Coupling Reactions and Molecular Conformations in the Modeling of Shear Banding in Wormlike Micelar Systems

Antony N. Beris, Natalie Germann* and Pam Cook*

University of Delaware Chemical and Biomolecular Engineering

*Department of Mathematical Sciences

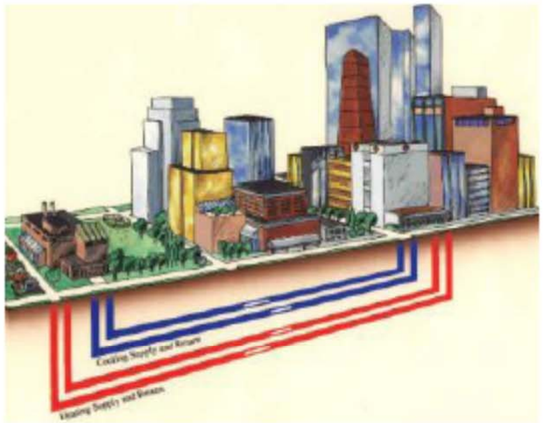
6th International Workshop on Nonequilibrium Thermodynamics
And 3rd Lars Onsager Symposium
August 20, 2012

1. **Motivation**
2. **Introduction to Micellar Systems and Shear Banding**
3. **NET Treatment of Chemical Reactions**
4. **Application to Micellar Systems and Homogeneous Flow Results**

New Application: Rod-like Micellar Systems

Applications:

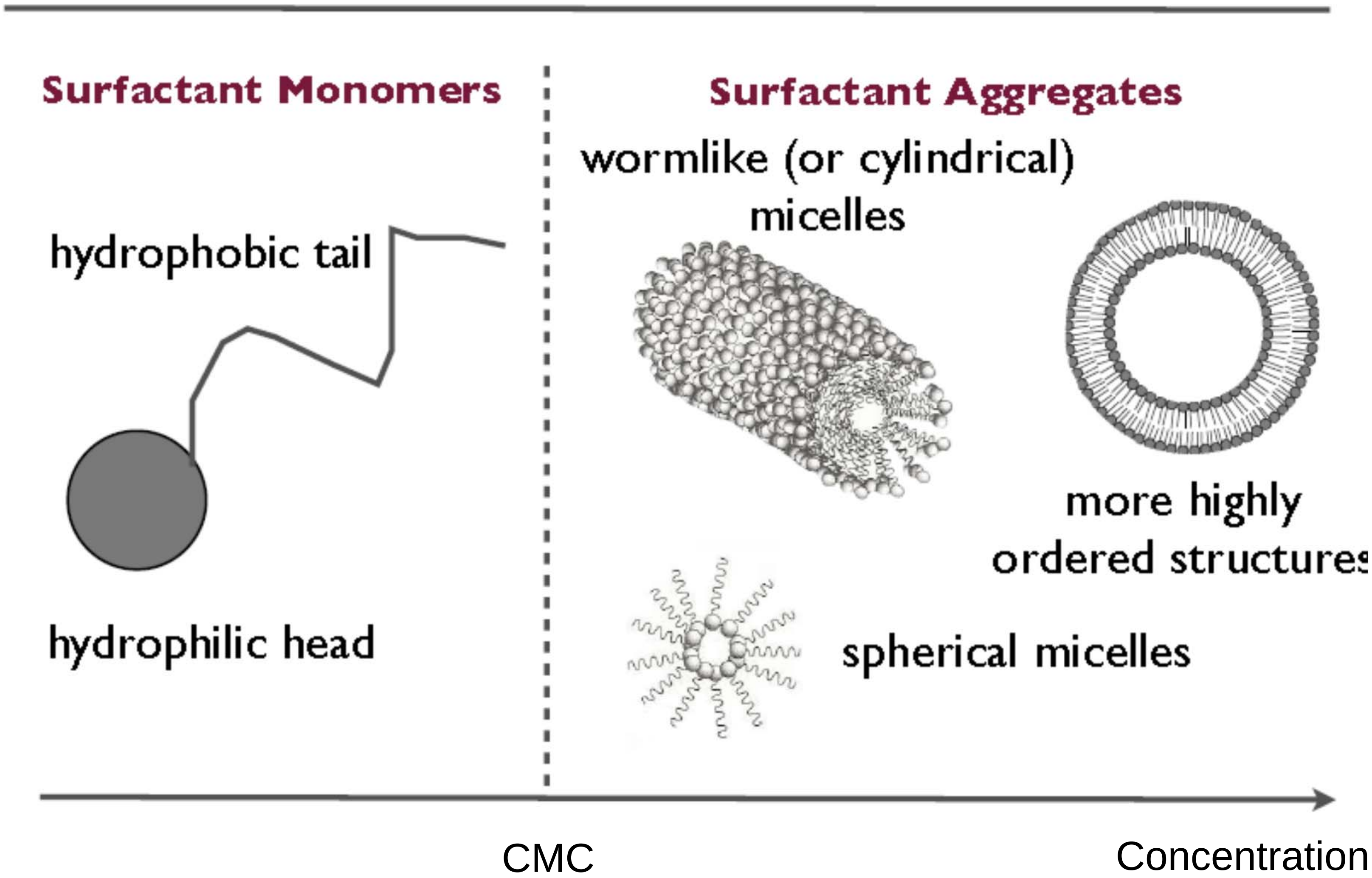
District heating & cooling systems



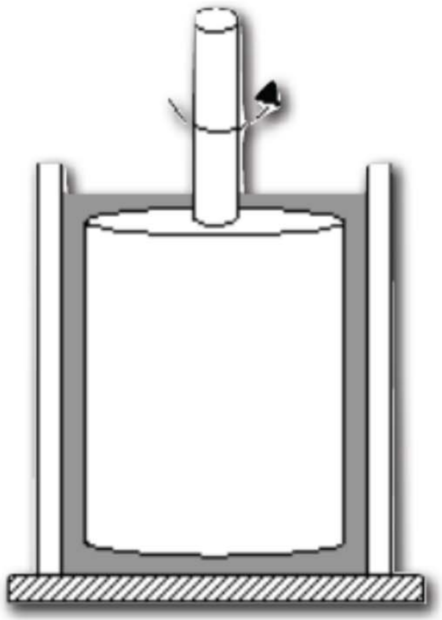
Oil industry

Home & personal care products

Micellar systems: concentrated suspensions of surfactants

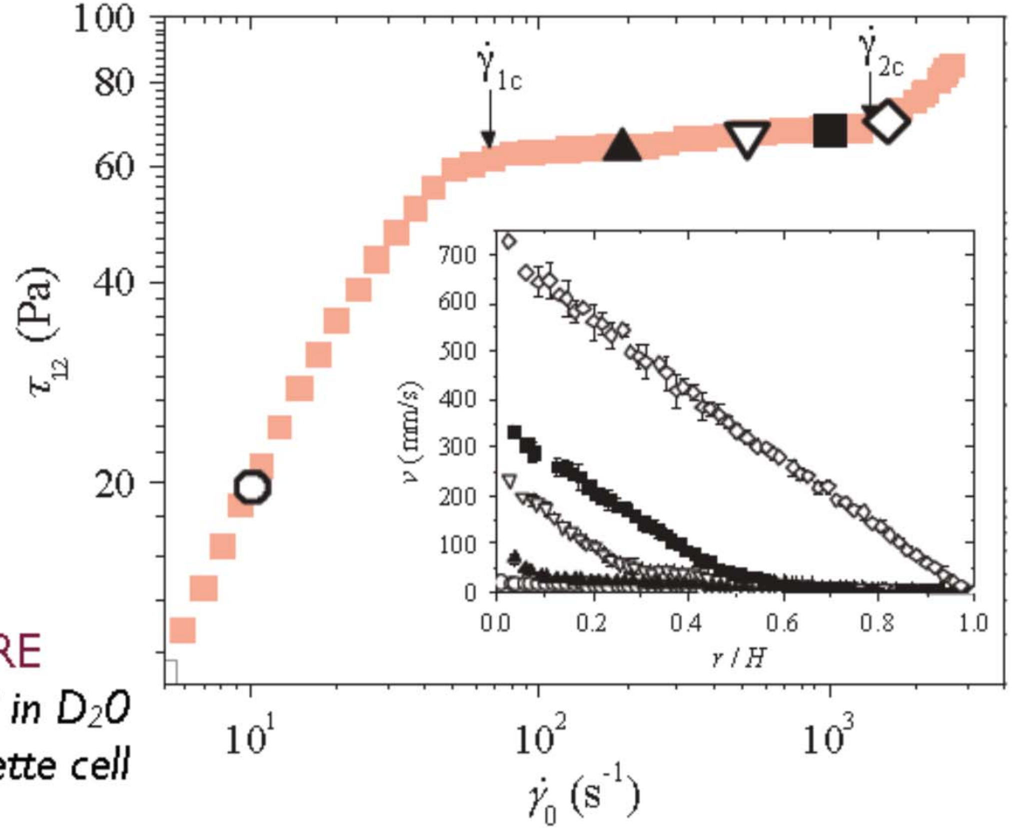


Rodlike Micellar Systems: Shear-Banding



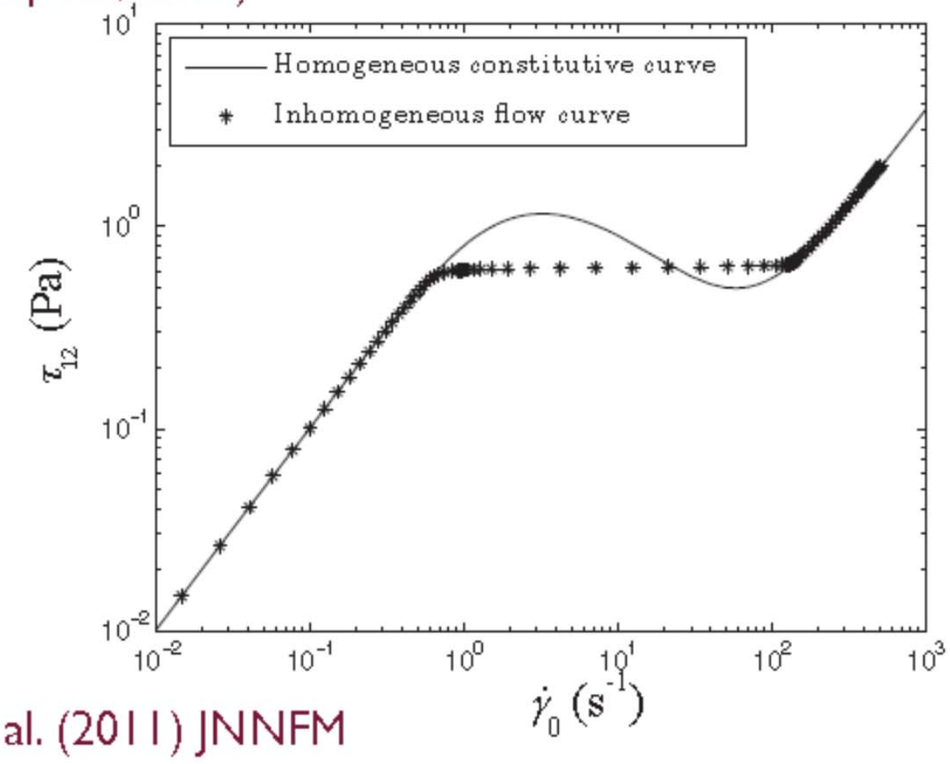
Helgeson *et al.* (2010a) PRE

- *16.7 wt.% CTAB dissolved in D_2O*
- *Shear-rate controlled Couette cell*



Previous Models for Rodlike Micellar Solutions

- Johnson-Segalmann-Olmsted model (Olmsted *et al.*, J. Rheol., 2000)
- Giesekus model with stress-driven diffusion (Helgeson *et al.*, J. Rheol., 2009)
- Vasquez-Cook-McKinley (VCM) model (Vasquez *et al.*, JNNFM., 2007; Zhou *et al.*, accepted, 2012)

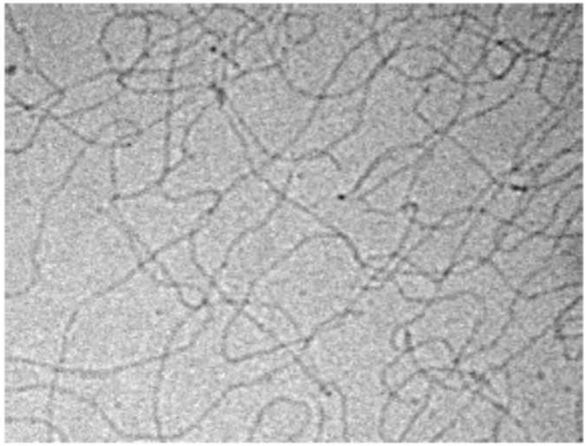


Cromer et al. (2011) JNNFM

Current Approach Extends VCM under NET

Frameworks:

- Generalized bracket approach (Beris & Edwards, Thermodynamics of Flowing Systems, 1994)
- General equation for the non-equilibrium reversible-irreversible coupling (GENERIC) (Öttinger, Beyond Equilibrium Thermodynamics, 2005)



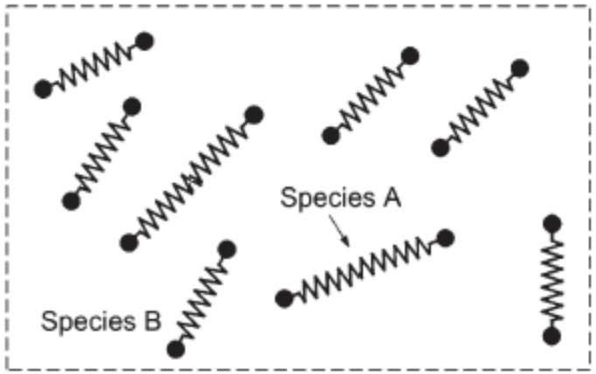
→ Breakable/reformable elastic dumbbells + viscous solvent

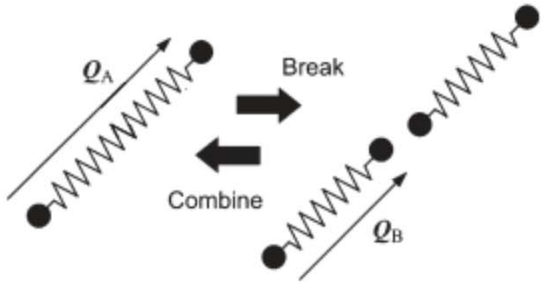
Clausen *et al.* (1992) J. Phys. Chem.

VCM Central Concept: A -> B Reaction

Two-species represenation of population:

- Species A ("longer chains")
- Species B ("shorter chains")





Source: Yamamoto & Sawa (2011) JSRJ

System variables

Number Densities: $n_A = \rho_A / M_A \, N_A$; $n_B = \rho_B / M_B \, N_A$

Conformation Tensor Densities: $C_A = n_A \mathbf{c}_A$; $C_B = n_B \mathbf{c}_B$; $\mathbf{c}_i = \langle \mathbf{Q}_i \mathbf{Q}_i \rangle$

$\langle \mathbf{Q}_i \mathbf{Q}_i \rangle$ is the second moment of the end-to-end connection vector, $\mathbf{Q}_i$, for component i

Momentum Density: $\mathbf{M}=\rho\mathbf{v}$; $\rho=\rho_A + \rho_B + \rho_S$

General reaction kinetics in multicomponent systems

- Assume that the system:
  - involves *n* components, optionally with internal structure and
  - participates in *l* chemical reactions
- For each component, $i = 1, 2, \ldots n$, the following primary variables are defined:
  - the mass density, ρ_i
  - the momentum density, $\mathbf{m}^i$, $\mathbf{m}^i = \rho_i \mathbf{v}^i$
  - (optionally) the internal structural tensor parameter density, $\mathbf{C}^i$, $\mathbf{C}^i = n_i \, \mathbf{c}^i$

where:

$\mathbf{v}^i$ is the mass-based velocity of component i

$n_i = \rho_i / M_i \, N_A$ is the number density of component i

$\mathbf{c}^i$ is the conformation tensor of component i; $\mathbf{c}^i = \langle \mathbf{Q}^i \mathbf{Q}^i \rangle$

$\langle \mathbf{Q}^i \mathbf{Q}^i \rangle$ is the second moment of the end-to-end connection vector, $\mathbf{Q}^i$, for component i

NET Extension for Chemical Reaction Rates

- It preserves standard transition theory kinetics that assigns for the corresponding forward (-) and reverse (+) flux of the reaction *I*, an Arhenius dependence on the corresponding affinity:

$$J_I^{\mp} = k_I\left(P,T\right)\exp\left(-\frac{A_I^{\mp}}{RT}\right)$$

- However, a generalized affinity is proposed in order to also accommodate other, nonequilibrium, changes associated with the reaction *I*, such as momentum and conformation (for entropy one needs a more general (GENERIC) formulation):

$$A_I^{\mp} = -\sum_{k=1}^{n} \gamma_{Ik}^{\mp} M_k \left(\frac{\delta H}{\delta \rho_k} + \frac{m_\alpha^k}{\rho_k}\left(\frac{\delta H}{\delta m_\alpha^k}\right)_G + \frac{C_{\alpha\beta}^k}{\rho_k}\frac{\delta H}{\delta C_{\alpha\beta}^k} \right)$$

where $\left(\dfrac{\delta H}{\delta m_\alpha^k}\right)_G$ represents the Galilean invariant contribution:

$$\left(\frac{\delta H}{\delta m_\alpha^k}\right)_G \equiv v_\alpha^k - v_\alpha = \frac{\delta H}{\delta m_\alpha^k} - \frac{\delta H}{\delta m_\alpha} = \frac{\delta H}{\delta m_\alpha^k} - \sum_{m=1}^{n} \frac{\rho_m}{\rho}\frac{\delta H}{\delta m_\alpha^m}$$

Corresponding Dissipation Bracket*

$$
\begin{aligned}
[F,H]_I = J_I^- & \left(-\sum_{k=1}^{n} \gamma_{Ik}^- M_k \left(\begin{array}{l} \dfrac{\delta F}{\delta \rho_k} + \dfrac{m_\alpha^k}{\rho_k}\left(\dfrac{\delta F}{\delta m_\alpha^k}\right)_G + \dfrac{C_{\alpha\beta}^k}{\rho_k}\dfrac{\delta F}{\delta C_{\alpha\beta}^k} \\ -\dfrac{1}{\sum_{k'=1}^{n} \gamma_{Ik'}^+ M_{k'}} \sum_{k''=1}^{n} \gamma_{Ik''}^+ M_{k''} \left(\dfrac{\delta F}{\delta \rho_{k''}} + \dfrac{m_\alpha^k}{\rho_k}\left(\dfrac{\delta F}{\delta m_\alpha^{k''}}\right)_G + \dfrac{C_{\alpha\beta}^k}{\rho_k}\dfrac{\delta F}{\delta C_{\alpha\beta}^{k''}} \right) \end{array} \right) \right) \\
+ J_I^+ & \left(-\sum_{k=1}^{n} \gamma_{Ik}^+ M_k \left(\begin{array}{l} \dfrac{\delta F}{\delta \rho_k} + \dfrac{m_\alpha^k}{\rho_k}\left(\dfrac{\delta F}{\delta m_\alpha^k}\right)_G + \dfrac{C_{\alpha\beta}^k}{\rho_k}\dfrac{\delta F}{\delta C_{\alpha\beta}^k} \\ -\dfrac{1}{\sum_{k'=1}^{n} \gamma_{Ik'}^- M_{k'}} \sum_{k''=1}^{n} \gamma_{Ik''}^- M_{k''} \left(\dfrac{\delta F}{\delta \rho_{k''}} + \dfrac{m_\alpha^k}{\rho_k}\left(\dfrac{\delta F}{\delta m_\alpha^{k''}}\right)_G + \dfrac{C_{\alpha\beta}^k}{\rho_k}\dfrac{\delta F}{\delta C_{\alpha\beta}^{k''}} \right) \end{array} \right) \right)
\end{aligned}
$$

- It duly satisfies Onsager's reciprocity relations
- It does not affect the overall momentum equation
- It redistributes among the products the excess momentum and conformation

* to within an entropy correction term, not needed for isothermal processes

NET Implementation for Homogeneous Micellar System

Breakage & reformation kinetics

Approach: Extension of chemical reaction kinetics in (Beris & Edwards, Thermodynamics of Flowing Systems, 1994) to viscoelastic systems

Stoichiometric equation

$$A \underset{c_B}{\overset{c_A}{\rightleftharpoons}} 2\,B$$

Flux: $J^{\mp} = k \exp\left(-\frac{A^{\mp}}{RT}\right)$

Affinity: $A^{\mp} = -\Sigma_k \gamma_k^{\mp} M_k \left(\underbrace{\frac{\delta H}{\delta \rho_k}}_{\rho_k\text{-transfer}} + \underbrace{\frac{C^k_{\alpha\beta}}{\rho_k} \frac{\delta H}{\delta C^k_{\alpha\beta}}}_{C^k_{\alpha\beta}\text{-transfer}} \right) \quad (k = \mathrm{A}, \mathrm{B})$

Key Element: Dissipation Induced by the Reaction

Dissipation bracket

Transfer of properties

donor | receiver

$$[F,H] = \int_\Omega J^- \left(-\Sigma_k \gamma_k^- M_k \left(\frac{\delta F}{\delta \rho_k} + \frac{C_{\alpha\beta}^k}{\rho_k} \frac{\delta F}{\delta C_{\alpha\beta}^k} \right.\right.$$

$$\left.\left. - \frac{1}{\Sigma_{k'} \gamma_{k'}^+ M_{k'}} \Sigma_{k''} \gamma_{k''}^+ M_{k''} \left(\frac{\delta F}{\delta \rho_{k''}} + \frac{C_{\alpha\beta}^k}{\rho_k} \frac{\delta F}{\delta C_{\alpha\beta}^{k''}} \right) \right) \right) \mathrm{d}^3 x$$

$$+ \int_\Omega J^+ \left(-\Sigma_k \gamma_k^+ M_k \left(\frac{\delta F}{\delta \rho_k} + \frac{C_{\alpha\beta}^k}{\rho_k} \frac{\delta F}{\delta C_{\alpha\beta}^k} \right.\right.$$

$$\left.\left. - \frac{1}{\Sigma_{k'} \gamma_{k'}^- M_{k'}} \Sigma_{k''} \gamma_{k''}^- M_{k''} \left(\frac{\delta F}{\delta \rho_{k''}} + \frac{C_{\alpha\beta}^k}{\rho_k} \frac{\delta F}{\delta C_{\alpha\beta}^{k''}} \right) \right) \right) \mathrm{d}^3 x$$

$(k = \mathrm{A}, \mathrm{B}; k' = \mathrm{A}, \mathrm{B}; k'' = \mathrm{A}, \mathrm{B})$

Final Equations

Model (without momentum & stress equations)

$$\frac{\partial n_A}{\partial t} = -\nabla_\alpha (v_\alpha n_A) - c_A n_A + \frac{1}{2} c_B n_B^2$$

$$\frac{\partial n_B}{\partial t} = -\nabla_\alpha (v_\alpha n_B) + 2 c_A n_A - c_B n_B^2$$

$$\frac{\partial C^A_{\alpha\beta}}{\partial t} = -\nabla_\gamma (v_\gamma C^A_{\alpha\beta}) + C^A_{\gamma\alpha} \nabla_\gamma v_\beta + C^A_{\gamma\beta} \nabla_\gamma v_\alpha - \frac{1}{\lambda_A}\left(C^A_{\alpha\beta} - \frac{n_A k_B T}{K_A} \delta_{\alpha\beta} \right) - c_A C^A_{\alpha\beta} + c_B n_B C^B_{\alpha\beta}$$

$$\frac{\partial C^B_{\alpha\beta}}{\partial t} = -\nabla_\gamma (v_\gamma C^B_{\alpha\beta}) + C^B_{\gamma\alpha} \nabla_\gamma v_\beta + C^B_{\gamma\beta} \nabla_\gamma v_\alpha - \frac{1}{\lambda_B}\left(C^B_{\alpha\beta} - \frac{n_B k_B T}{K_B} \delta_{\alpha\beta} \right) + c_A C^A_{\alpha\beta} - c_B n_B C^B_{\alpha\beta}$$

$$c_A = c_{Aeq} \frac{\exp\left(\frac{\mathrm{tr}\,\sigma^A}{2 n_A k_B T} \right)}{\sqrt{\det\left(\frac{K_A \mathbf{C}^A}{n_A k_B T} \right)}} \qquad c_B = c_{Beq} \frac{\exp\left(\frac{\mathrm{tr}\,\sigma^B}{n_B k_B T} \right)}{\det\left(\frac{K_B \mathbf{C}^B}{n_B k_B T} \right)}$$

Parameters

Dissipative terms:

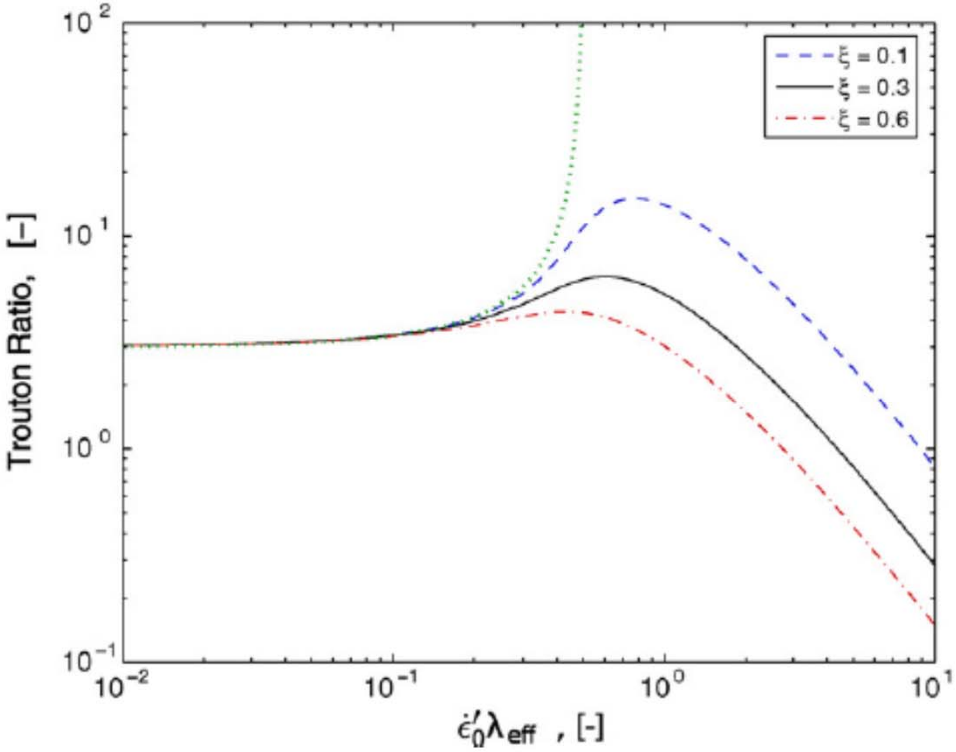
- *breakage*
- *reformation*
- *relaxation*

Comparison with the VCM Model

Impact of parameter ξ in extension (Vasquez *et al.*, JNNFM, 2007)

additional parameter

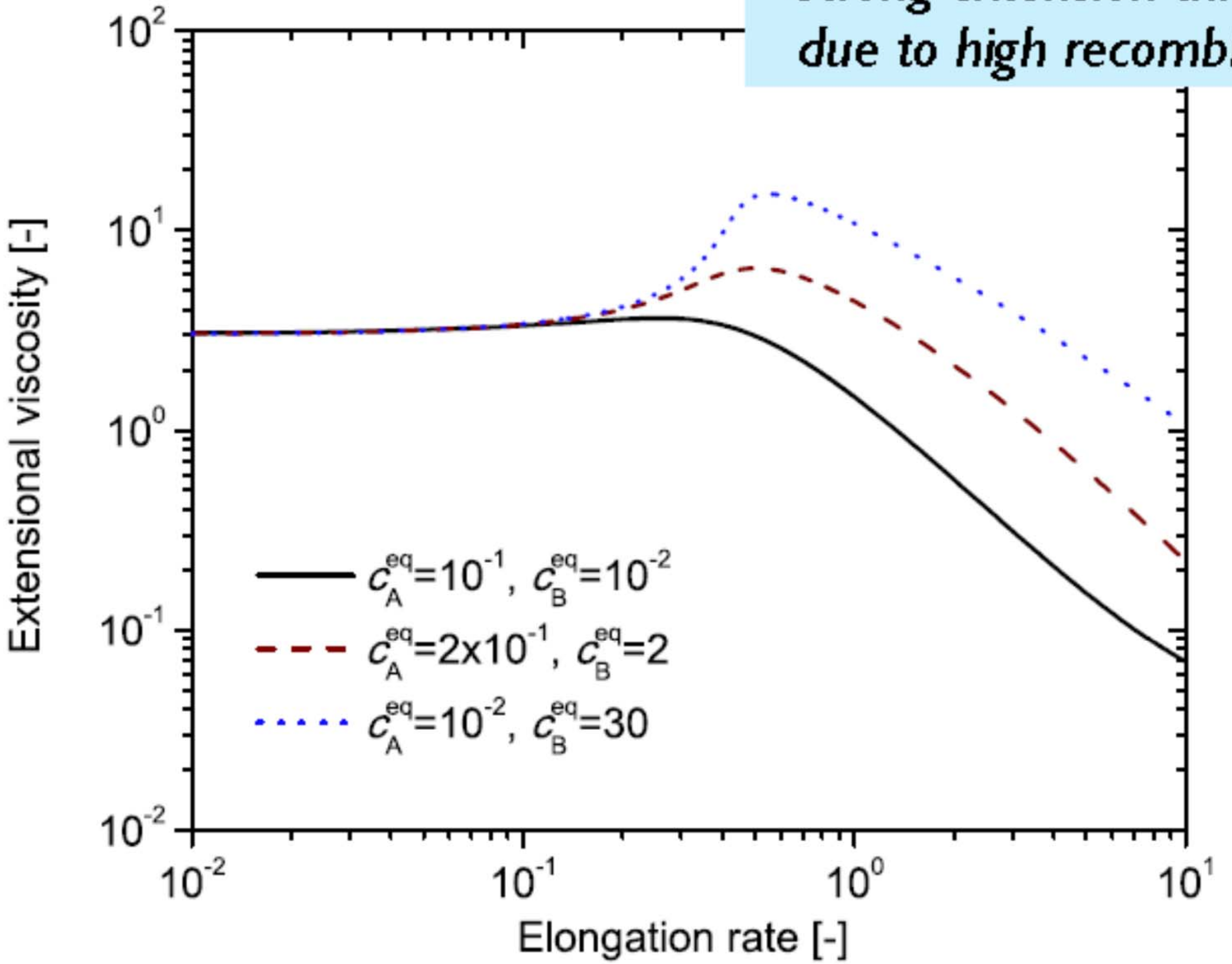
$$c_A = c_{Aeq} + \frac{1}{3}\xi\left(\nabla \mathbf{v} + \nabla \mathbf{v}^T\right) : \frac{\mathbf{C}^A}{n_A} \qquad c_B = c_{Beq}$$



New Model Predictions

Parameters: $\beta = 7 \times 10^{-5}$; $\varepsilon = 10^{-4}$

Strong extension thickening due to high recombination!



Model Non-Dimensionalization & Parameters

Non-dimensionalization

Time: $\widetilde{t} = t/\lambda_{\text{eff}}$ Length: $\widetilde{x}_\alpha = x_\alpha/H$ Pressure: $\widetilde{p} = p/G_0$

Number density: $\widetilde{n}_k = n_k/n_{\text{Aeq}}$ $(k = \text{A}, \text{B})$

Conformation: $\widetilde{c}^k_{\alpha\beta} = (K_\text{A}/(k_\text{B}T)) c^k_{\alpha\beta}$ $(k = \text{A}, \text{B})$

Stress: $\widetilde{\sigma}^k_{\alpha\beta} = \sigma^k_{\alpha\beta}/G_0$ $(k = \text{A}, \text{B}, \text{total}, \text{solvent})$

Dimensionless numbers

Reynolds number: $Re = \rho H^2/(\lambda^2_{\text{eff}} G_0)$

Deborah number: $De = \lambda_{\text{eff}} V/H$

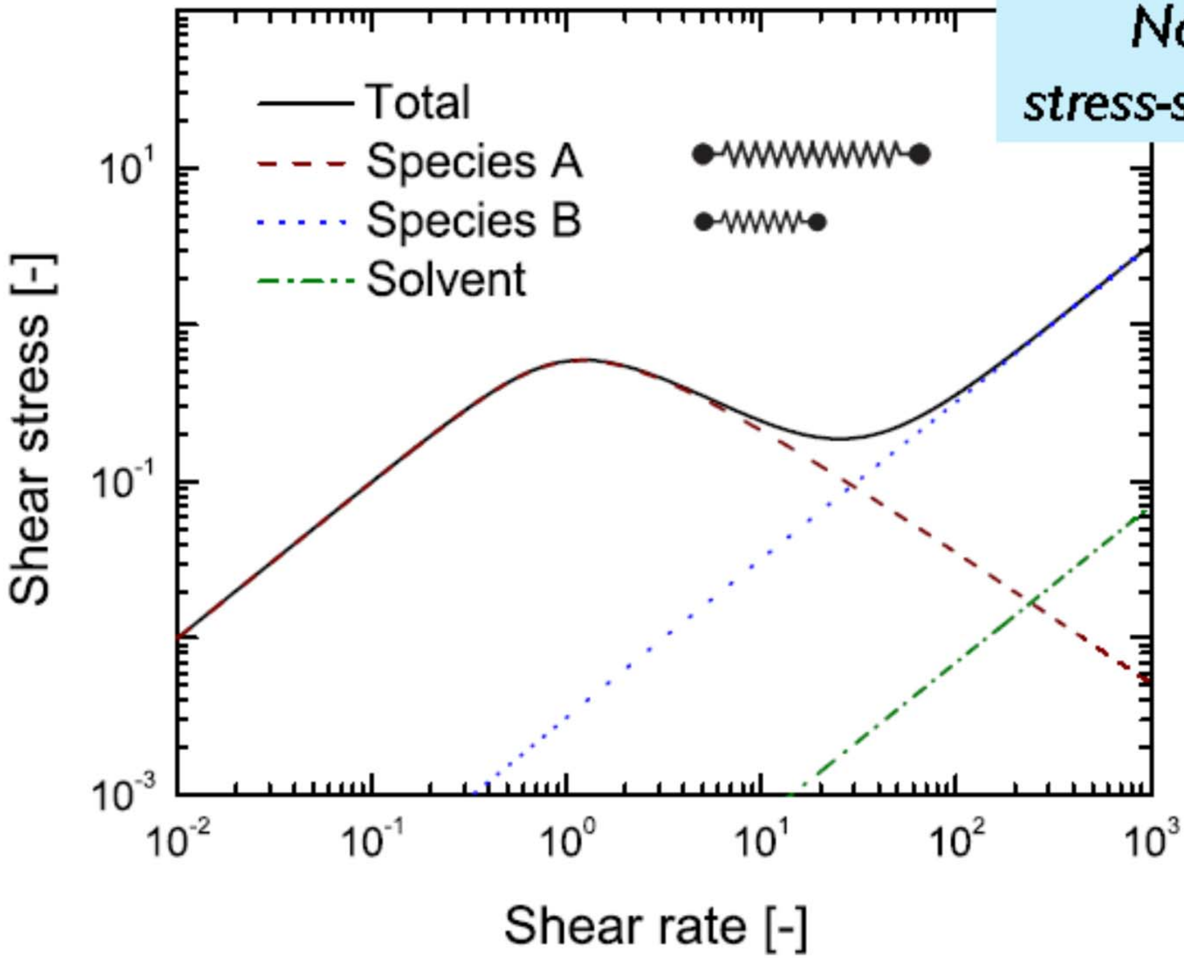
Viscosity ratio: $\beta = \eta_s/\eta_0$ Relaxation time ratio: $\varepsilon = \lambda_\text{B}/\lambda_\text{A}$

Reaction rate: $\widetilde{c}_{\text{Aeq}} = \lambda_\text{A} c_{\text{Aeq}}$

Reformation rate: $\widetilde{c}_{\text{Beq}} = \lambda_\text{A} c_{\text{Beq}} n_{\text{Aeq}}$

Homogeneous Shear Flow Predictions -1

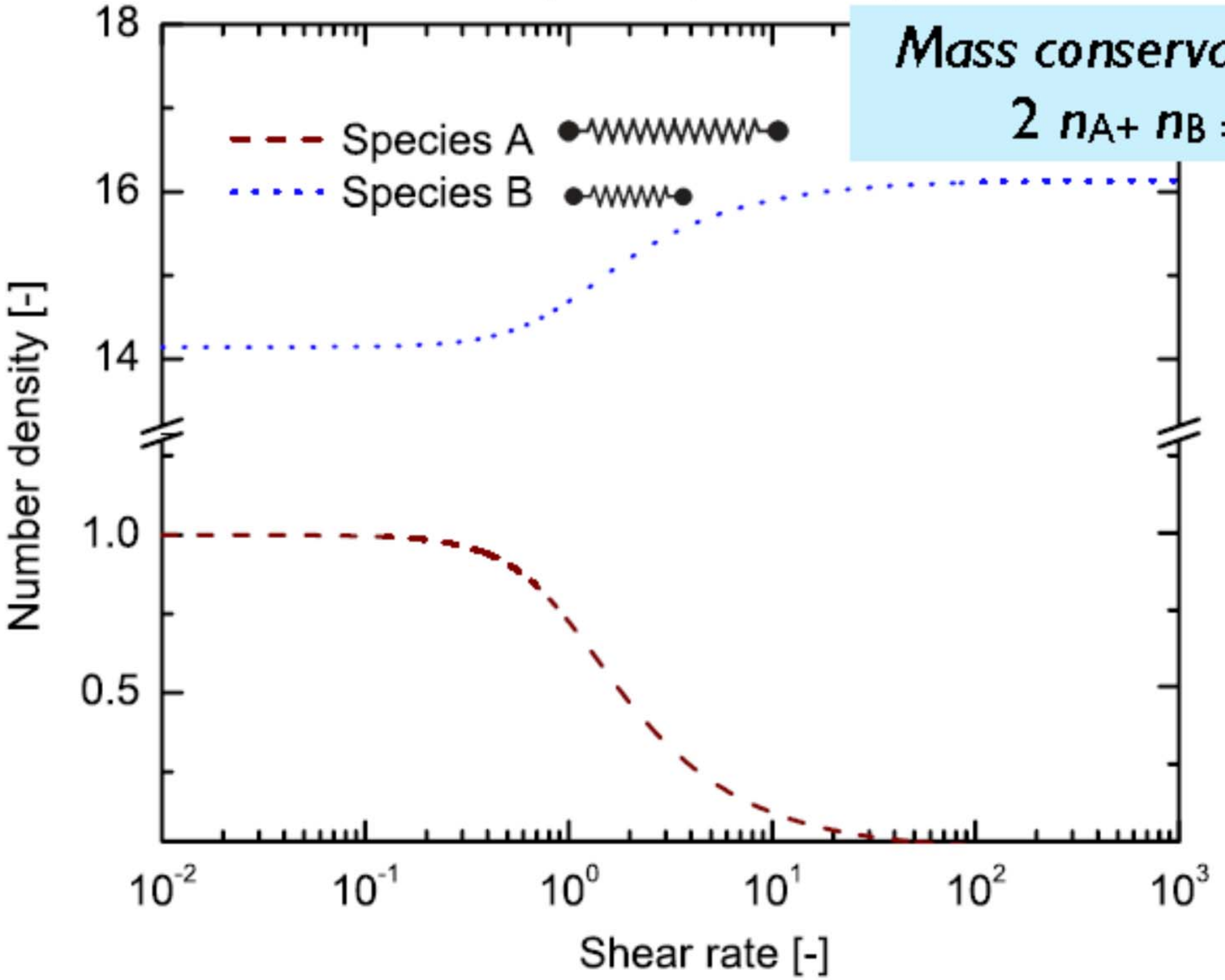
Parameters: $\beta = 7 \times 10^{-5}\,;\, \varepsilon = 10^{-4}\,;\, \widetilde{c}_{\mathrm{Aeq}} = 1\,;\, \widetilde{c}_{\mathrm{Beq}} = 10^{-2}$



Non-monotone stress-stain relationship!

Homogeneous Shear Flow Predictions -2

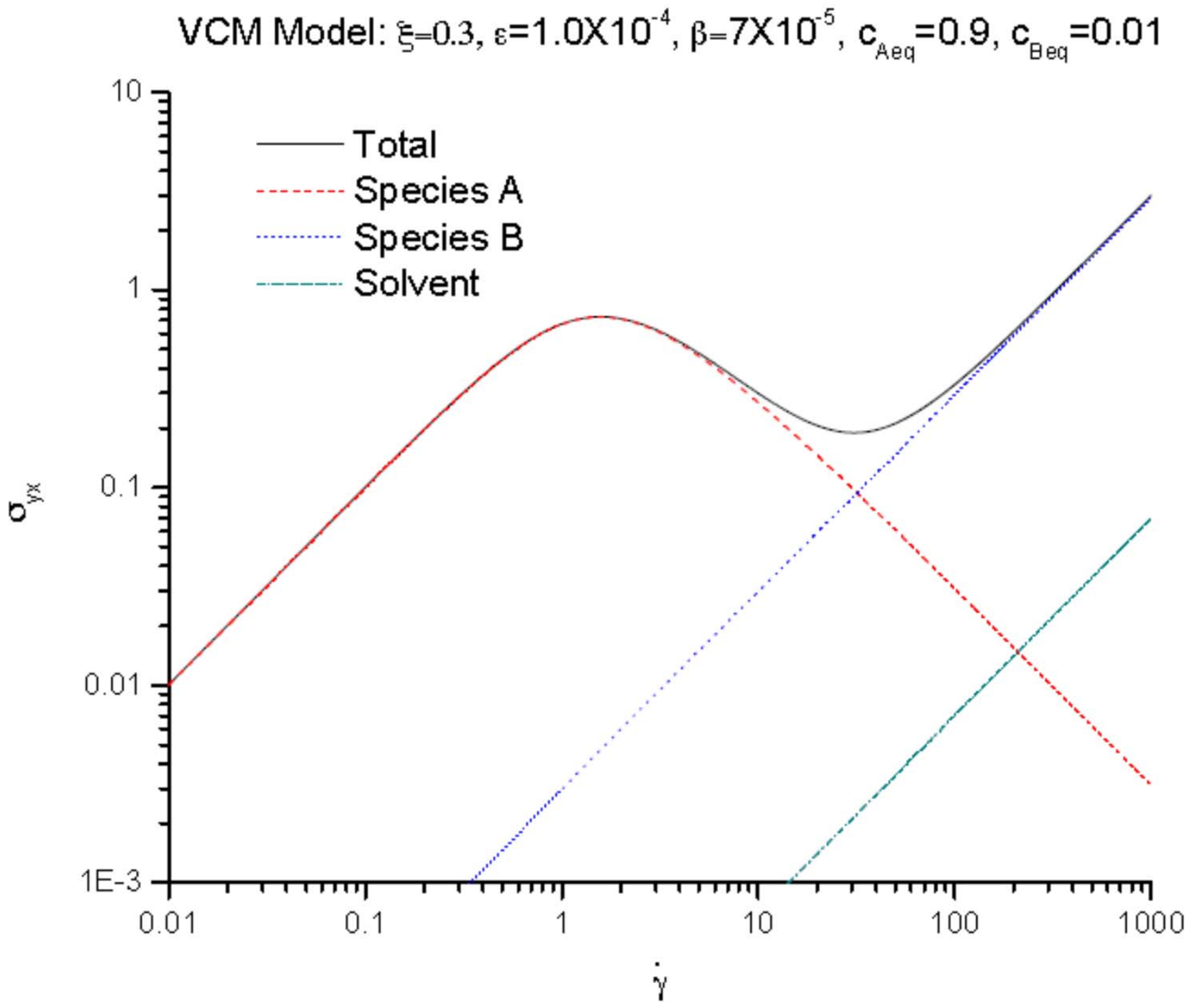
Parameters: $\beta = 7 \times 10^{-5}\,;\, \varepsilon = 10^{-4}\,;\, \widetilde{c}_{\mathrm{Aeq}} = 1\,;\, \widetilde{c}_{\mathrm{Beq}} = 10^{-2}$



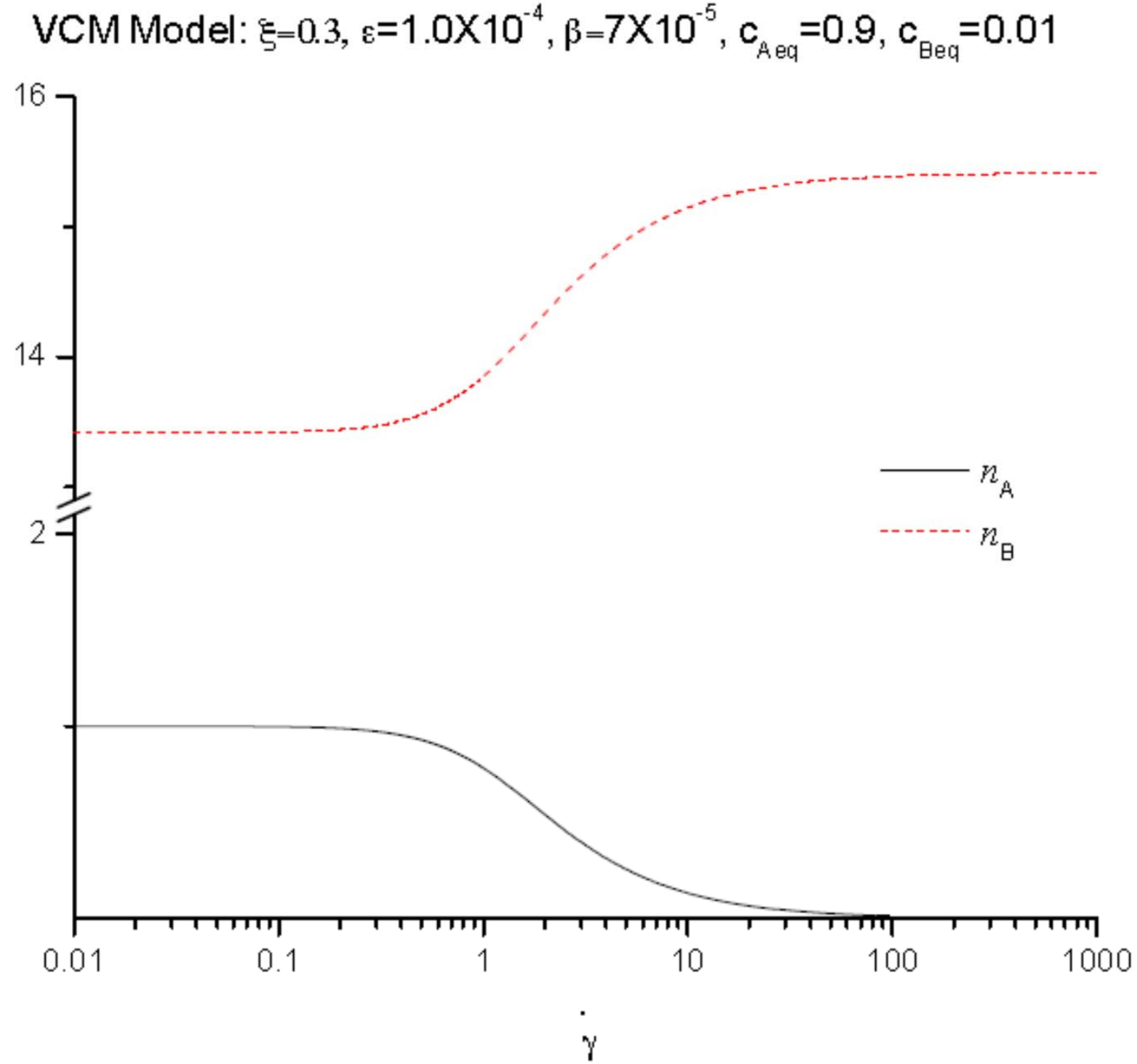
Mass conservation requires

$2\,n_A + n_B = \text{const.}$

Comparison Against the VCM Model - 1



Comparison Against the VCM Model - 2



Three-Species Model

Non-dimensionalization

Time: $\tilde{t} = t/\lambda_{\mathrm{eff}}$ Length: $\tilde{x}_\alpha = x_\alpha/H$ Pressure: $\tilde{p} = p/G_0$

Number density: $\tilde{n}_k = n_k/n_{\mathrm{Aeq}}$ $(k = \mathrm{A, B, C})$

Conformation: $\tilde{c}^k_{\alpha\beta} = (K_\mathrm{A}/(k_\mathrm{B}T)\, c^k_{\alpha\beta}$ $(k = \mathrm{A, B, C})$

Stress: $\tilde{\sigma}^k_{\alpha\beta} = \sigma^k_{\alpha\beta}/G_0$ $(k = \mathrm{A, B, C, solvent})$

Dimensionless numbers

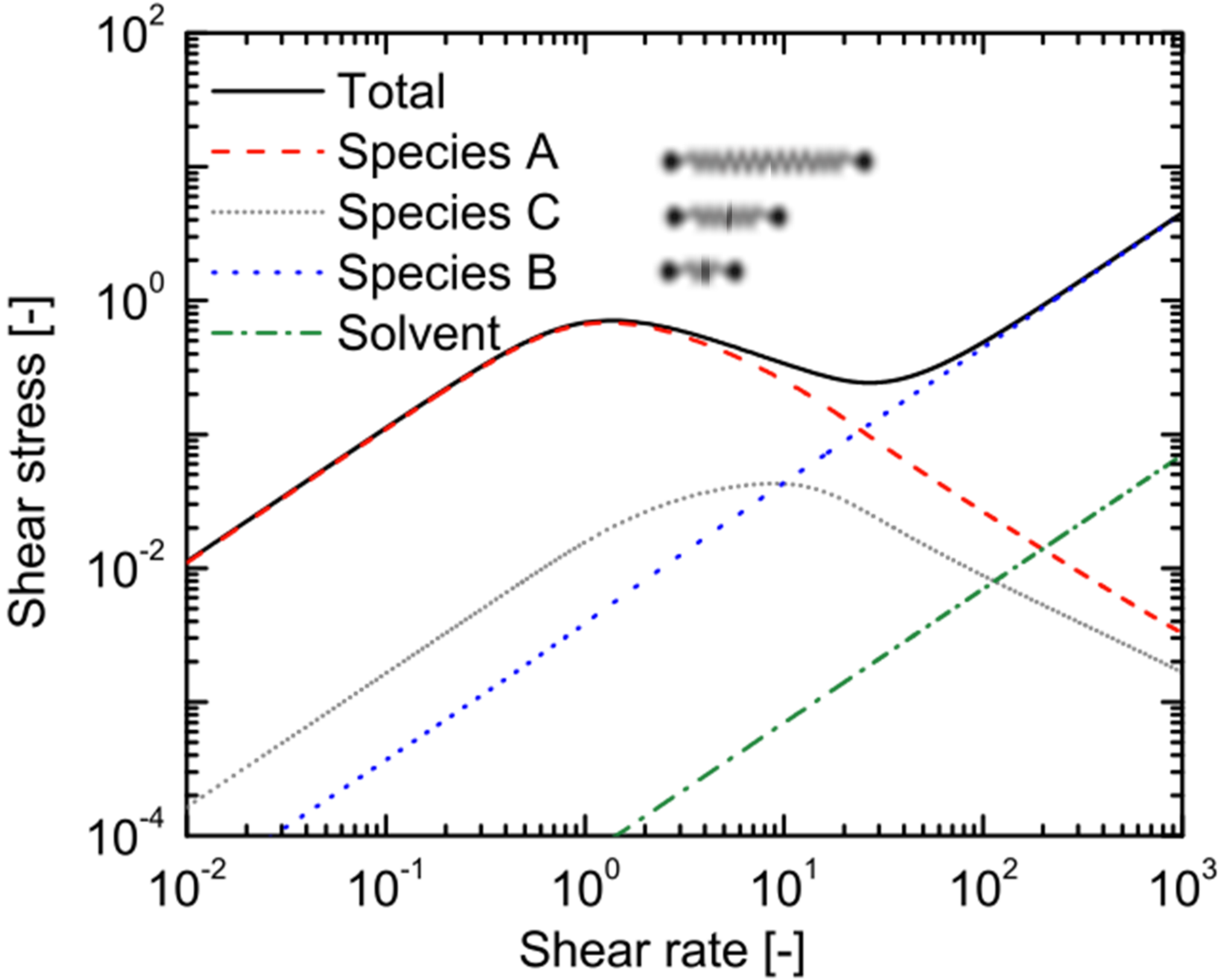
Viscosity ratio: $\beta = \eta_s/\eta_0 = 7 \times 10^{-5}$

Ratios of relaxation times: $\varepsilon = \lambda_\mathrm{B}/\lambda_\mathrm{A} = 10^{-4}$ $\zeta = \lambda_\mathrm{C}/\lambda_\mathrm{A} = 0.01$

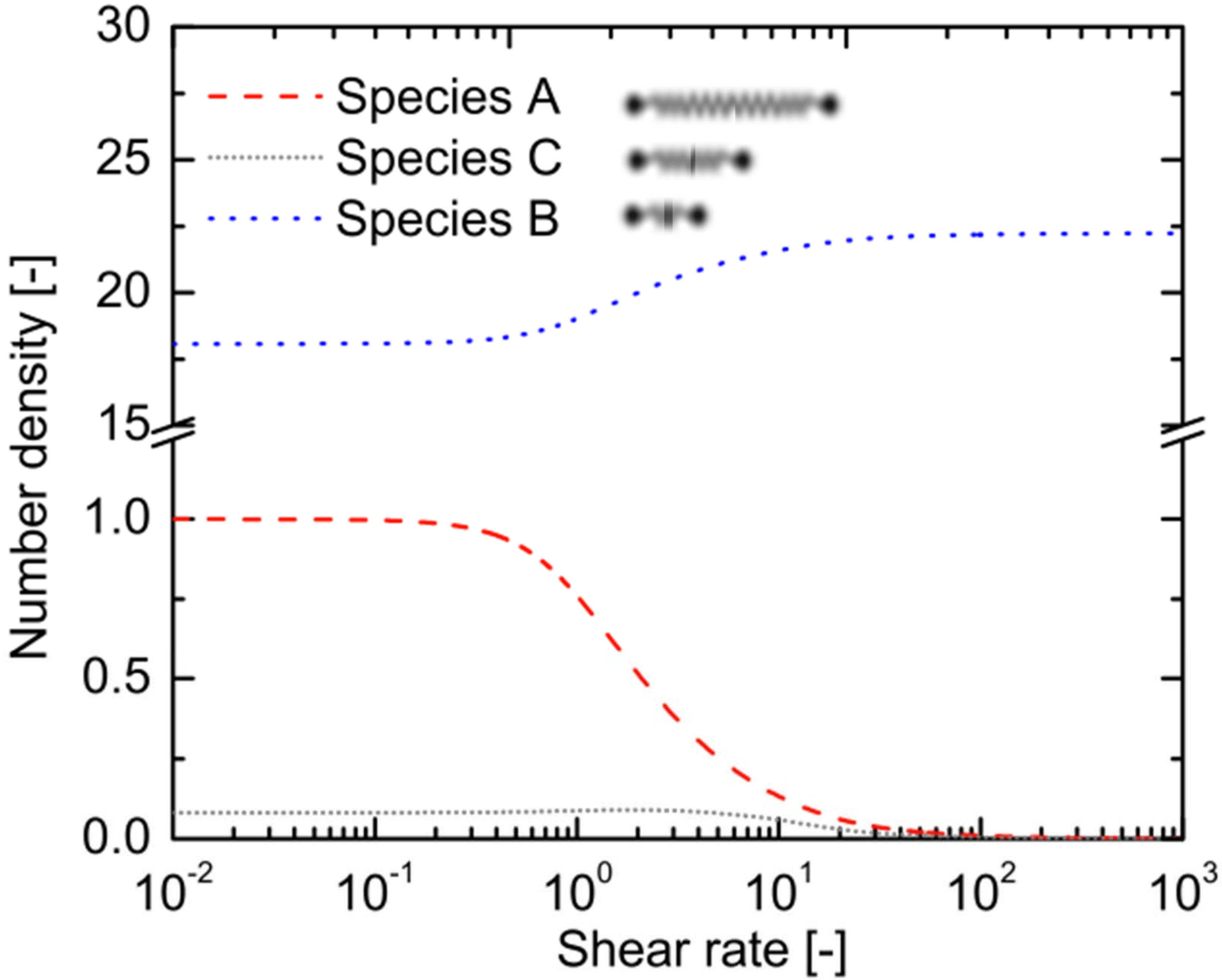
Reaction rates: $\tilde{c}_{\mathrm{Aeq},1} = \lambda_\mathrm{A} c_{\mathrm{Aeq},1} = 1$ $\tilde{c}_{\mathrm{Beq},2} = \lambda_\mathrm{A} c_{\mathrm{Beq},2} = 0.01$

$\tilde{c}_{\mathrm{Ceq},1} = \lambda_\mathrm{A} c_{\mathrm{Ceq},1} = 300$ $\tilde{c}_{\mathrm{Ceq},2} = \lambda_\mathrm{A} c_{\mathrm{Ceq},2} = 20$

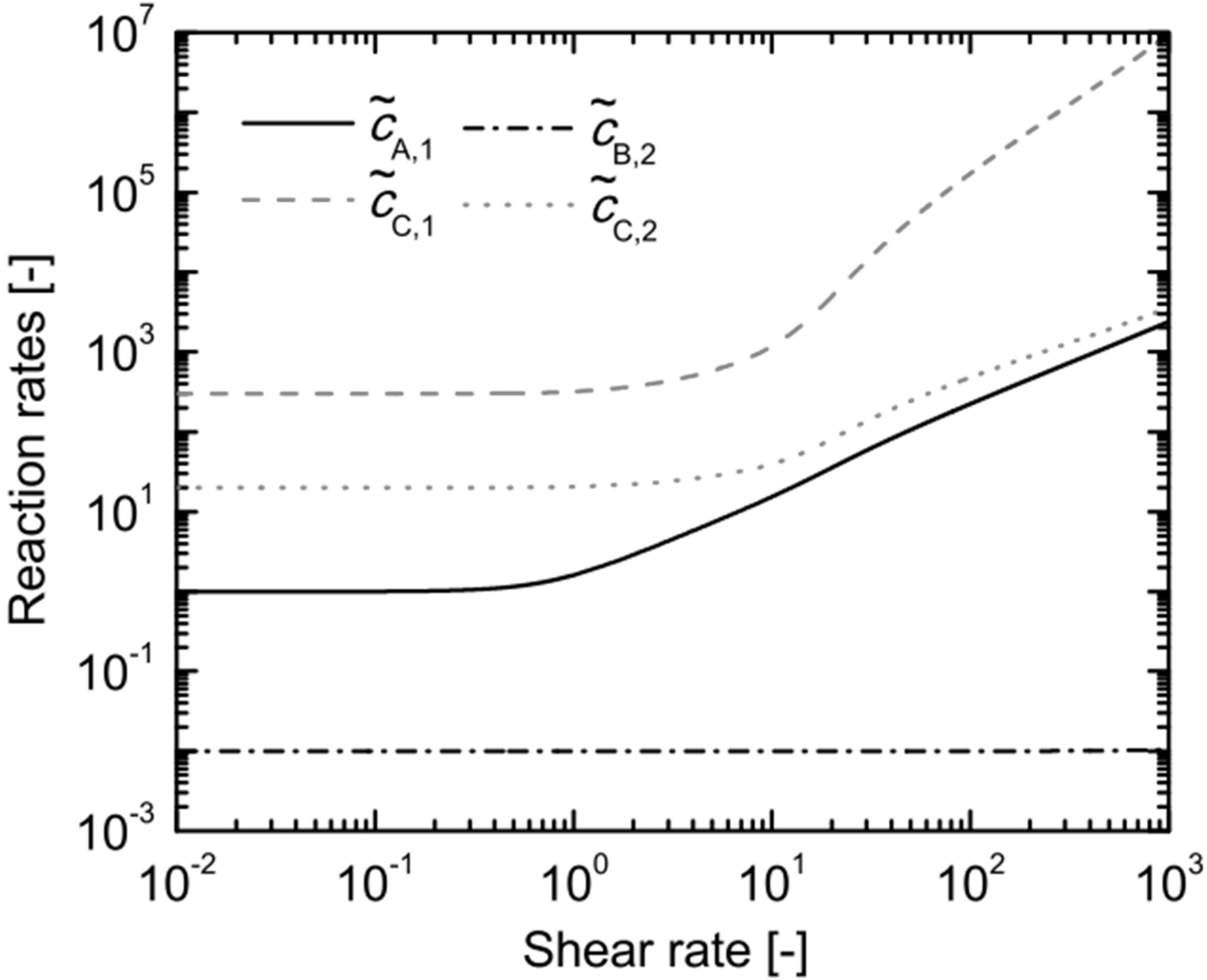
Three-Species Model: Planar Couette Flow



Three-Species Model: Planar Couette Flow



Three-Species Model: Planar Couette Flow



Conclusions

- We have corrected and significantly extended the description within NET that first appeared in our previous work [Beris and Edwards, 1994] of chemical reactions taking into account momentum and (for systems with internal structure) conformation transfers during each elementary reaction

- The new description allows for reaction rates that are conformation-dependent:
  - This can explain some very recent experiments on DNA scission under extension [Muller et al., ICR Lisbon, 2012]
  - The new description has been applied to the modeling of a system of concentrated rodlike micelles:
    - The new model produces very similar, non-monotonic shear stress vs. shear rate, predictions for homogeneous shear flows, while being thermodynamically consistent and requiring fewer parameters
    - The new model can be easily extended to more physically realistic situations (for example, allowing for a third species)

- Future work: Extension of the model to nonhomogeneous flows, along the lines of a multifluid approach in order to simulate shear-banding phenomena.

Acknowledgments

Prof. Norman J. Wagner (UD, C&B Engineering)

Prof. Hans Christian Oettinger (ETH, Zurich)

Additional Slides

Dimensional Two-Species Model

Reaction:

$$A \underset{c_{\mathrm{B}}}{\overset{c_{\mathrm{A}}}{\rightleftharpoons}} 2B$$

Dimensional model equations:

$$\frac{\partial n_{\mathrm{A}}}{\partial t} = -\nabla_\alpha \left(v_\alpha n_{\mathrm{A}}\right) - c_{\mathrm{A}} n_{\mathrm{A}} + \frac{1}{2} c_{\mathrm{B}} n_{\mathrm{B}}^2$$

$$\frac{\partial n_{\mathrm{B}}}{\partial t} = -\nabla_\alpha \left(v_\alpha n_{\mathrm{B}}\right) + 2 c_{\mathrm{A}} n_{\mathrm{A}} - c_{\mathrm{B}} n_{\mathrm{B}}^2$$

$$\rho \frac{\partial v_\alpha}{\partial t} = -\rho v_\beta \nabla_\beta v_\alpha - \nabla_\alpha p + \nabla_\beta \sigma_{\alpha\beta}$$

$$\frac{\partial C^{\mathrm{A}}_{\alpha\beta}}{\partial t} = -\nabla_\gamma \left(v_\gamma C^{\mathrm{A}}_{\alpha\beta}\right) + C^{\mathrm{A}}_{\gamma\alpha} \nabla_\gamma v_\beta + C^{\mathrm{A}}_{\gamma\beta} \nabla_\gamma v_\alpha - \frac{1}{\lambda_{\mathrm{A}}} \left(C^{\mathrm{A}}_{\alpha\beta} - \frac{n_{\mathrm{A}} k_{\mathrm{B}} T}{K_{\mathrm{A}}} \delta_{\alpha\beta} \right) - c_{\mathrm{A}} C^{\mathrm{A}}_{\alpha\beta} + c_{\mathrm{B}} n_{\mathrm{B}} C^{\mathrm{B}}_{\alpha\beta}$$

$$\frac{\partial C^{\mathrm{B}}_{\alpha\beta}}{\partial t} = -\nabla_\gamma \left(v_\gamma C^{\mathrm{B}}_{\alpha\beta}\right) + C^{\mathrm{B}}_{\gamma\alpha} \nabla_\gamma v_\beta + C^{\mathrm{B}}_{\gamma\beta} \nabla_\gamma v_\alpha - \frac{1}{\lambda_{\mathrm{B}}} \left(C^{\mathrm{B}}_{\alpha\beta} - \frac{n_{\mathrm{B}} k_{\mathrm{B}} T}{K_{\mathrm{B}}} \delta_{\alpha\beta} \right) + c_{\mathrm{A}} C^{\mathrm{A}}_{\alpha\beta} - c_{\mathrm{B}} n_{\mathrm{B}} C^{\mathrm{B}}_{\alpha\beta}$$

$$\sigma_{\alpha\beta} = \sigma^{\mathrm{A}}_{\alpha\beta} + \sigma^{\mathrm{B}}_{\alpha\beta} + \sigma^{\mathrm{s}}_{\alpha\beta}$$

$$\sigma^{\mathrm{A}}_{\alpha\beta} = K_{\mathrm{A}} C^{\mathrm{A}}_{\alpha\beta} - n_{\mathrm{A}} k_{\mathrm{B}} T \delta_{\alpha\beta}$$

$$\sigma^{\mathrm{B}}_{\alpha\beta} = K_{\mathrm{B}} C^{\mathrm{B}}_{\alpha\beta} - n_{\mathrm{B}} k_{\mathrm{B}} T \delta_{\alpha\beta}$$

$$\sigma^{\mathrm{s}}_{\alpha\beta} = \eta_{\mathrm{s}} \left(\nabla_\alpha v_\beta + \nabla_\beta v_\alpha\right)$$

$$c_{\mathrm{A}} = c_{\mathrm{Aeq}} \frac{\exp\left(\frac{\mathrm{tr}\,\sigma^{\mathrm{A}}}{2 n_{\mathrm{A}} k_{\mathrm{B}} T}\right)}{\sqrt{\det\left(\frac{K_{\mathrm{A}} \mathrm{C}^{\mathrm{A}}}{n_{\mathrm{A}} k_{\mathrm{B}} T}\right)}}$$

$$c_{\mathrm{B}} = c_{\mathrm{Beq}} \frac{\exp\left(\frac{\mathrm{tr}\,\sigma^{\mathrm{B}}}{n_{\mathrm{B}} k_{\mathrm{B}} T}\right)}{\det\left(\frac{K_{\mathrm{B}} \mathrm{C}^{\mathrm{B}}}{n_{\mathrm{B}} k_{\mathrm{B}} T}\right)}$$

Dimensional Three-Species Model

Reactions:

$$A \underset{c_{\mathrm{C},1}}{\overset{c_{\mathrm{A},1}}{\rightleftharpoons}} 2C$$

$$C \underset{c_{\mathrm{B},2}}{\overset{c_{\mathrm{C},2}}{\rightleftharpoons}} 2B$$

Dimensional model equations:

$$\frac{\partial n_{\mathrm{A}}}{\partial t} = -\nabla_\alpha \left(v_\alpha n_{\mathrm{A}}\right) - c_{\mathrm{A},1} n_{\mathrm{A}} + \frac{1}{2} c_{\mathrm{C},1} n_{\mathrm{C}}^2$$

$$\frac{\partial n_{\mathrm{C}}}{\partial t} = -\nabla_\alpha \left(v_\alpha n_{\mathrm{C}}\right) + 2c_{\mathrm{A},1} n_{\mathrm{A}} - c_{\mathrm{C},1} n_{\mathrm{C}}^2 - c_{\mathrm{C},2} n_{\mathrm{C}} + \frac{1}{2} c_{\mathrm{B},2} n_{\mathrm{B}}^2$$

$$\frac{\partial n_{\mathrm{B}}}{\partial t} = -\nabla_\alpha \left(v_\alpha n_{\mathrm{B}}\right) + 2c_{\mathrm{C},2} n_{\mathrm{C}} - c_{\mathrm{B},2} n_{\mathrm{B}}^2$$

$$\rho \frac{\partial v_\alpha}{\partial t} = -\rho v_\beta \nabla_\beta v_\alpha - \nabla_\alpha p + \nabla_\beta \sigma_{\alpha\beta}$$

$$\frac{\partial C^{\mathrm{A}}_{\alpha\beta}}{\partial t} = -\nabla_\gamma \left(v_\gamma C^{\mathrm{A}}_{\alpha\beta}\right) + C^{\mathrm{A}}_{\gamma\alpha} \nabla_\gamma v_\beta + C^{\mathrm{A}}_{\gamma\beta} \nabla_\gamma v_\alpha - \frac{1}{\lambda_{\mathrm{A}}} \left(C^{\mathrm{A}}_{\alpha\beta} - \frac{n_{\mathrm{A}} k_{\mathrm{B}} T}{K_{\mathrm{A}}} \delta_{\alpha\beta} \right) - c_{\mathrm{A},1} C^{\mathrm{A}}_{\alpha\beta} + c_{\mathrm{C},1} n_{\mathrm{C}} C^{\mathrm{C}}_{\alpha\beta}$$

$$\frac{\partial C^{\mathrm{C}}_{\alpha\beta}}{\partial t} = -\nabla_\gamma \left(v_\gamma C^{\mathrm{C}}_{\alpha\beta}\right) + C^{\mathrm{C}}_{\gamma\alpha} \nabla_\gamma v_\beta + C^{\mathrm{C}}_{\gamma\beta} \nabla_\gamma v_\alpha - \frac{1}{\lambda_{\mathrm{C}}} \left(C^{\mathrm{C}}_{\alpha\beta} - \frac{n_{\mathrm{C}} k_{\mathrm{B}} T}{K_{\mathrm{B}}} \delta_{\alpha\beta} \right) + c_{\mathrm{A},1} C^{\mathrm{A}}_{\alpha\beta} - c_{\mathrm{C},1} n_{\mathrm{C}} C^{\mathrm{C}}_{\alpha\beta} - c_{\mathrm{C},2} C^{\mathrm{C}}_{\alpha\beta} + c_{\mathrm{B},2} n_{\mathrm{B}} C^{\mathrm{B}}_{\alpha\beta}$$

$$\frac{\partial C^{\mathrm{B}}_{\alpha\beta}}{\partial t} = -\nabla_\gamma \left(v_\gamma C^{\mathrm{B}}_{\alpha\beta}\right) + C^{\mathrm{B}}_{\gamma\alpha} \nabla_\gamma v_\beta + C^{\mathrm{B}}_{\gamma\beta} \nabla_\gamma v_\alpha - \frac{1}{\lambda_{\mathrm{B}}} \left(C^{\mathrm{B}}_{\alpha\beta} - \frac{n_{\mathrm{B}} k_{\mathrm{B}} T}{K_{\mathrm{C}}} \delta_{\alpha\beta} \right) + c_{\mathrm{C},2} C^{\mathrm{C}}_{\alpha\beta} - c_{\mathrm{B},2} n_{\mathrm{B}} C^{\mathrm{B}}_{\alpha\beta}$$

$$\sigma_{\alpha\beta} = \sigma^{\mathrm{A}}_{\alpha\beta} + \sigma^{\mathrm{C}}_{\alpha\beta} + \sigma^{\mathrm{B}}_{\alpha\beta} + \sigma^{\mathrm{s}}_{\alpha\beta}$$

$$\sigma^{\mathrm{A}}_{\alpha\beta} = K_{\mathrm{A}} C^{\mathrm{A}}_{\alpha\beta} - n_{\mathrm{A}} k_{\mathrm{B}} T \delta_{\alpha\beta}$$

$$\sigma^{\mathrm{C}}_{\alpha\beta} = K_{\mathrm{C}} C^{\mathrm{C}}_{\alpha\beta} - n_{\mathrm{C}} k_{\mathrm{B}} T \delta_{\alpha\beta}$$

$$\sigma^{\mathrm{B}}_{\alpha\beta} = K_{\mathrm{B}} C^{\mathrm{B}}_{\alpha\beta} - n_{\mathrm{B}} k_{\mathrm{B}} T \delta_{\alpha\beta}$$

$$\sigma^{\mathrm{s}}_{\alpha\beta} = \eta_s \left(\nabla_\alpha v_\beta + \nabla_\beta v_\alpha \right)$$

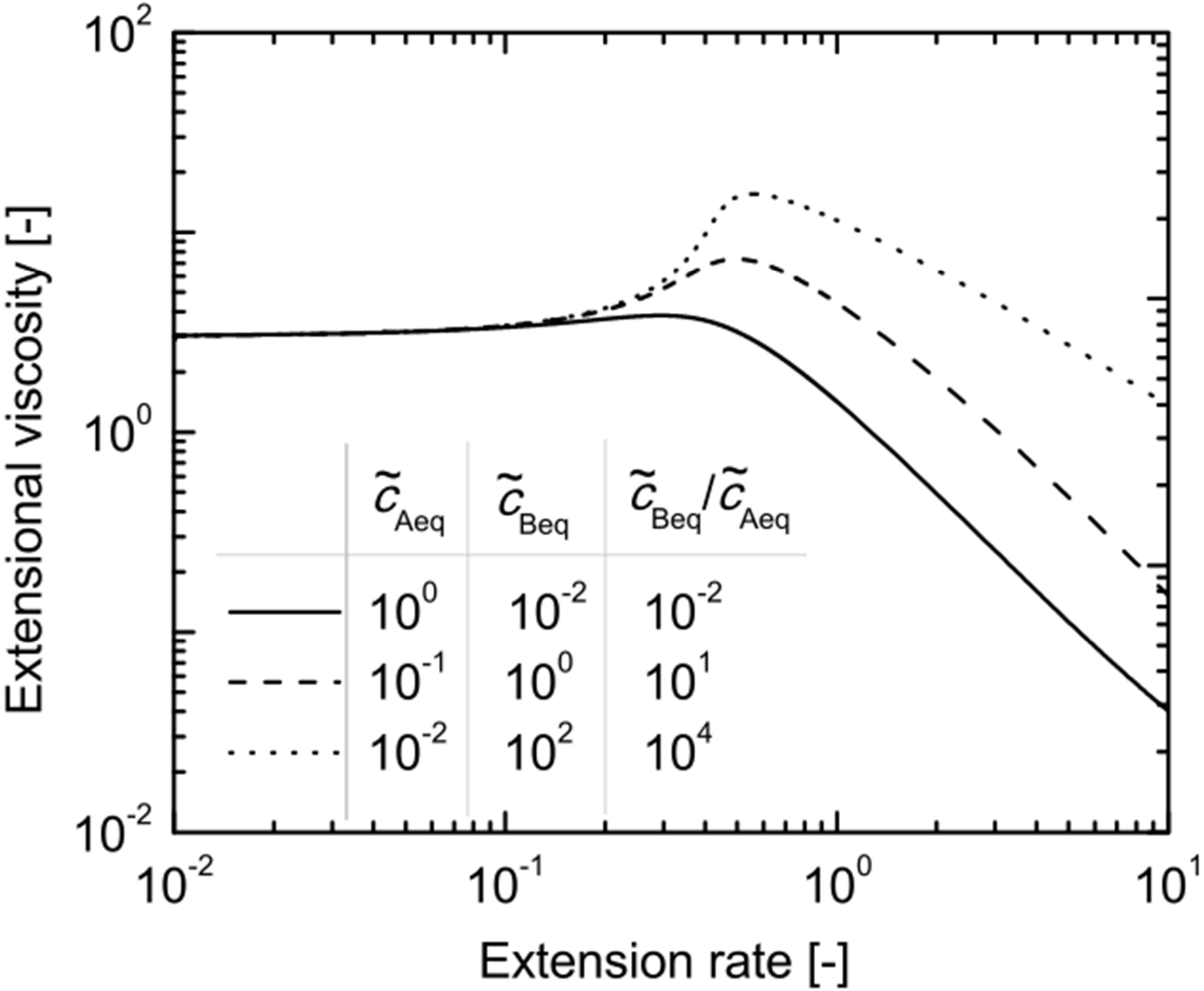
$$c_{\mathrm{A},1} = c_{\mathrm{Aeq},1} \frac{\exp\left(\frac{\mathrm{tr}\sigma^{A}}{2 n_{\mathrm{A}} k_{\mathrm{B}} T} \right)}{\sqrt{\det\left(\frac{K_{\mathrm{A}} C^{A}}{n_{\mathrm{A}} k_{\mathrm{B}} T} \right)}}$$

$$c_{\mathrm{C},1} = c_{\mathrm{Ceq},1} \frac{\exp\left(\frac{\mathrm{tr}\sigma^{C}}{n_{\mathrm{C}} k_{\mathrm{B}} T} \right)}{\det\left(\frac{K_{\mathrm{C}} C^{C}}{n_{\mathrm{C}} k_{\mathrm{B}} T} \right)}$$

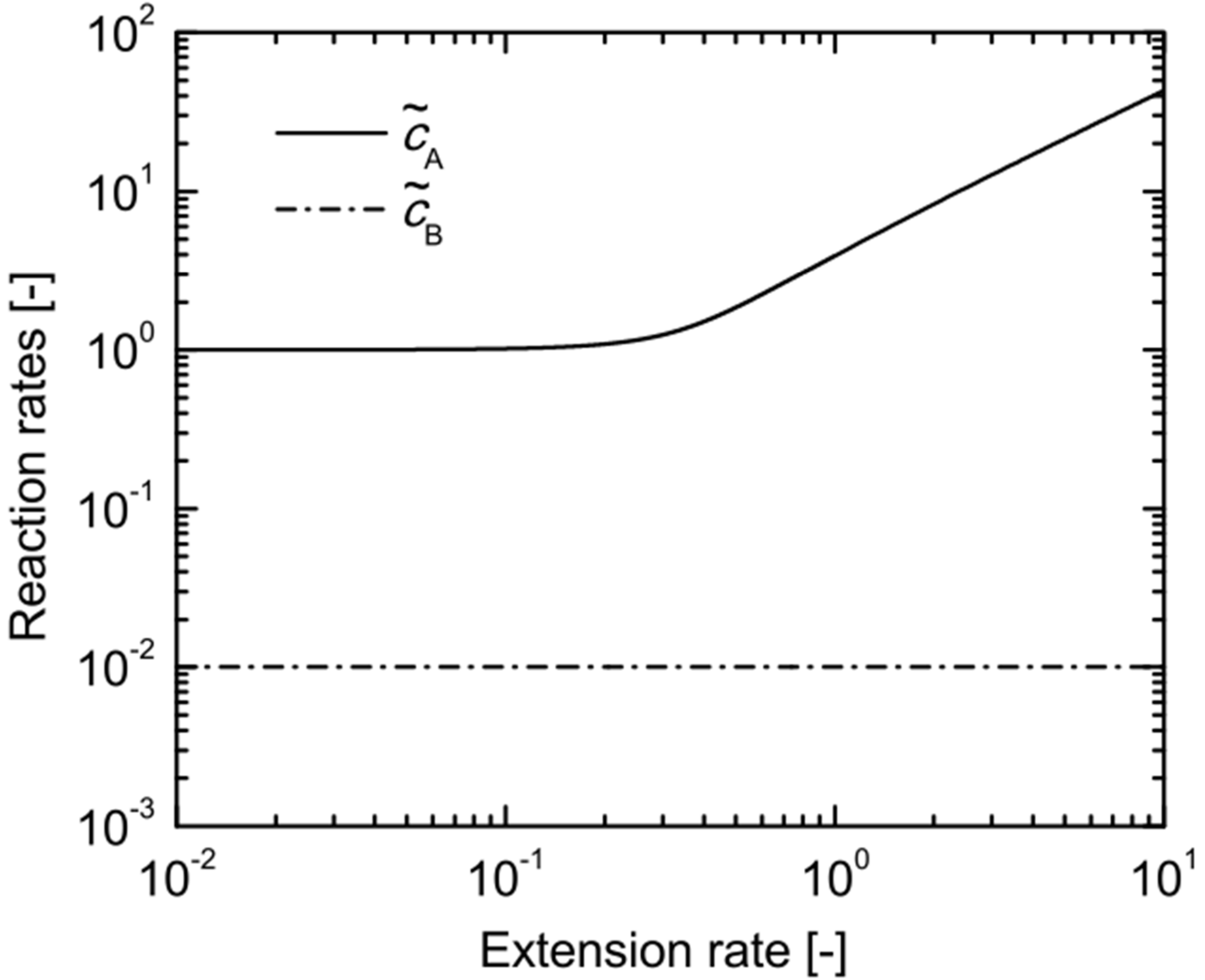
$$c_{\mathrm{C},2} = c_{\mathrm{Ceq},2} \frac{\exp\left(\frac{\mathrm{tr}\sigma^{C}}{2 n_{\mathrm{C}} k_{\mathrm{B}} T} \right)}{\sqrt{\det\left(\frac{K_{\mathrm{C}} C^{C}}{n_{\mathrm{C}} k_{\mathrm{B}} T} \right)}}$$

$$c_{\mathrm{B},2} = c_{\mathrm{Beq},2} \frac{\exp\left(\frac{\mathrm{tr}\sigma^{B}}{n_{\mathrm{B}} k_{\mathrm{B}} T} \right)}{\det\left(\frac{K_{\mathrm{B}} C^{B}}{n_{\mathrm{B}} k_{\mathrm{B}} T} \right)}$$

Two-Species Model: Uniaxial Extension

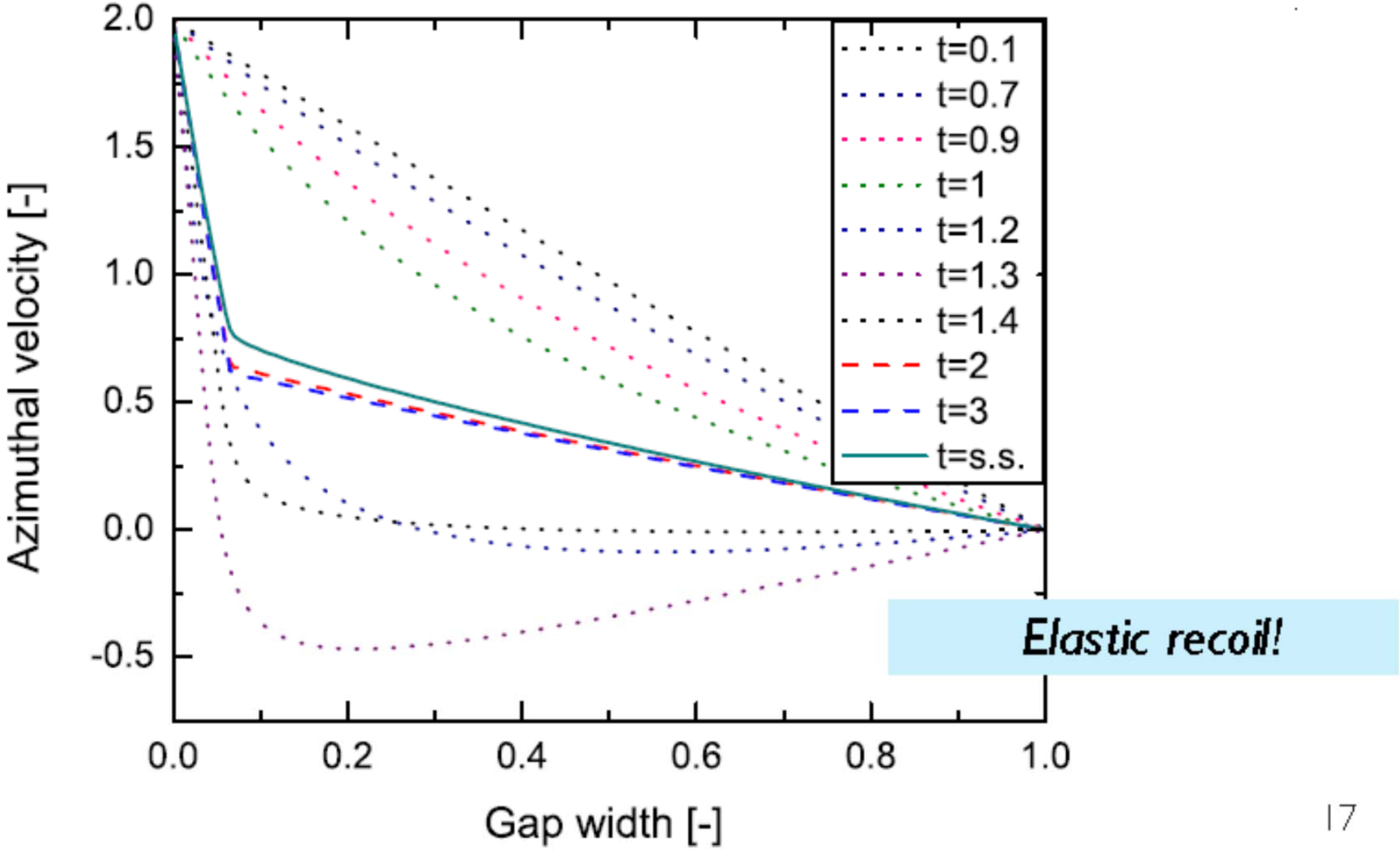


Two-Species Model: Uniaxial Extension



Cylindrical Couette Flow*: Shear Banding!

Parameters: $Re = 0;\ De = 2;\ \beta = 6.8 \times 10^{-5};\ \varepsilon = 4.5 \times 10^{-4};$
$\widetilde{c}_{\mathrm{Aeq}} = 4.7;\ \widetilde{c}_{\mathrm{Beq}} = 7.3$



* Preliminary results based on simplified diffusion model