Dynamics of the Conformation Tensor in Viscoelastic FENE Polymer Models

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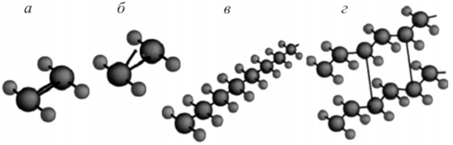
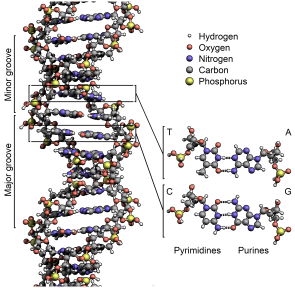
STRUCTURE OF POLYMER

- 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.



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

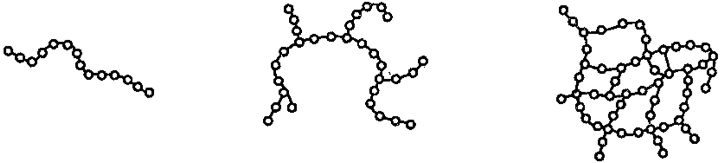


$L \approx 2\mathrm{m}!, \quad m \approx 10^{-12}\mathrm{g}$

STRUCTURE OF POLYMER

Microstructures of a polymer

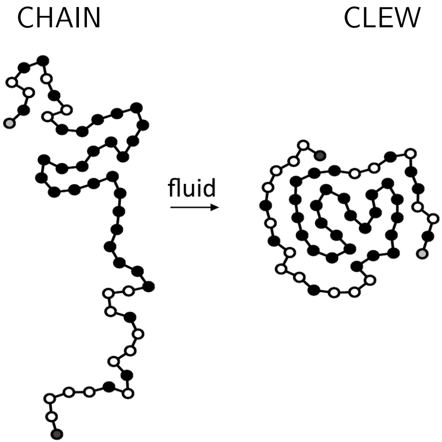
From long line chain $\longrightarrow$ To clew, ball



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.

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

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

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

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

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

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

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

for FENE models.

Lie Derivatives

In Equations for $\boldsymbol{C}$:

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

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

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

SOLUTION for FENE model

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

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

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

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

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

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

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

SOLUTION for FENE-CR model

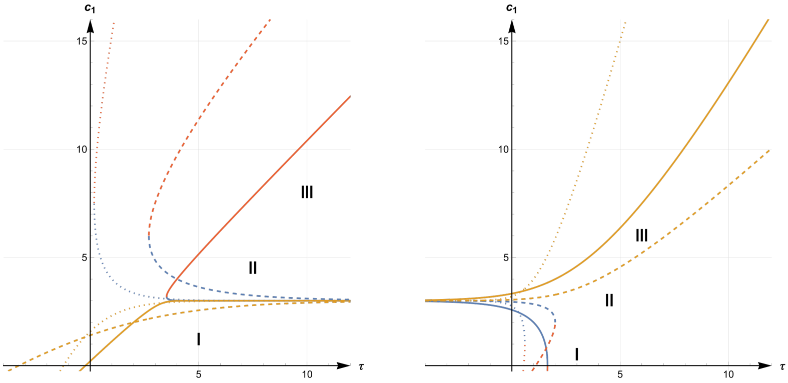


Figure: Graph of the function $c_1(\tau)$: a) for $L^2 > 3$, b) for $L^2 < 3$. Different branches are denoted by different colors, curves for different parameters l and L^2 are separated by different hatching.

$y_1 = c_1 - 3$ - 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

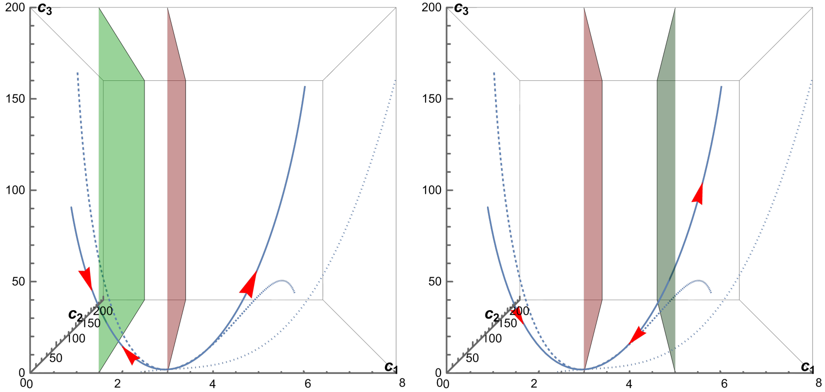


Figure: Behavior of the trajectories of the dynamical system: a) for $L^2 < 3$, b) for $L^2 > 3$, planes $c_1 = 3$ and $c_1 = L^2$. Curves for different initial data are separated by different hatching.

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

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

Dynamical system for invariants y_i:

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

STRUCTURE DYNAMICS OF INVARIANTS c_i

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

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

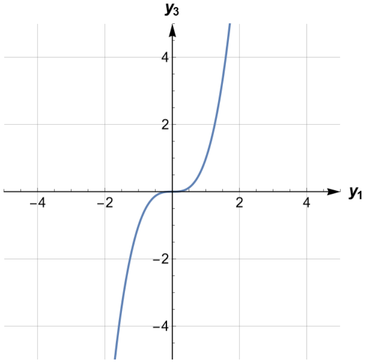
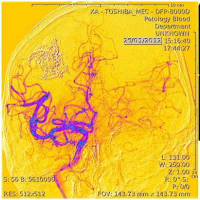


Figure: $y_3^2 = y_2^3$ - Neil parabola

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

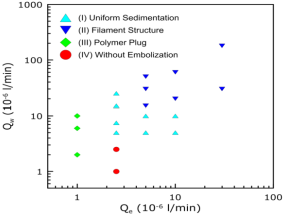
Arteriovenous Malformation (AVM)



AVM is embolized

AVM During Microsurgery

Experimentally Observed Regimes Map

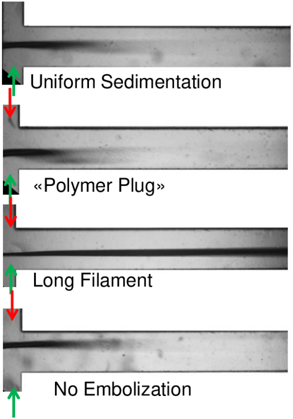


Q_w = 5 µl/min
Q_e = 2,5 µl/min

Q_w = 10 µl/мин
Q_e = 1 µl/мин

Q_w = 60 µl/min
Q_e = 10 µl/min

Q_w = 2,5 µl/min
Q_e = 2,5 µl/min



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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.

Thanks for your attention!