# Modeling of Extrusion Film Casting (EFC) Process using Multi-mode UCM and PTT Constitutive Equations

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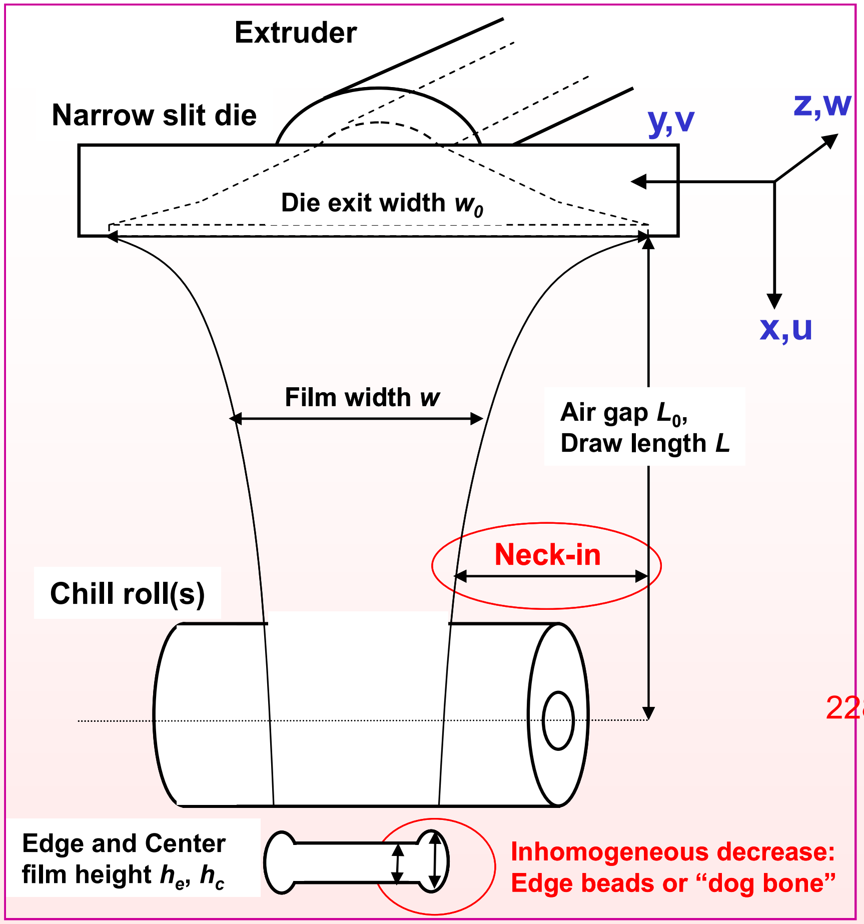
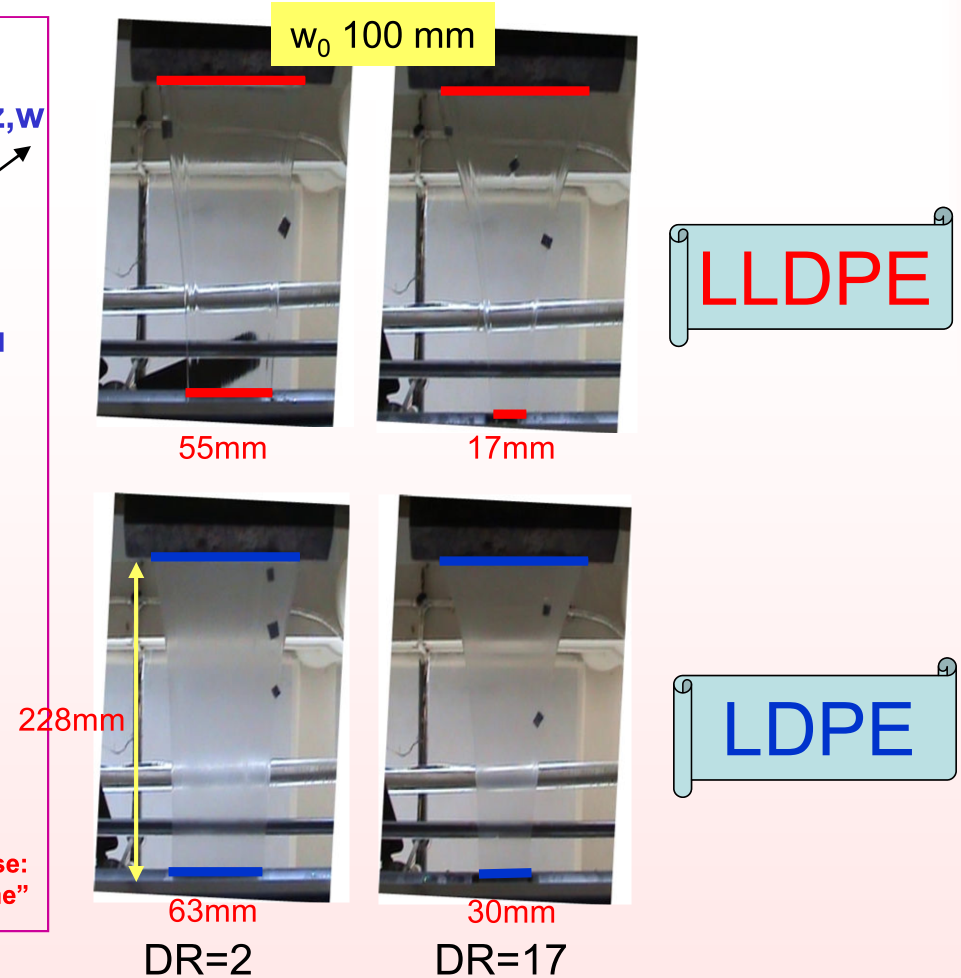
# Introduction




Objective: to study the effect of *polymer chain architecture* on *neck-in length and thickness distribution* of extrusion cast films using a combination of experiments and simulations.

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# Flow kinematics[2] and MM-UCM CE

***Float Glass Approximation[1]: u = u(x), v = y f(x), w= z g(x)***

$$\tilde{\tau}_{xx}^{i} + De^{i}\left\{\tilde{u}\frac{d\tilde{\tau}_{xx}^{i}}{d\tilde{x}} - 2\tilde{\tau}_{xx}^{i}\frac{d\tilde{u}}{d\tilde{x}}\right\} = 2E^{i}\frac{d\tilde{u}}{d\tilde{x}}$$

$$\tilde{\tau}_{yy}^{i} + De^{i}\left\{\tilde{u}\frac{d\tilde{\tau}_{yy}^{i}}{d\tilde{x}} - 2\tilde{\tau}_{yy}^{i}\frac{\tilde{u}}{\tilde{L}}\frac{d\tilde{L}}{d\tilde{x}}\right\} = 2E^{i}\frac{\tilde{u}}{\tilde{L}}\frac{d\tilde{L}}{d\tilde{x}}$$

$$\tilde{\tau}_{zz}^{i} + De^{i}\left\{\tilde{u}\frac{d\tilde{\tau}_{zz}^{i}}{d\tilde{x}} - 2\tilde{\tau}_{zz}^{i}\frac{\tilde{u}}{\tilde{e}}\frac{d\tilde{e}}{d\tilde{x}}\right\} = 2E^{i}\frac{\tilde{u}}{\tilde{e}}\frac{d\tilde{e}}{d\tilde{x}}$$

Obtained from MM-UCM after substituting velocity b.c.'s

$$\frac{d\tilde{L}}{d\tilde{x}} = -A\sqrt{\frac{\tilde{\tau}_{yy} - \tilde{\tau}_{zz}}{\tilde{\tau}_{xx} - \tilde{\tau}_{zz}}}$$

Boundary condition

$$\left(\tilde{\tau}_{xx} - \tilde{\tau}_{zz}\right)\tilde{L}\tilde{e} = 1$$

Force balance

$$\tilde{e}\tilde{L}\tilde{u} = 1$$

Mass balance

No. of unknowns is 6 : $\tilde{\tau}_{xx}^{i}$ $\tilde{\tau}_{yy}^{i}$ $\tilde{\tau}_{zz}^{i}$ $\tilde{L}$ $\tilde{e}$ $\tilde{u}$

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# Numerical Modeling using Matlab®

*Solving a system of coupled, non-linear ODE's*

$$\begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & -1 & 0 & 1 \\ \frac{e}{L} & \frac{e}{u} & 1 & 0 & 0 & 0 \\ 0 & -2De\tau_{xx}-2E & 0 & Deu & 0 & 0 \\ \left\{-2\tau_{yy}De\frac{u}{L}-2E\frac{u}{L}\right\} & 0 & 0 & 0 & Deu & 0 \\ 0 & \left\{-2\tau_{zz}De\frac{u}{e}-2E\frac{u}{e}\right\} & 0 & 0 & 0 & Deu \end{bmatrix} * \begin{bmatrix} \frac{dL}{dx} \\ \frac{du}{dx} \\ \frac{de}{dx} \\ \frac{d\tau_{xx}}{dx} \\ \frac{d\tau_{yy}}{dx} \\ \frac{d\tau_{zz}}{dx} \end{bmatrix} = \begin{bmatrix} -A\sqrt{\frac{\tau_{yy}-\tau_{zz}}{\tau_{xx}-\tau_{zz}}} \\ 0 \\ 0 \\ -\tau_{xx} \\ -\tau_{yy} \\ -\tau_{zz} \end{bmatrix}$$

1. Equations solved using stiff solver of MATLAB.
2. Newton's shooting method with an in built optimizer routine

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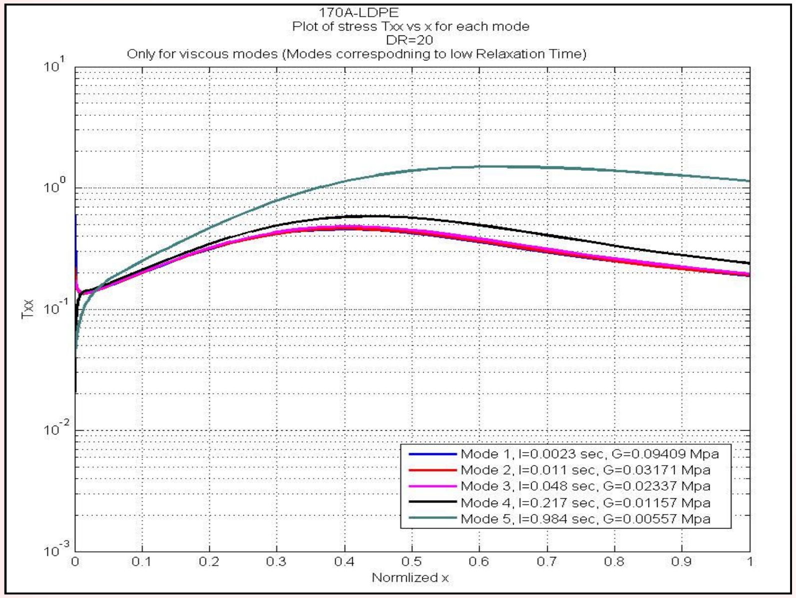
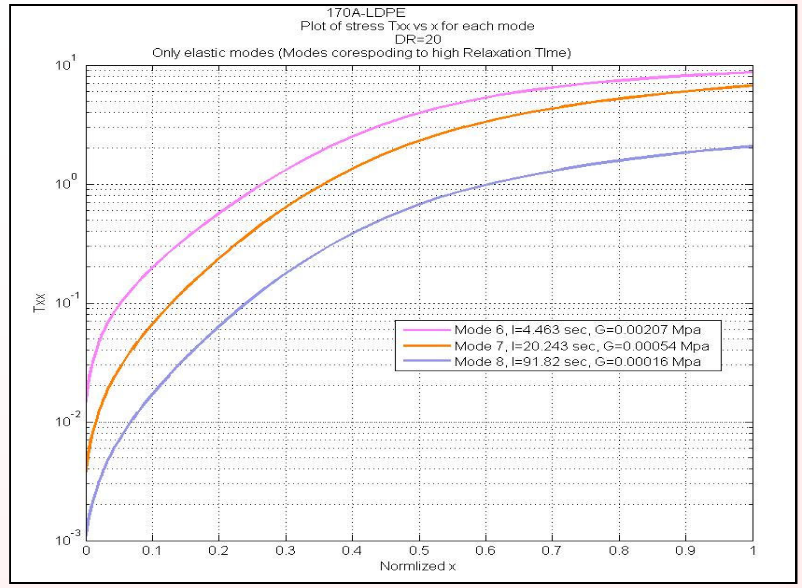
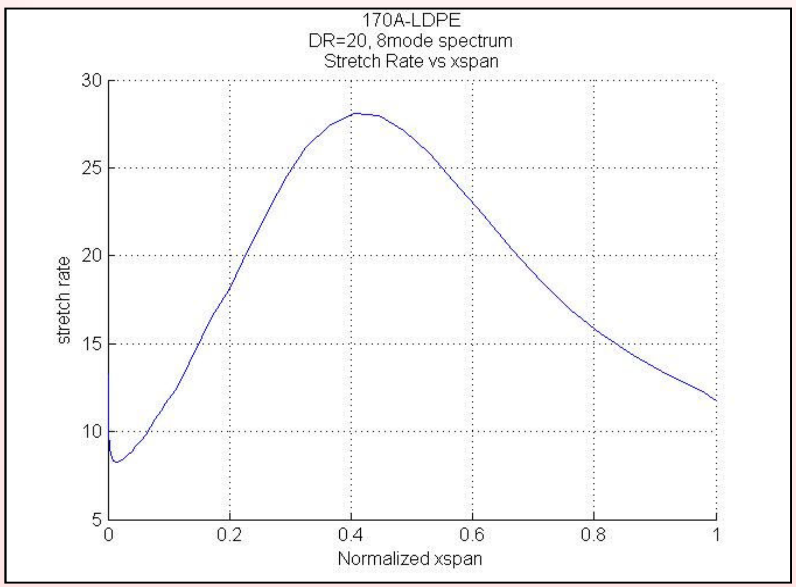
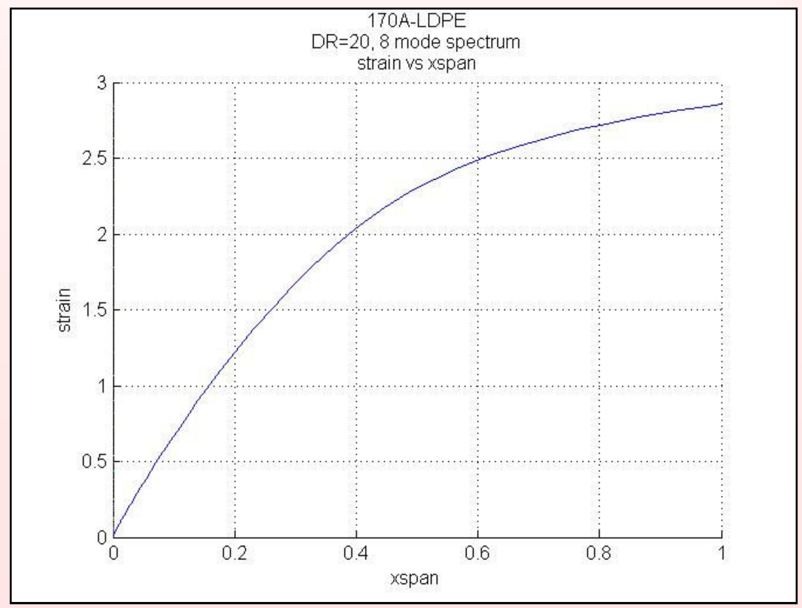
# Predictions using MM-UCM CE

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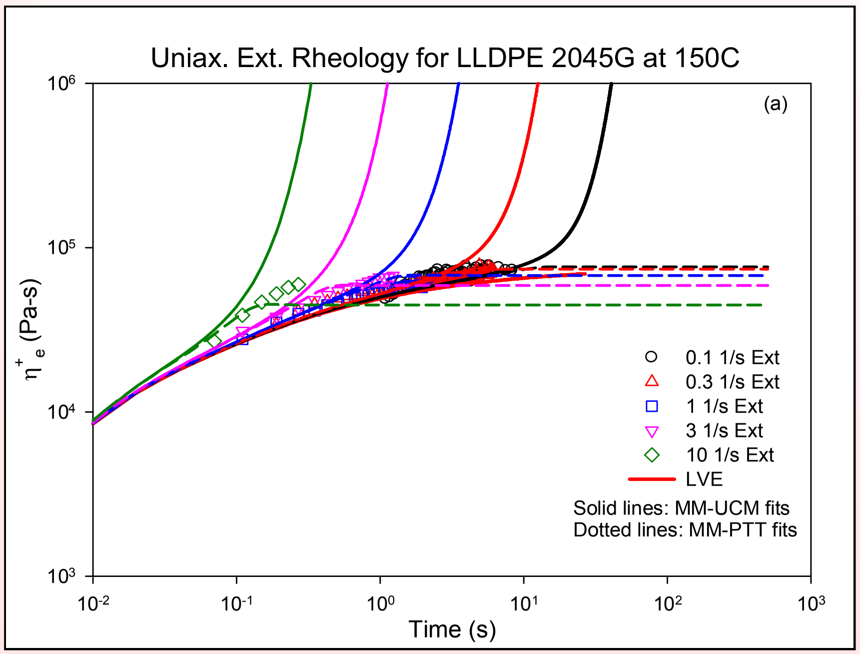
# Realistic CEs

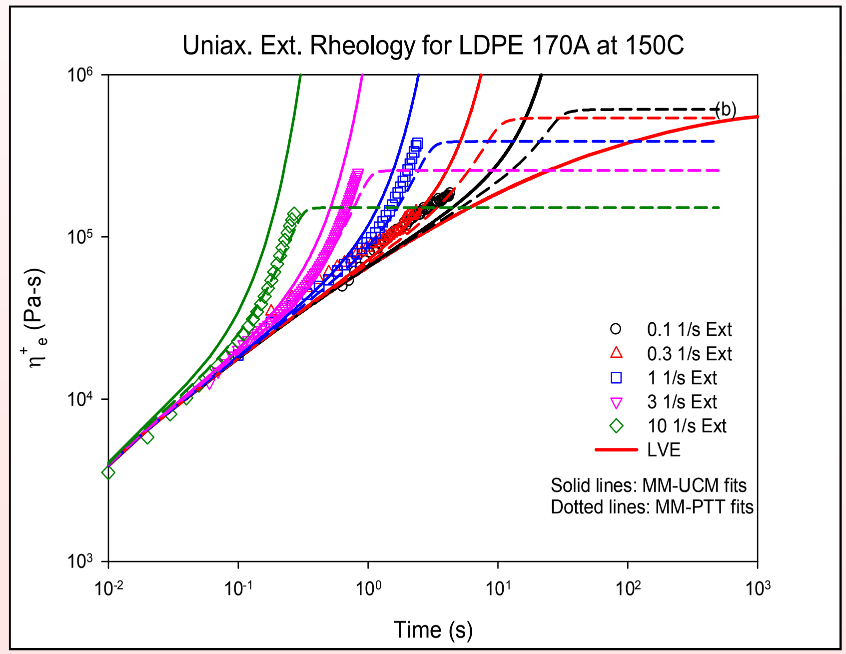
## *Phan Thein Tanner CE*

$$\sum_i \overset{\nabla}{\underline{\underline{\tau}}}{}^i \lambda^i + \sum_i \exp\left(\frac{\lambda^i \varepsilon}{G^i \lambda^i} \operatorname{tr}\left(\underline{\underline{\tau}}^i\right)\right)\underline{\underline{\tau}}^i + \sum_i \lambda^i \xi \left(\underline{\underline{2D}} \cdot \underline{\underline{\tau}}^i + \underline{\underline{\tau}}^i \cdot \underline{\underline{2D}}\right) = \sum_i G^i \lambda^i \left(\underline{\underline{2D}}\right)$$

$$\underline{\underline{2D}} = \left\{ \left(\nabla \underline{v}\right) + \left(\nabla \underline{v}\right)^T \right\}$$

and i goes from 1 to n where n are total number of modes of poly-disperse polymer

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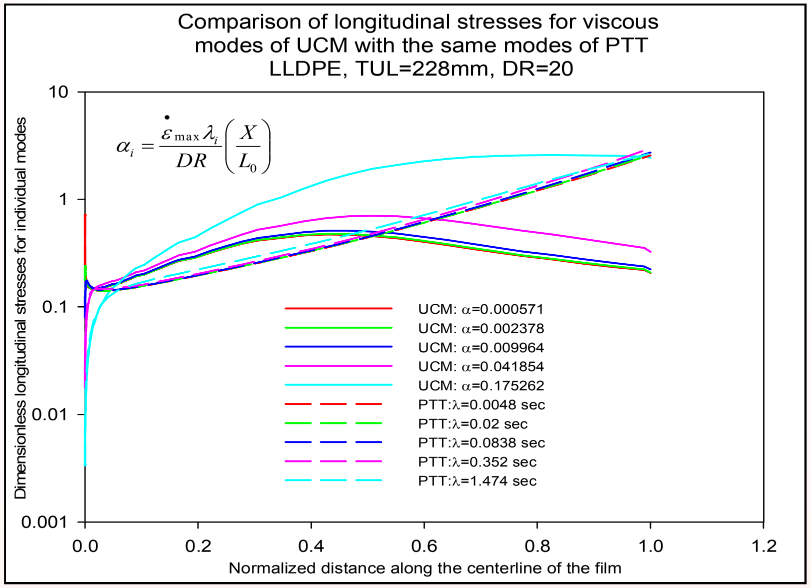
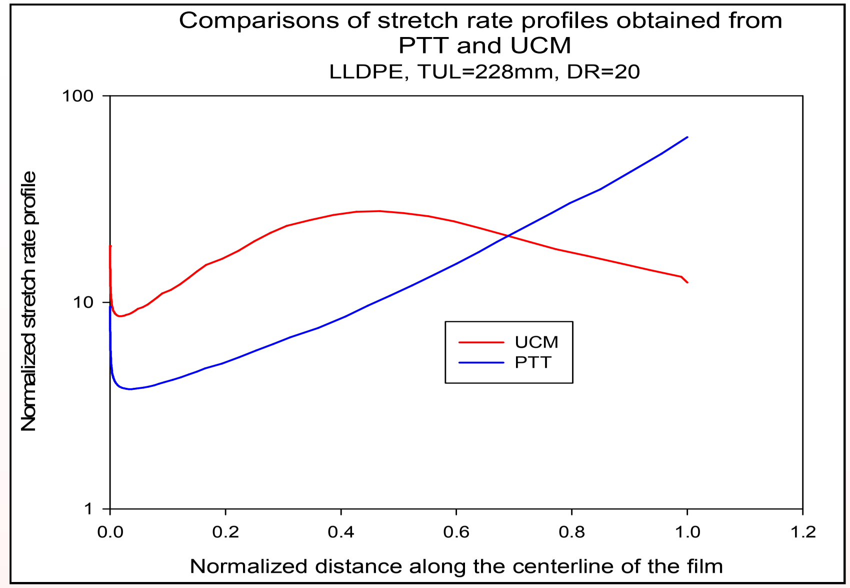
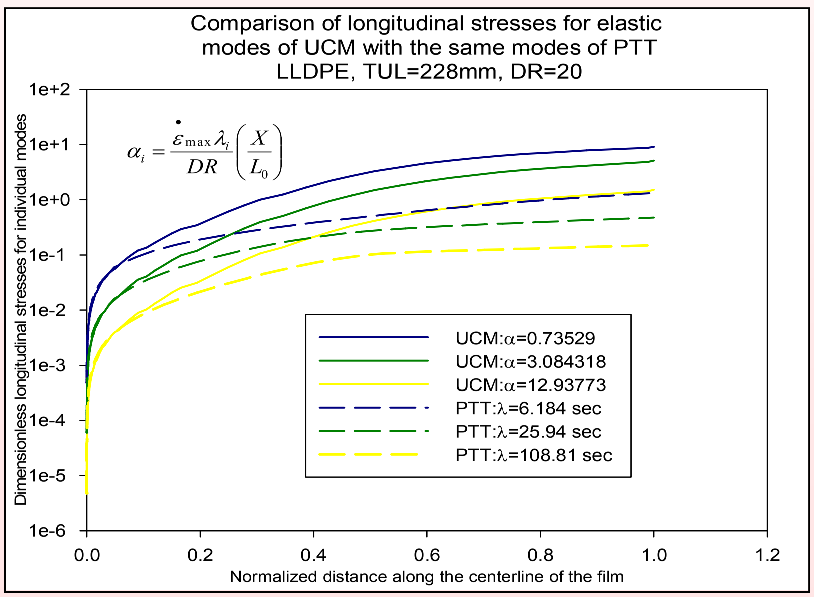
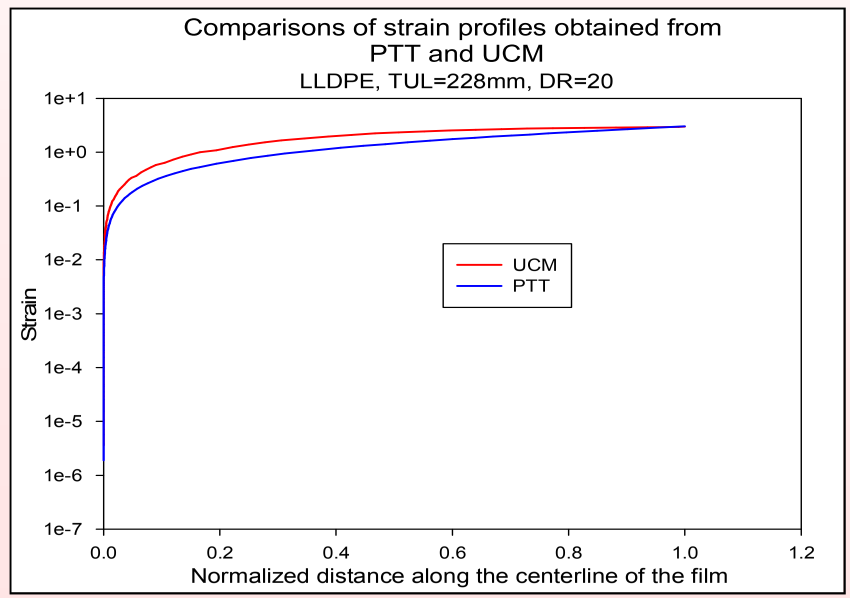
# PTT vs UCM: Relaxation mode stresses

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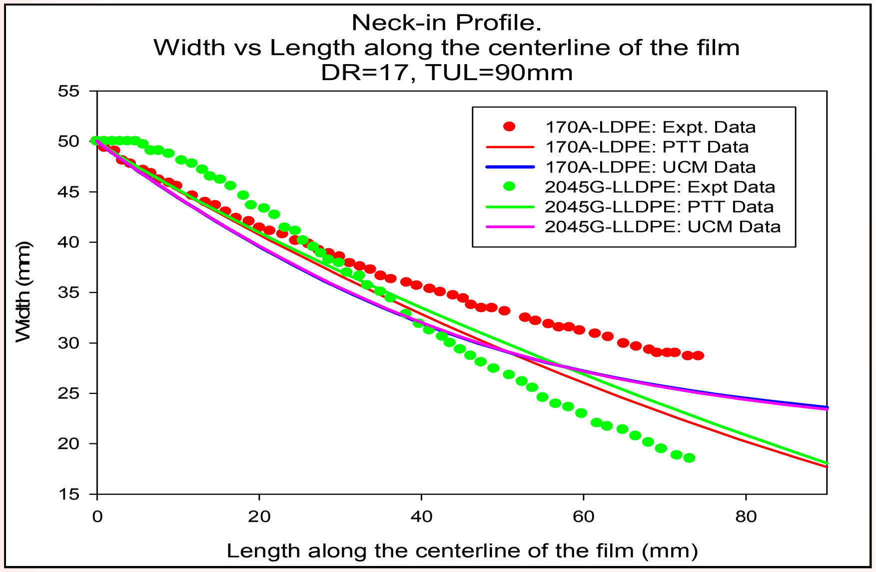
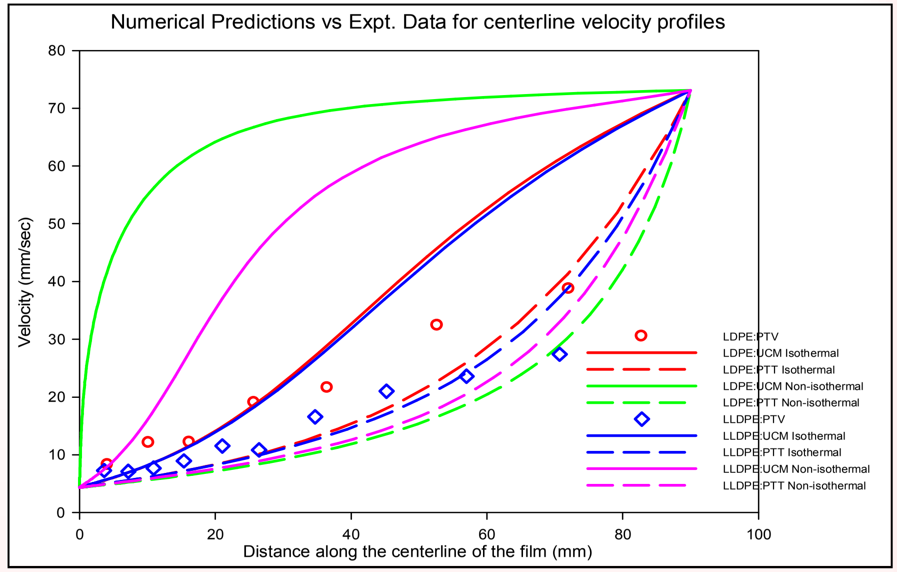
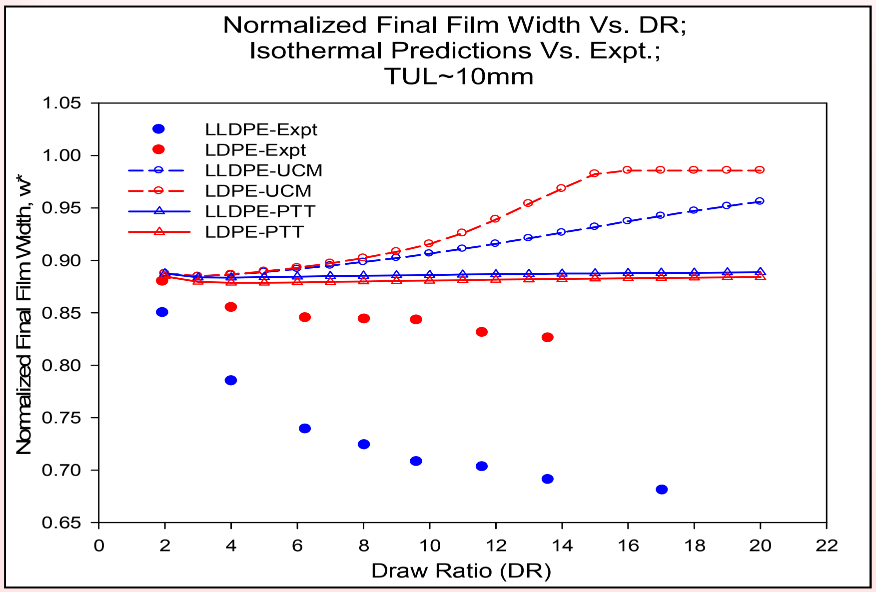
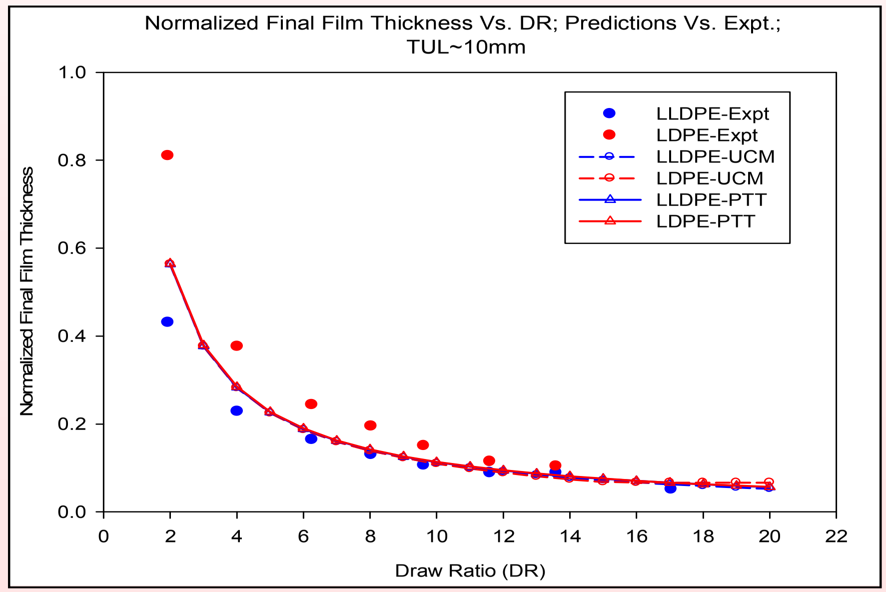
# Numerical Predictions vs. Experiments

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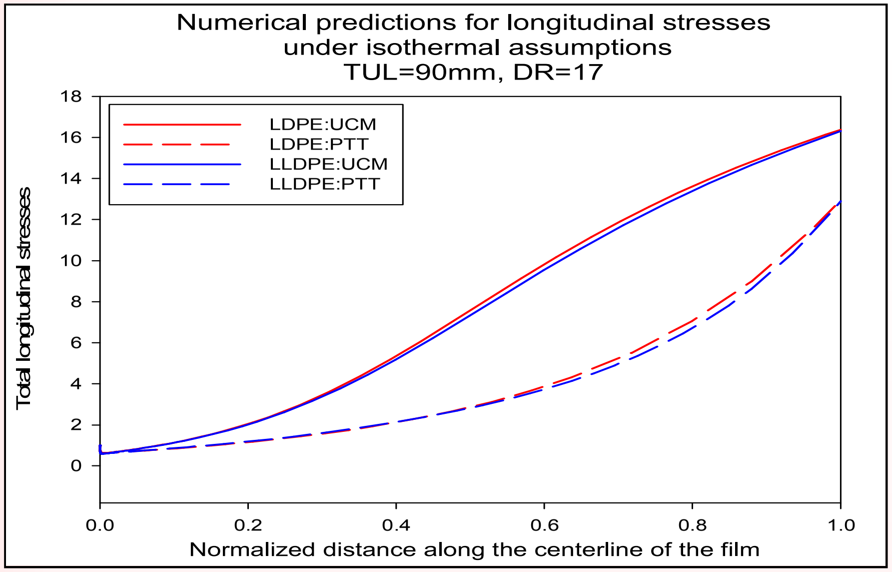
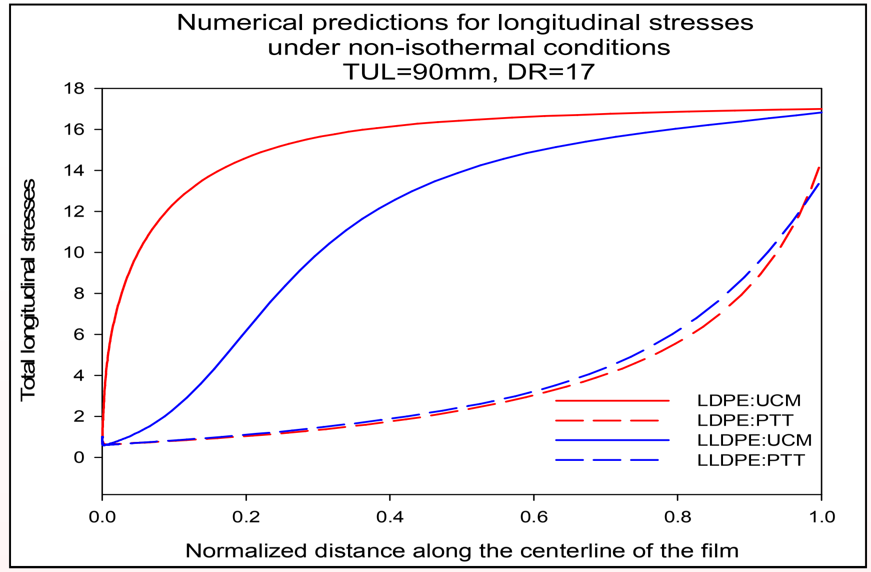
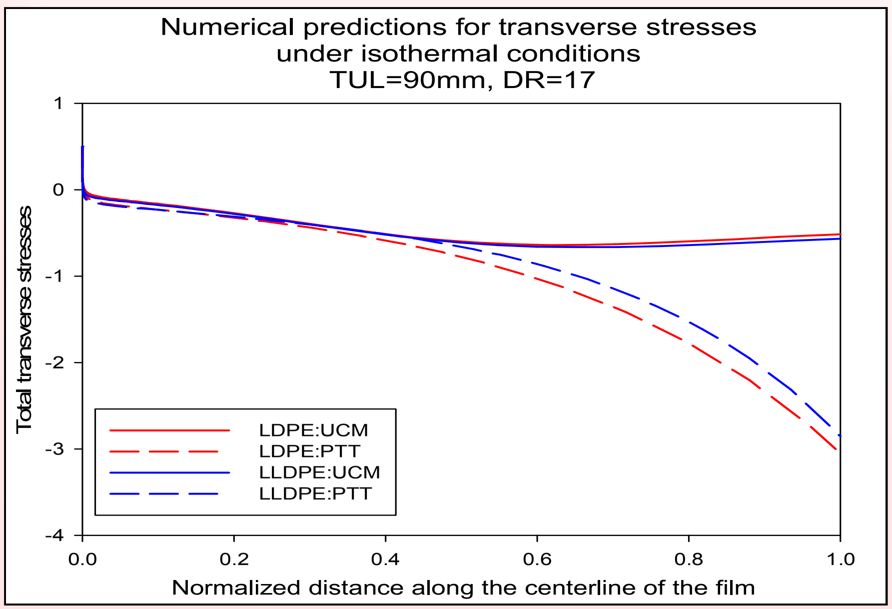
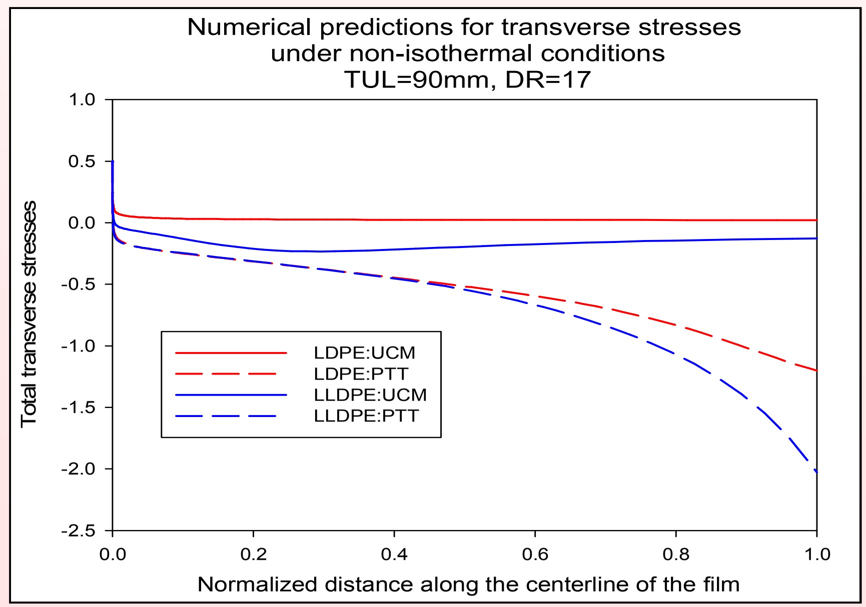
# Predictions of Longitud. and Transv. stresses

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# Conclusions

- The rheological behavior of both linear and branched polymers is better described by the multi-mode PTT CE than the UCM CE.

- Numerical predictions of EFC process using Silagy et al.[2] framework utilizing multi-mode UCM and PTT CE's show poor quantitative comparison with experimental data.

- A distinct separation of the fast and slow relaxing modes (utilizing a non-dimensionless number $\alpha$ ) is possible when the MM UCM CE is used wherein
  - fast relaxing modes exhibit stresses ~ stretch (or strain) rate (viscous behavior) till $\alpha$~0.2 whereas,
  - the slow relaxing modes exhibit stresses ~ strain for $\alpha$>0.5 (elastic or Hookean behavior).

- A separation of viscous and elastic modes is not possible for the more complex PTT CE.

- More realistic flow kinematics is required for quantitative comparisons with experiments.

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# Future Work

- Undertake 2-D ALE based FEM simulations of EFC process.
- Carry out detailed EFC expts. to capture details of exact flow kinematics and PSD using PTV and rheo-optical techniques.
- Utilize more advanced coarse-grained ‘molecular CE’s like XPP or Rolie-Polie.

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