Biopolymer flow dynamics

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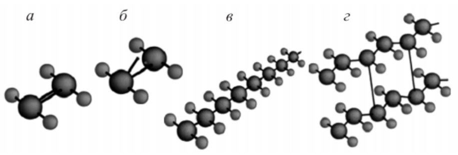
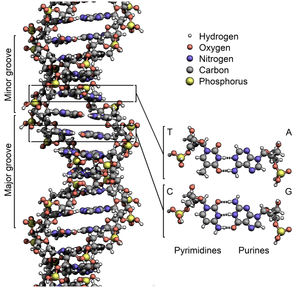
STRUCTURE OF POLYMER

- POLYMER consists of very large molecules, macromolecules with many repeating subunits.
- One or more species of MONOMERS.
- EXAMPLES: polyethylene, nylon and so on.
- BIOLOGY: polypeptides, polynucleotides, DNA, RNA.



$L \approx 1 - 10\,\mathrm{nm} \quad (10^{-9} - 10^{-8}\,\mathrm{m})$

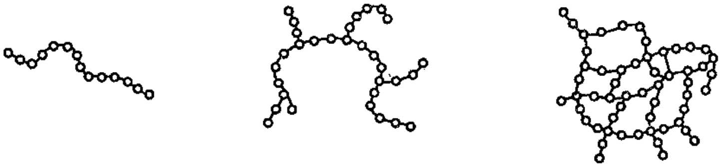


$L \approx 2\mathrm{m}!, \quad m \approx 10^{-12}\mathrm{g}$

STRUCTURE OF POLYMER

Microstructures of a polymer

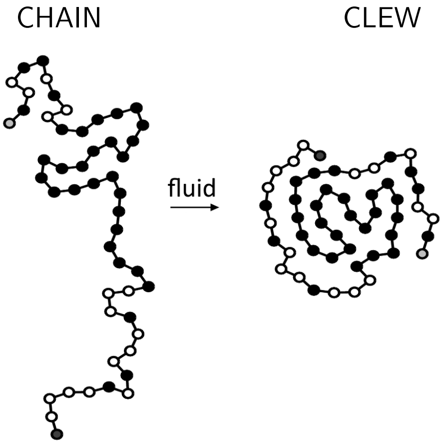
From long line chain $\longrightarrow$ To clew, ball



Chain conformation

Radius of gyration = average distance from the center of mass of the chain to the chain itself

POLYMER CHAIN IN FLUID



Micro - thermal fluctuations covalent bond, noncovalent weak chemical attractions, hydrogen bonds Van der Waals forces.
Macro - drug force, Stokes' law.

STOCHASTIC, BROWN MOTION COMPONENT

Vector $\boldsymbol{r} = (r^i)$, MICROSCOPIC model, Langevin equation, stochastic DE.

$$\boldsymbol{r}_t = -\frac{1}{2\lambda} f(\boldsymbol{r})\boldsymbol{r} + \nabla \boldsymbol{u} \cdot \boldsymbol{r} + \sqrt{\frac{L^2}{\lambda}} \boldsymbol{W}(t)$$

Where:

- $\boldsymbol{u}$ - velocity
- λ - relaxation time
- L^2 - parameter of thermofluctuations
- $\boldsymbol{W}(t)$ - random fluctuating force (white noise)

Statistical Physics + Ito Calculus ⇒ Macromodel for TENSOR OF CONFORMATION

$$\boldsymbol{C} = \langle \boldsymbol{r} \otimes \boldsymbol{r} \rangle_W :$$

Equation for $\boldsymbol{C}$:

$$\boldsymbol{C}_t + (\boldsymbol{u} \cdot \nabla)\boldsymbol{C} - (\nabla \boldsymbol{u})^T \cdot \boldsymbol{C} - \boldsymbol{C} \cdot (\nabla \boldsymbol{u}) + \mathcal{E}(c_1)(\boldsymbol{E} \cdot \boldsymbol{C} + \boldsymbol{C} \cdot \boldsymbol{E}) = \\ = \frac{-1}{\lambda \mathcal{Z}(c_1)} \left[\mathcal{F}(c_1)\boldsymbol{C} - \mathcal{G}(c_1)\boldsymbol{I} \right],$$

- Tensor $\boldsymbol{C}$: $\boldsymbol{C}^T = \boldsymbol{C}$, $\boldsymbol{C} = (C^{ij})$, differentiable, $C > 0$.
- $\boldsymbol{I}$-unit tensor.
- $2\boldsymbol{E} = \nabla \boldsymbol{u} + (\nabla \boldsymbol{u})^T$.
- $\mathcal{F}, \mathcal{G}, \mathcal{Z}$ - dimensionless functions, $c_1 = \mathrm{Tr}\boldsymbol{C}$.
- Finite Extensible Nonlinear Elasticity models = FENE models.

Equation of Polymer Motion

$$\boldsymbol{C}_t + (\boldsymbol{u}\cdot\nabla)\boldsymbol{C} - (\nabla\boldsymbol{u})^T\cdot\boldsymbol{C} - \boldsymbol{C}\cdot(\nabla\boldsymbol{u}) + \mathcal{E}(c_1)(\boldsymbol{E}\cdot\boldsymbol{C} + \boldsymbol{C}\cdot\boldsymbol{E}) = \\ = \frac{-1}{\lambda\mathcal{Z}(c_1)}\left[\mathcal{F}(c_1)\boldsymbol{C} - \mathcal{G}(c_1)\boldsymbol{I}\right],$$

$$\boldsymbol{u}_t + (\boldsymbol{u}\cdot\nabla)\boldsymbol{u} + \nabla\cdot(p + \boldsymbol{\tau}_s + \boldsymbol{\tau}_p) = 0,$$

$$\nabla\cdot\boldsymbol{u} = 0,$$

$$\boldsymbol{\tau}_s = 2\eta_s\boldsymbol{E},$$

$$\boldsymbol{\tau}_p = \frac{\eta_p}{\lambda}[\mathcal{F}(c_1)\boldsymbol{C} - \mathcal{G}(c_1)\boldsymbol{I}]$$

for FENE models.

Lie Derivatives

In Equations for $\boldsymbol{C}$:

$$L_{\boldsymbol{v}}\boldsymbol{C} = \boldsymbol{C}_t + (\boldsymbol{u}\cdot\nabla)\cdot\boldsymbol{C} - (\nabla\boldsymbol{u})^T\cdot\boldsymbol{C} - \boldsymbol{C}\cdot\nabla\boldsymbol{u}$$

is Lie derivatives for $\boldsymbol{C}$

$$L_{\boldsymbol{v}}C^{ij} = \partial_t C^{ij} + u^k\frac{\partial C^{ij}}{\partial x^k} - C^{kj}\partial_k u^i - C^{ik}\partial_k u^j, \quad (i,j,k=1,2,3),$$

$$\boldsymbol{C}' = L_{\boldsymbol{v}}\boldsymbol{C}, \qquad \frac{d\boldsymbol{x}}{dt} = \boldsymbol{v}(\boldsymbol{x}), \qquad \boldsymbol{x}|_{t=t_0} = \boldsymbol{X}, \qquad \boldsymbol{x} = \boldsymbol{x}(t,\boldsymbol{X})$$

Lie Equations for vector field $\boldsymbol{v}$

Canonical parameter: $\boldsymbol{v} = \partial_t + u^k\partial_k \to \partial_1$

History and References

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Main Goal = Dynamics of Tensor C

We have two equations for $\boldsymbol{C}$:

$$\begin{cases} L_{\boldsymbol{v}}\boldsymbol{C} = -\frac{1}{\lambda \mathcal{Z}(c_1)}\left[\mathcal{F}(c_1)\boldsymbol{C} - \mathcal{G}(c_1)\boldsymbol{I}\right], & (2) \\ \boldsymbol{C}^3 - c_1\boldsymbol{C}^2 + c_2\boldsymbol{C} - c_3\boldsymbol{I} = 0, & (3) \end{cases}$$

(3) - Hamilton-Cayley equations for Tensor $\boldsymbol{C}$.

$c_1 = \mathrm{Tr}\boldsymbol{C}$, $\quad c_2 = \frac{1}{2}\left[(\mathrm{Tr}\boldsymbol{C})^2 - \mathrm{Tr}\boldsymbol{C}^2\right]$, $\quad c_3 = \det \boldsymbol{C}$ are invariants of Tensor $\boldsymbol{C}$.

(2) + (3) is overdetermined system DE for $\boldsymbol{C}$. Compatibility conditions, Reduce to Involutions (Cartan, Pommaret).

SOLUTION for FENE model

Let $\mathcal{F}(c_1) = \mathcal{G}(c_1) = \frac{1}{1-c_1/L^2}$, $\quad g(c_1) = -\frac{\mathcal{F}(c_1)}{\lambda \mathcal{Z}(c_1)}$,
where L is the maximum chain length, $c_1/L^2 < 1$. System DE

$$\begin{cases} L_{\boldsymbol{v}} \boldsymbol{C} = g(c_1)(\boldsymbol{C} - \boldsymbol{I}), \\ \boldsymbol{C}^3 - c_1 \boldsymbol{C}^2 + c_2 \boldsymbol{C} - c_3 \boldsymbol{I} = 0, \end{cases} \tag{4}$$

Динамическая система для инвариантов для двумерного случая ($n = 3$ громоздкая).

$$\boldsymbol{C}^T = \boldsymbol{C}, \quad \boldsymbol{C} > 0 \implies \boldsymbol{C} = \boldsymbol{Q}\boldsymbol{\Lambda}\boldsymbol{Q}^T, \quad \boldsymbol{Q}\boldsymbol{Q}^T = \boldsymbol{I}$$

где

$$\boldsymbol{\Lambda} = \mathrm{diag}(\lambda_1, \lambda_2), \quad \lambda_i > 0$$

$$\boldsymbol{E} = \frac{1}{2}(\nabla \boldsymbol{u} + (\nabla \boldsymbol{u})^T), \quad \boldsymbol{E}^T = \boldsymbol{E}, \quad \mathrm{tr}\,\boldsymbol{E} = 0$$

$$\boldsymbol{E} = \boldsymbol{R}\boldsymbol{M}\boldsymbol{R}^T, \quad \boldsymbol{R}\boldsymbol{R}^T = \boldsymbol{I}$$

где

$$\boldsymbol{M} = \mathrm{diag}(e, -e)$$

Устанавливается подобие матричных операторов, следствием чего является теорема.

Теорема (Динамическая система)

$$L_1 c_1 = g c_1 + 2 f c_{12} - 2h - \frac{4 e c_2}{\lambda_1 - \lambda_2}$$

$$L_1 c_2 = 2 g c_2 - h c_1 - 2 e c_2 \frac{\lambda_1 + \lambda_2}{\lambda_1 - \lambda_2}$$

где f, g, h — неотрицательные функции от c_1 из реологического уравнения, $c_{12} = \operatorname{tr} \boldsymbol{CE}$

Пусть $W = \frac{1}{4} c_1^2 - c_2$ — аналог функции Уиллмора.

Следствие

$$L_x W = 2gW + f c_1 c_2$$

где

$$g = g(c_1) < 0, \quad f = f(c_1) > 0$$

Функционал W монотонно убывает $\implies$ конфигурация стремится к окружности, области с минимумом функционала Уиллмора.

SOLUTION for FENE model

$$L_{\boldsymbol{v}}\,[(3)\text{=Hamilton-Cayley Eq.}] \overset{L_{\boldsymbol{v}}\boldsymbol{C}}{\Longrightarrow}$$

$$3g\,\boldsymbol{C}^3 - (c_1' + 3g + 3gc_1)\boldsymbol{C}^2 + (c_2' + 2gc_1 + gc_2)\boldsymbol{C} - (c_3' + gc_2)\boldsymbol{I} = 0$$

for $L_{\boldsymbol{v}}\boldsymbol{I} = 0$

$$\Rightarrow \begin{cases} c_1' = g(c_1 - 3), \\ c_2' = 2g(c_2 - c_1), \\ c_3' = g(3c_3 - c_2) \end{cases} \qquad (5)$$

$$g = g(c_1) \quad \Rightarrow \quad c_1 = c_1(\tau), \quad c_2 = c_2(c_1(\tau)), \quad c_3 = c_3(c_1(\tau))$$

SOLUTION for FENE-CR model

$$\mathcal{Z} = 1 \quad \Rightarrow \quad g(c_1) = \frac{-1}{\lambda(1 - c_1/L^2)} \tag{6}$$

Theorem 1. Invariants of $\boldsymbol{C}$ are solutions of umplicite system of equations

$$\begin{cases} (3 - L^2)\ln|c_1 - 3| + c_1 = \frac{L^2}{\lambda}(\tau - \tau_0), \\ c_2 = \alpha_1(c_1 - 3)^2 + 2c_1 - 3, \\ c_3 = \alpha_2(c_1 - 3)^3 + \alpha_1(c_1 - 3)^2 + c_1 - 2, \end{cases} \tag{7}$$

where τ_0, α_1, α_2 are arbitrary functions of parameters $\boldsymbol{X}$.

SOLUTION for FENE-CR model

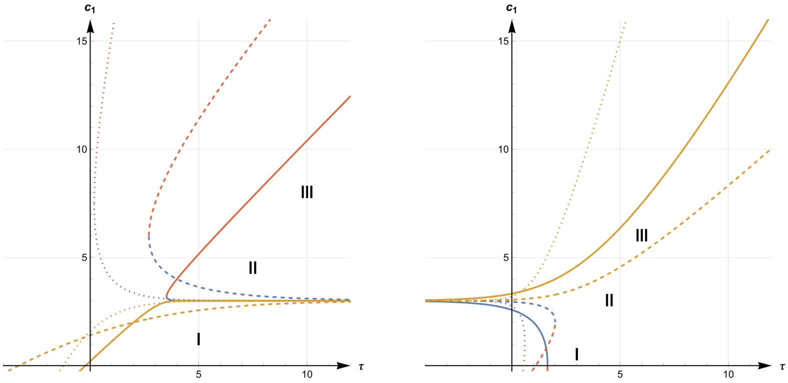


Figure: Graph of the function $c_1(\tau)$: a) for $L^2 > 3$, b) for $L^2 < 3$. Different branches are denoted by different colors, curves for different parameters l and L^2 are separated by different hatching.

$y_1 = c_1 - 3$ - Lambert function: $$L^2 \ln |y_1| + y_1 = \frac{L^2}{\lambda}(\tau - \tau_0)$$

SOLUTION for FENE-CR model

Two singular points of system (5) on the planes: $c_1 = 3$ -singular point and $c_1 = L^2$ - singular manifold.

Let's investigate the behavior of the solutions $c_i = c_i(\tau)$ of system (5) near these singularities.

The singular point on the plane $c_1 = 3$ has coordinates $c_1 = 3, c_2 = 3, c_3 = 1$. It is a node, repelling for $L^2 < 3$ and attracting for $L^2 > 3$.

SOLUTION for FENE-CR model

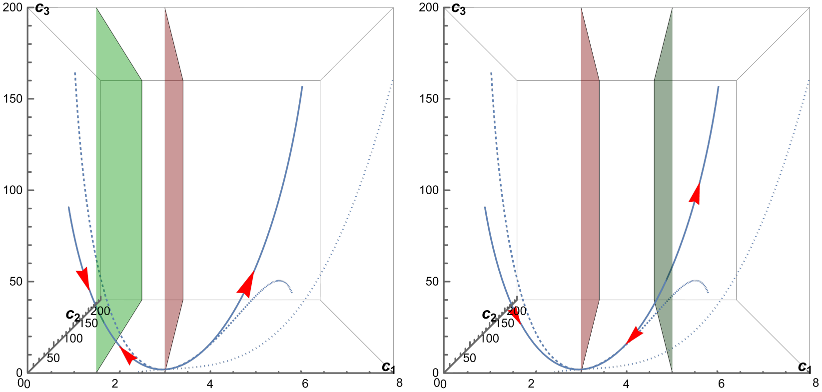


Figure: Behavior of the trajectories of the dynamical system: a) for $L^2 < 3$, b) for $L^2 > 3$, planes $c_1 = 3$ and $c_1 = L^2$. Curves for different initial data are separated by different hatching.

Problem formulation: FENE-CR model

We consider incompressible viscoelastic 2D flow governed by Navier–Stokes equations coupled with the FENE-CR model.

Momentum equation

$$\rho\left(\frac{\partial \boldsymbol{u}}{\partial t} + (\boldsymbol{u}\cdot\nabla)\boldsymbol{u}\right) = -\nabla p + \mu\Delta\boldsymbol{u} + \nabla\cdot\boldsymbol{\tau}_p$$

Continuity equation

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

Polymer stress tensor

$$\boldsymbol{\tau}_p = \frac{1-\beta}{\lambda}\frac{\boldsymbol{C}-\boldsymbol{I}}{1-\mathrm{tr}(\boldsymbol{C})/L^2}$$

- $\boldsymbol{u}$ — velocity
- p — pressure
- $\boldsymbol{C}$ — conformation tensor
- λ — relaxation time
- L — extensibility parameter

Transport equation for conformation tensor

The conformation tensor satisfies the FENE-CR equation:

$$\frac{\partial \boldsymbol{C}}{\partial t} + (\boldsymbol{u} \cdot \nabla)\boldsymbol{C} - (\nabla \boldsymbol{u})\boldsymbol{C} - \boldsymbol{C}(\nabla \boldsymbol{u})^T = -\frac{1}{\lambda\left(1 - \frac{\mathrm{tr}(\boldsymbol{C})}{L^2}\right)}(\boldsymbol{C} - \boldsymbol{I})$$

Properties

- $\boldsymbol{C}^T = \boldsymbol{C}$
- $\boldsymbol{C} > 0$
- $\mathrm{tr}(\boldsymbol{C}) < L^2$

Lie derivative form:

$$\mathcal{L}_u \boldsymbol{C} = -\frac{1}{\lambda\,(1 - \mathrm{tr}(\boldsymbol{C})/L^2)}(\boldsymbol{C} - \boldsymbol{I})$$

Initial and boundary conditions

Initial conditions

$$\boldsymbol{u}(y,0) = \boldsymbol{u}_0(y) = 4U_{max}y\,(1-y)\,.$$

$$\boldsymbol{C}(x,y,0) = \boldsymbol{I}$$

Boundary conditions

- Inlet:

$$\boldsymbol{u} = \boldsymbol{u}_0(y)$$

- Wall:

$$\boldsymbol{u} = 0$$

- Outlet:

$$p = 0, \quad \frac{d\boldsymbol{u}}{dt} = 0$$

Numerical results 1 $\lambda = 0.04$, $L^2 = 5$:

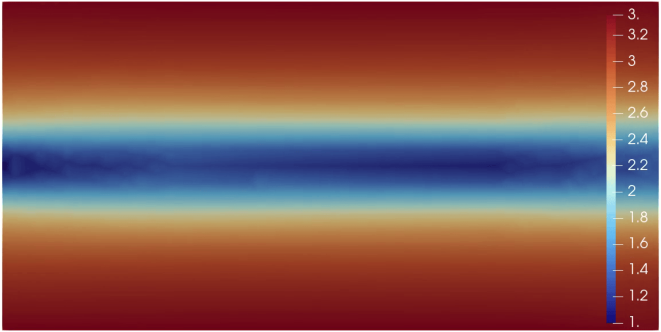


Figure: Distribution of C_{11} at $t = 0.03$

- $C_{22} = 1$
- Flow establishment within 0.3 seconds
- $max(trace(\boldsymbol{C})) = 4 < L^2 = 5$

Numerical results 1 $\lambda = 0.04$, $L^2 = 5$:

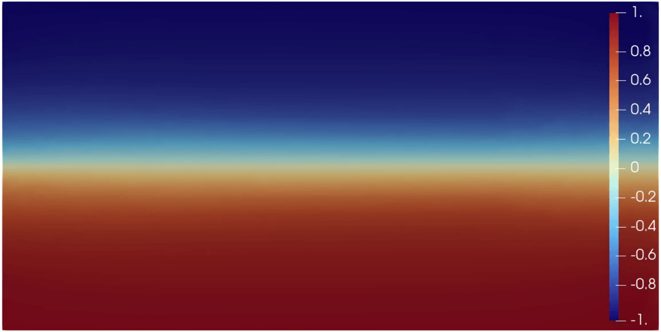


Figure: Distribution of C_{12} at $t = 0.03$

- $C_{22} = 1$
- Flow establishment within 0.3 seconds
- $max(trace(\boldsymbol{C})) = 4 < L^2 = 5$

Numerical results 2 $\lambda = 0.04$, $L^2 = 10$:

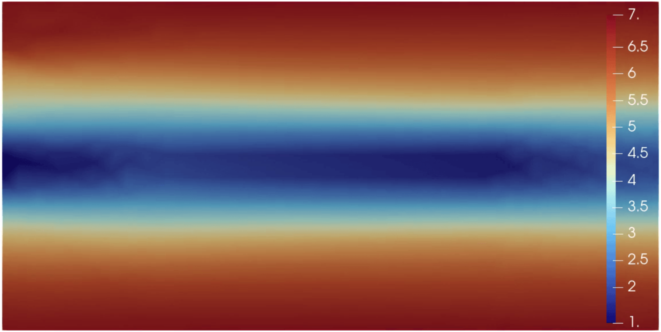


Figure: Distribution of C_{12} at $t = 0.03$

- $C_{22} = 1$
- Flow establishment within 0.3 seconds
- $max(trace(\boldsymbol{C})) = 8 < L^2 = 10$

Numerical results 2 $\lambda = 0.04$, $L^2 = 10$:

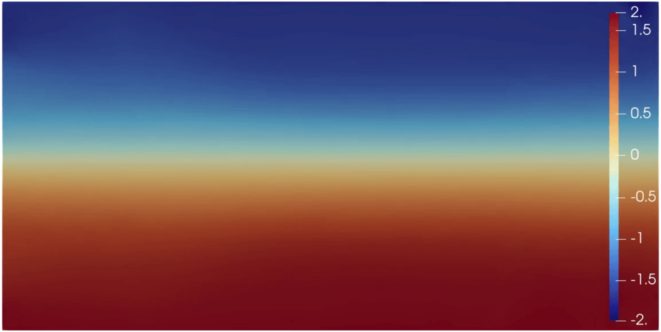


Figure: Distribution of C_{12} at $t = 0.03$

- $C_{22} = 1$
- Flow establishment within 0.3 seconds
- $max(trace(\boldsymbol{C})) = 8 < L^2 = 10$

SOLUTION for Model FENE-CD

$$\mathcal{Z} = 1 - \varkappa + \varkappa\sqrt{c_1/3} \Rightarrow g(c_1) = \frac{-1}{\lambda(1-c_1/L^2)(1-\varkappa+\varkappa\sqrt{c_1/3})} \qquad (8)$$

Theorem 2. Invariants of $\boldsymbol{C}$ are solutions of umplicite system of equations

$$\begin{cases} \frac{\varkappa}{\sqrt{3}}\left[\frac{3}{2}c_1\sqrt{c_1} + 2(3-L^2)\sqrt{c_1} + (3-L^2)\ln\left|\frac{\sqrt{c_1}-\sqrt{3}}{\sqrt{c_1}+\sqrt{3}}\right|\right] + \\ +(1-\varkappa)\left[c_1 + (3-L^2)\ln|c_1-3|\right] = \frac{L^2}{\lambda}(\tau-\tau_0), \\ c_2 = \alpha_1(c_1-3)^2 + 2c_1 - 3, \\ c_3 = \alpha_2(c_1-3)^3 + \alpha_1(c_1-3)^2 + c_1 - 2 \end{cases} \qquad (9)$$

Identical formulas for $c_\alpha = c_\alpha(c_1)$, $\alpha = 2, 3$ for FENE-CR and FENE-CD.

STRUCTURE DYNAMICS OF INVARIANTS c_i

Change $\boldsymbol{C} \to \boldsymbol{Y} = \boldsymbol{C} - \boldsymbol{I} \qquad (c_i > 0, i = 1, 2, 3)$

$$\begin{cases} y_1 = c_1 - 3, \\ y_2 = c_2 - 2c_1 + 3, \\ y_3 = c_3 - c_2 + c_1 - 1. \end{cases} \tag{10}$$

Dynamical system for invariants y_i:

$$\Sigma : \begin{array}{l} y_1 = y_1(\tau), \\ \begin{cases} y_2 = \alpha_1 (y_1)^2, \\ y_3 = \alpha_2 (y_1)^3. \end{cases} \end{array} \tag{11}$$

STRUCTURE DYNAMICS OF INVARIANTS c_i

Curve Σ in space $\mathbb{R}^3(\boldsymbol{y})$ has curvature k and torsion κ:

$$k = 2\left[\frac{9\alpha_2^2 y_1^4 + \alpha_1^2(1 + 9\alpha_2^2 y_1^4)}{(1 + 4\alpha_1^2 y_1^2 + 9\alpha_2^2 y_1^4)^3}\right]^{1/2}, \qquad \kappa = \frac{3\alpha_1\alpha_2}{\alpha_1^2 + 9\alpha_2^2 y_1^2 + 9\alpha_1^2\alpha_2^2 y_1^4}$$

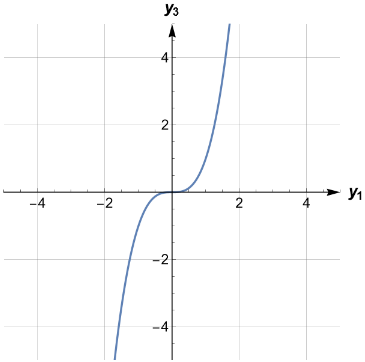
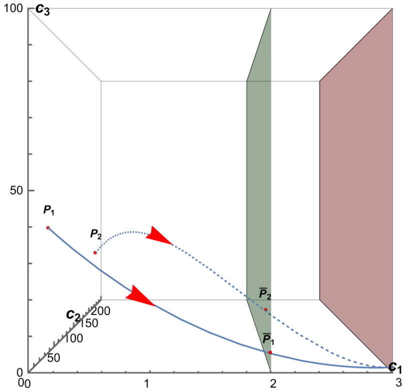
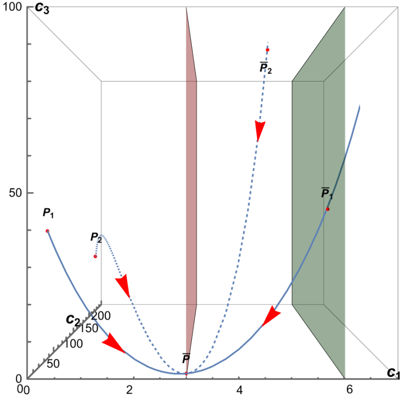


Figure: $y_3^2 = y_2^3$ - Neil parabola

Embolizates – Advanced Polymers for Minimally Invasive Treatment of Vascular Pathologies. Experiment.

DIFFERENT MODES





$P1 = P1', C1 = 3, C2 = 3, S < 1$

Polymer fills an extended formation. Can be used for channel embolization.

$P_i \in \Pi, \quad P_i' \in C1 \to L^2$

Ball.
Can be used for targeted delivery, but only to a fixed point.

CONCLUSION

In this work, the equations for the dynamics of the invariants of the conformational tensor for FENE polymer solution models are derived and integrated.
Explicit formulas for the invariants as functions of the time parameter along the trajectory of fluid particles are obtained.
The invariants are represented as functions of the Lambert function.
A description of the qualitative behavior of the invariants under different regimes is given.

Publication

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Thanks for your attention!