Coarse-Grained Modeling in Polymer-Plasticizer System

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Objective

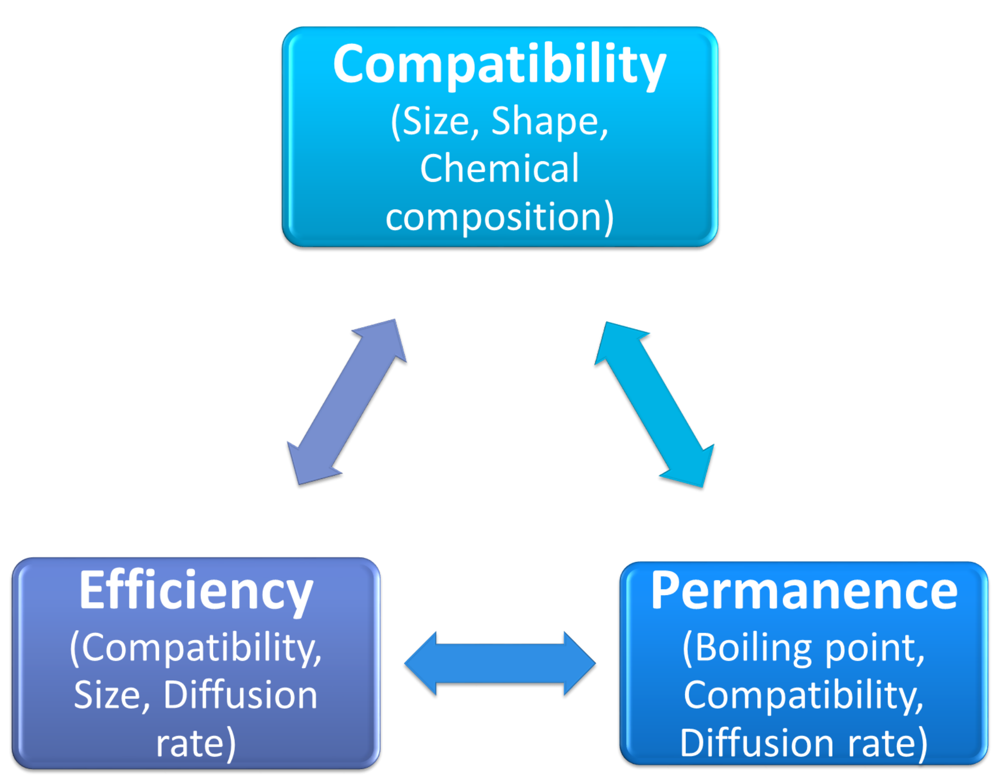
- Understanding glass-formation in amorphous polymers
- Major influences on plasticization , i.e. molecular architecture, hydrophobicity, energetics
- Optimize plasticizer design
- Migration and plasticization characterization

Background

- A Plasticizer is a polymer *additive*
- Effect on polymer properties: an important distinction from other additives
- Increases polymer flexibility, elongation or workability

Working Theories of Plasticization:

- Lubricity Theory
  - *These molecules act as lubricants for the polymer chains*
- Gel Theory
  - *Break interactions and masks the centers from each other, preventing re-formation*
- Free-Volume Theory
  - *"internal space" available in the polymer for the chains to move*



Simulation Design

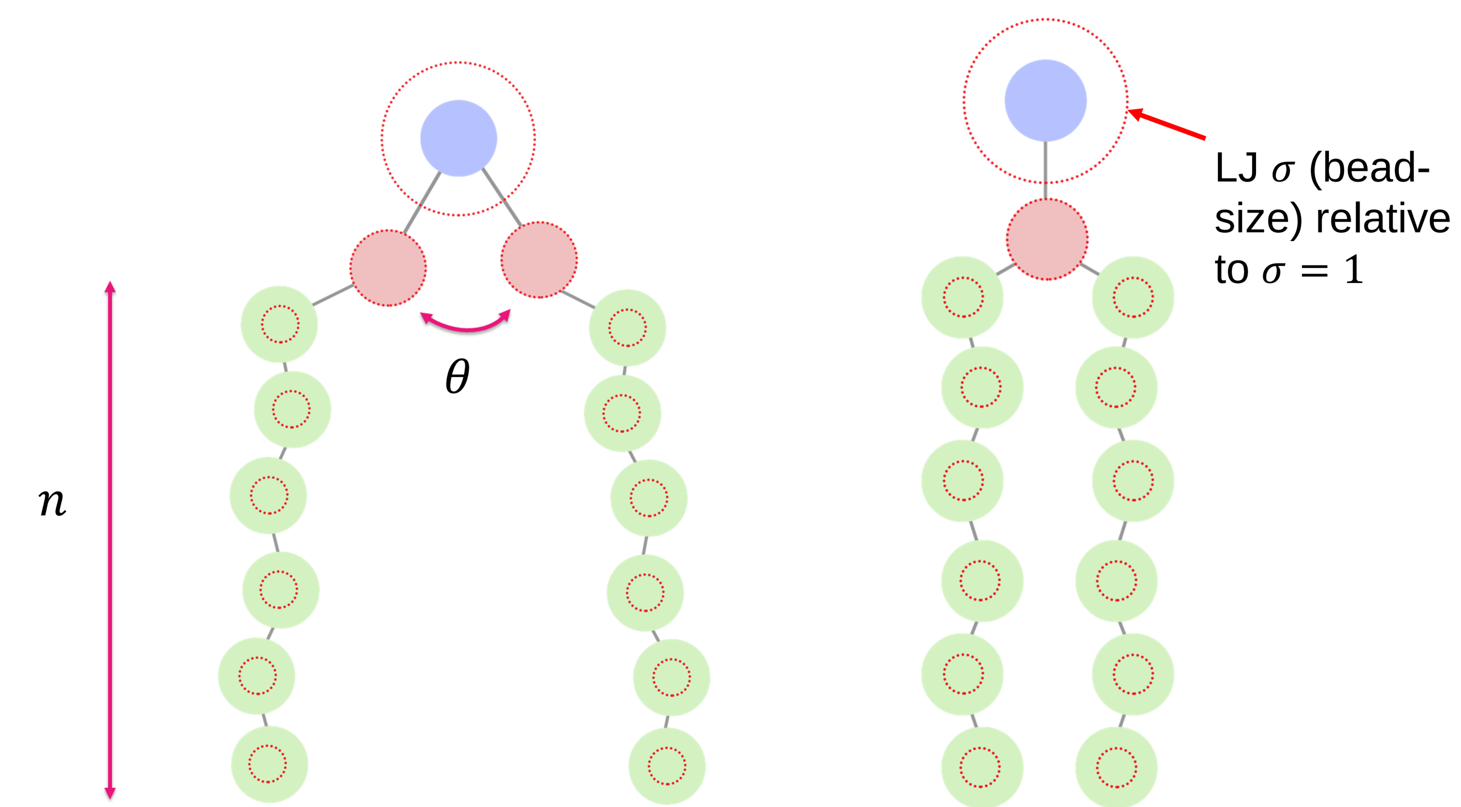
Force field setup with Lennard Jones (LJ) 12-6 model. For non-bonded potential energy.

$$E_{LJ}(r) = \begin{cases} 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right], & r \geq r_{cut} \\ 0, & r \leq r_{cut} \end{cases}$$

Bonded potential modeled by Finite Extensible Nonlinear Elastic (FENE) potential.

$$E = -0.5KR_0^2 \ln\left[1-\left(\frac{r}{R_0}\right)^2\right] + 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right] + \varepsilon$$

Complex plasticizers are being modeled to see how carbon chain length (n) and benzene positioning (θ) affect plasticization.



Future Work & Reference

- Evaluate best LJ parameters for plasticization
- Look into how polarity affects plasticization
- Using General Entropy Theory (GET) to help in direction of understanding glass-forming in amorphous polymers

[1] R. A. Riggleman, H. N. Lee, M. D. Ediger, and J. J. De Pablo, "Free volume and finite-size effects in a polymer glass under stress," *Phys. Rev. Lett.*, vol. 99, no. 21, pp. 1–4, 2007.

[2] E. H. Immergut and H. F. Mark, "Principles of Plasticization," *Plast. Plast. Process.*, vol. 48, pp. 1–26, 1965.

[3] D. S. Simmons, M. T. Cicerone, Q. Zhong, M. Tyagi, and J. F. Douglas, "Generalized localization model of relaxation in glass-forming liquids," *Soft Matter*, vol. 8, no. 45, p. 11455, 2012.

Acknowledgements

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