SIMULATION OF VISCOELASTIC FLUID FLOW IN A TWIN SCREW EXTRUDER

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Motivation

Advanced composite energetic materials are highly filled polymers with complex rheological properties that affect their microstructural evolution during Twin Screw Extrusion processing

Objectives

To simulate the flow of the material in the twin screw extruder for understanding the effects of operating conditions and screw configurations on the microstructure, and for visualizing it in a virtual reality environment

Research Approach

- Develop C code for 2-D Stokes Problem with various screw geometries
- Incorporate Carreau Model with Discontinuous Galerkin formulation

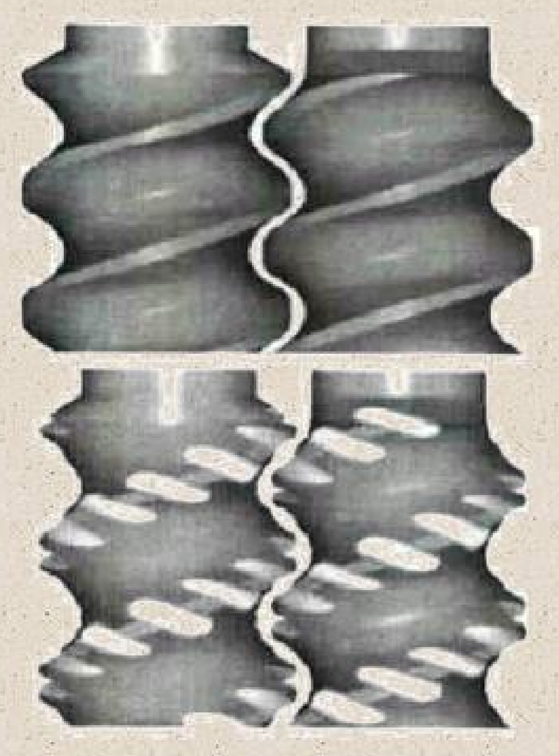
$$\tau = 2\eta \mathbf{D}$$

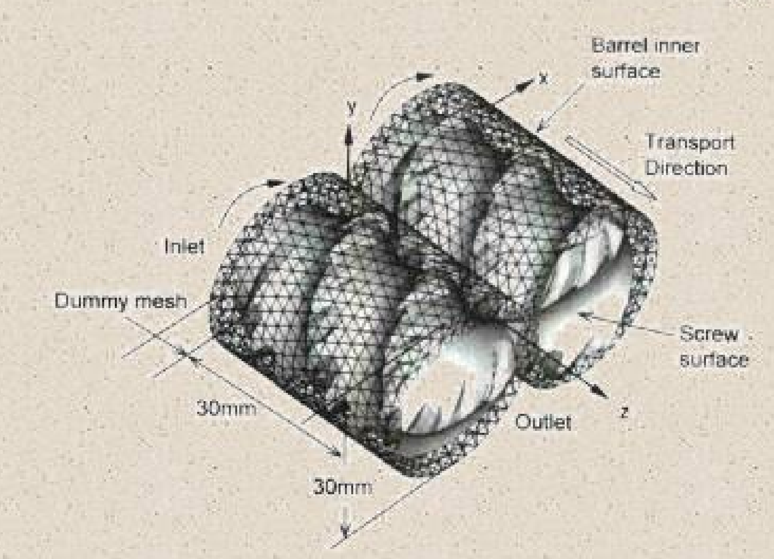
$$\eta = H(T)F(\dot{\gamma}\, H(T)),\ \ \dot{\gamma} = \sqrt{2II_D}$$

$$F = \eta_0[\,1 + \lambda_c^{\,2}\,(2II_D)\,]^{(n-1)/2}$$

- *No energy equation*: Isothermal (H(T)=1)
- Provides better understanding of the overall problem
- New ideas for addressing the problem

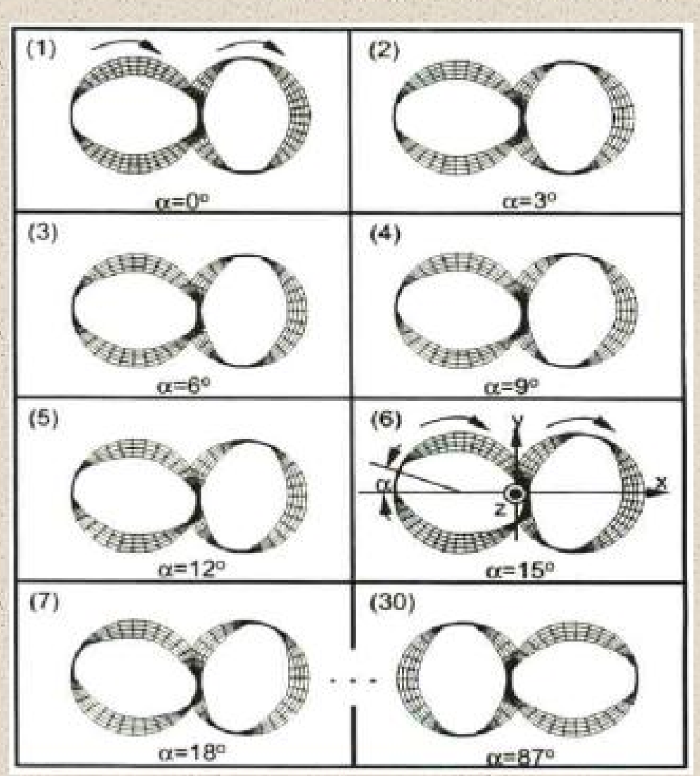
State-of-the-art Screw Design





Work by Ishikawa et. al.

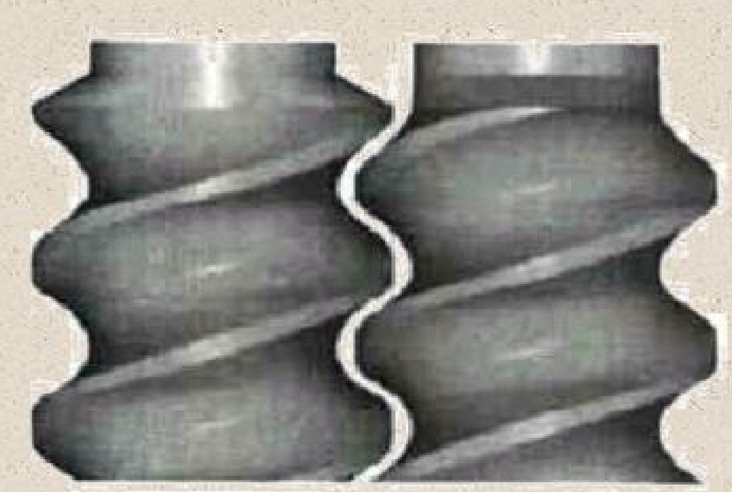
State-of-the-art Modeling



- *Mesh Generation*: IDEAS
- *Problem solution*: Customized Code Development
  1. *Constitutive equation*: Herschel-Bulkley
  2. *Geometry*: 30 different geometries in sequential manner with 3º increments.
  3. Compare results with unfolding techniques.

New Ideas: Storage Savings

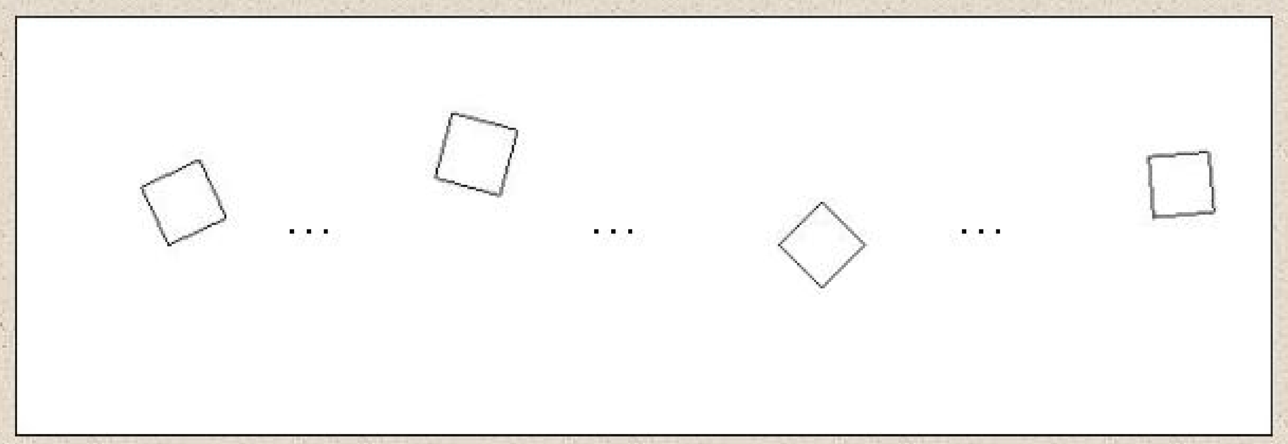
Rather than generating a mesh for this:



Generate a mesh for this:

- All computations can be done on this cell which will be "periodized".
- Outflow boundary conditions for previous cell are inflow boundary conditions for next cell.
- Meshing will be done on half of this cell.

New Ideas: Unmelted Pellets



An initial understanding of this problem could be formulated by studying the motion of a square pellet in channel flow.

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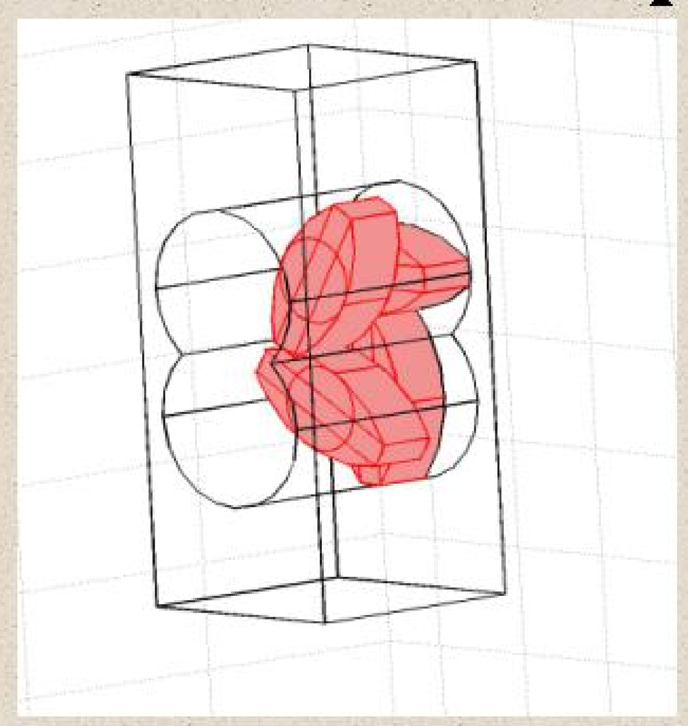
Code Development: FEMLAB



FEMLAB can be used to model some screw geometries, such as kneading blocks, but cannot produce more complex structures such as the transport elements. These more complex screw geometries will be modeled using IDEAS.

Other New Ideas

- State of the art visualization in *Virtual Reality Environment* (parallel effort with Mr. A. El Sabbagh and Dr. A. Baz at the University of Maryland).
  1. 2-D Navier-Stokes code has been implemented
  2. Benchmarking currently being conducted
- Implement other computation saving techniques, such as two-level methods which have been shown (see Liakos &Lee 2003, *Comput. Meth. Appl. Mech. Engr.)* both mathematically and numerically to have good convergence properties.

Future Work

- Design complex screw geometries using IDEAS - ANSYS
- Use Army HPC research codes for increasing solution speed and complexity of screw configurations and material behavior
- Further code development issues:
  1. Dynamic memory allocation
  2. Incorporation of Herschel-Buckley properties
  3. Simulation using Lattice Boltzmann method
  4. Extension from 2-D to 3-D geometric models
- Integration into Virtual Reality Environment

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