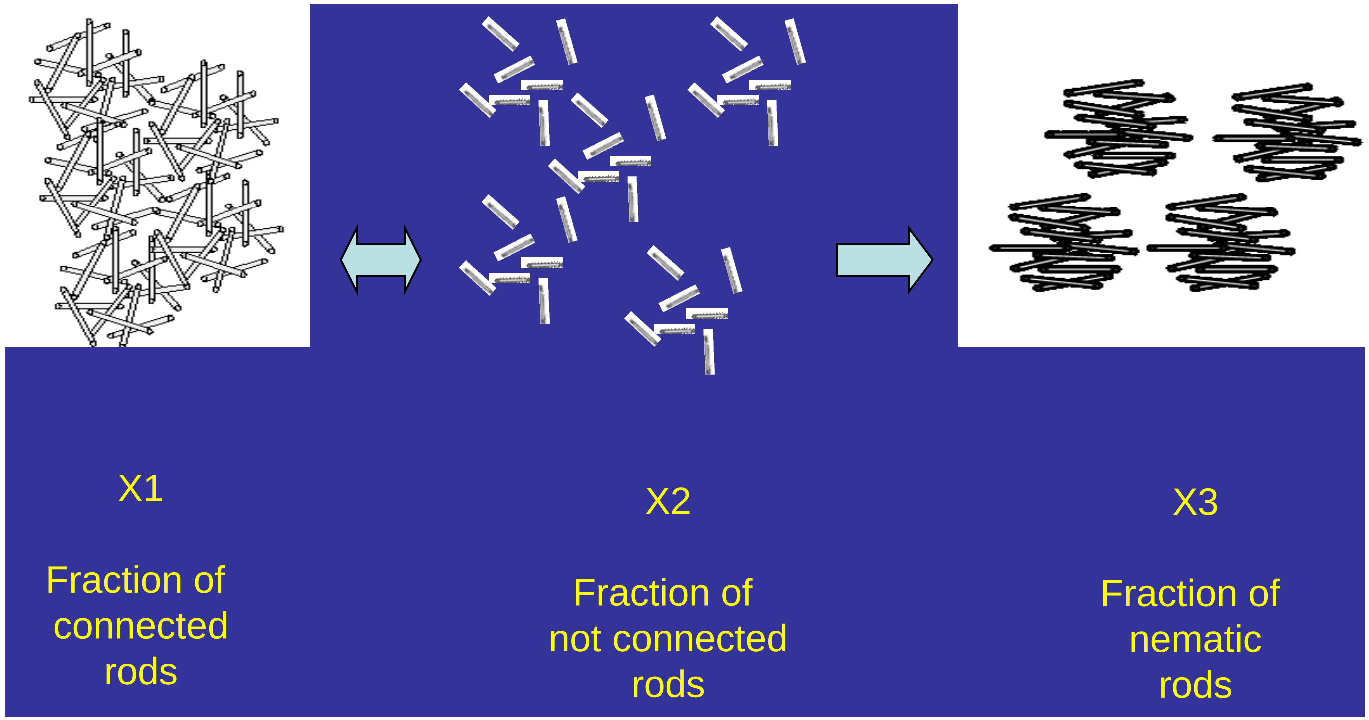
Time Sweep Oscillation

τ = 0 -900 sec





Empirical modeling



$$\frac{dX_1}{dt} = -(a_1 + b_1 \cdot \tau) \cdot X_1 + a_2 \cdot X_2$$

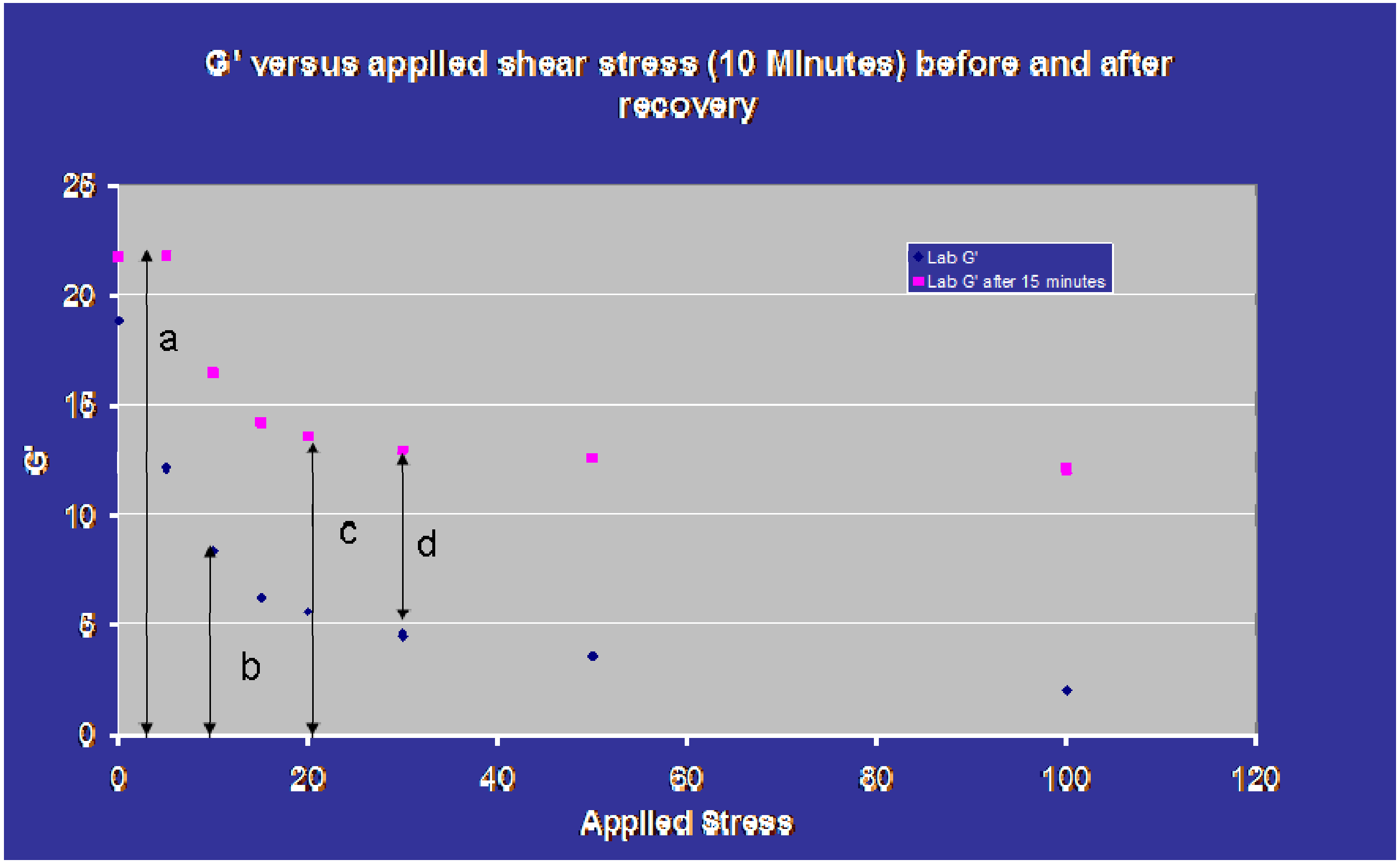
$$\frac{dX_2}{dt} = +(a_1 + b_1 \cdot \tau) \cdot X_1 - a_2 \cdot X_2 - (a_3 + b_3 \cdot \tau) \cdot X_2$$

$$X_3 = 1 - X_1 - X_2$$

Estimating Kinetics from Rheology

2 simple rules:

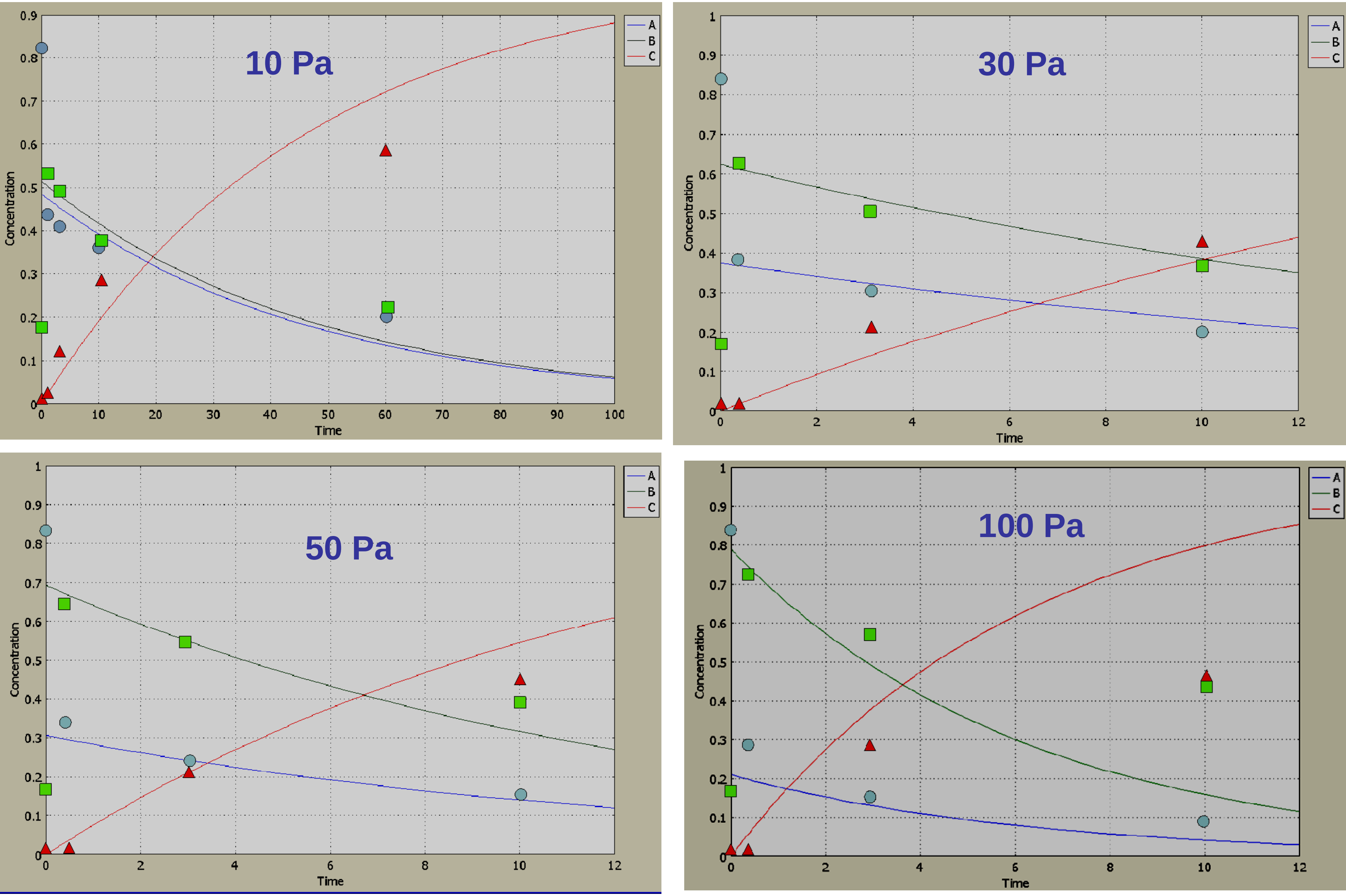
- *Elastic modulus depends only on phase 1*
  *G' = G'0 * X1*
- *After 15 minutes time sweep X2 =0*



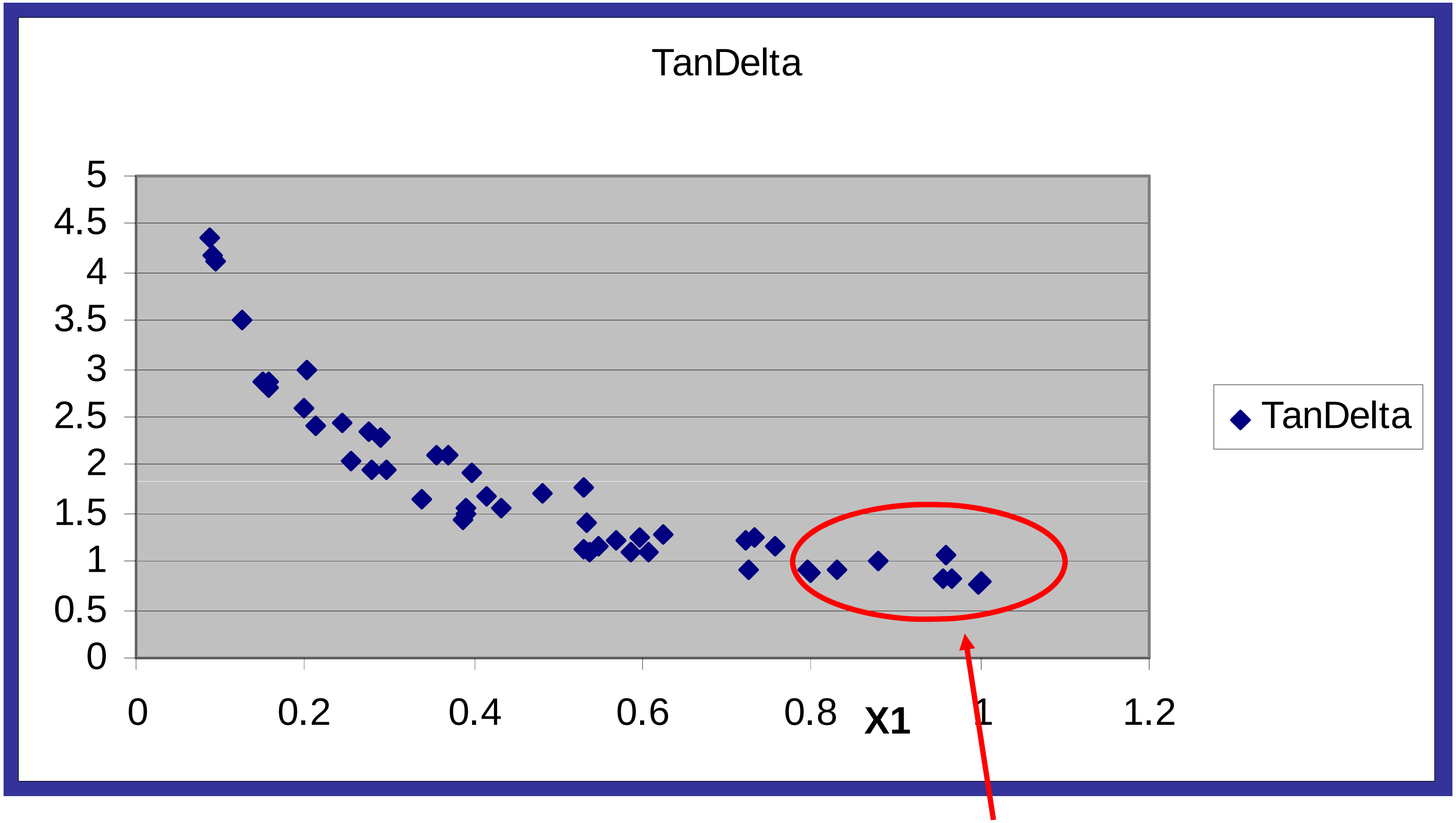
As flow stops:
X1 = b/a, X2, = d/a

After recovery:
X1 = c/a, X2 = 0

Model fitting: maximum likelihood parameter estimation



Gelification prediction



Area of interest for manufacturing

Conclusions

- Comsol is a very flexible platform, ideal to model rheology modification under flow
- Analogy with reactive flows allows modeling of both thixotropy and gelation with decent level of accuracy and predictability
- It is possible, a certain extent, to use 1 D rheology to extrapolate 3D behavior

Not all that glitters is gold

- Not everything scales with total shear rate!
- Need at least to distinguish the extensional and the pure shear components
- Single or double step reaction model are too crude, need to move to population balance
- Need to move from General viscous to Visco-elastic
- Need to describe the rods incorporation process (mixing + aggregates break up)

Thank You!

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