COMPUTATIONAL ANALYSIS AND DESIGN OF SINGLE SCREW EXTRUDERS HAVING SCREWS OF COMPLEX GEOMETRY WITH MIXING ELEMENTS

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The "heart" of every extruder is an ARCHIMEDEAN SCREW attributed to Archimedes 287-212 BC but, actually known to Egyptians for irrigation in the Nile Delta and the auger (screw drill) for carpentry was known to the Greeks before the 3rd Century BC.

See:

Chris Rorres, J.Hydraul.Eng., Vol.126, 71-80, (January 2000)

SINGLE SCREW EXTRUDER: Rotating screw in a heated barrel.

Early developments for rubber due to Thomas Hancock in 1820 in England.

Modern developments started in the 1950's.

MODELING of EXTRUSION started in the 1950's

Prominent names at DUPONT (USA)

- McKelvey
- o Gore
- Squires
 1950's

 Maillefer (parallel developments in Switzerland, 1950's)

- Maddock (Union Carbide) 1950's - McKelvey's book on P.P. appeared in 19
- McKelvey's book on P.P. appeared in 1962
- The book by Z. Tadmor and I. Klein appeared in 1970

MODELING OF EXTRUSION IS 60 YEARS OLD, BUT MANY CHALLENGES REMAIN

SINGLE SCREW EXTRUSION IS THE MOST COST-EFFECTIVE WAY TO MELT AND PUMP A POLYMER

SCREW DESIGN calls for

- OUTPUT MAXIMIZATION
- MELT TEMPERATURE MINIMIZATION
- EXTRUSION STABILITY
- MELT QUALITY
- **OPTIONS:**
- CONVENTIONAL single flighted screws
- BARRIER screws
- Screws with MIXING SECTIONS

Conventional single screw (also called: plasticating) extruders are composed of three sections:



In all screws at <u>least</u> the first 70% or so of melting is due to the shear stress in the melt film between the barrel and the solid bed surface.



BARRIER SCREW PRINCIPLE



- Increased melting.

- At least 80% is melted by <u>shear</u> over the solid bed (i.e. very little conductive melting).

MADDOCK (Union Carbide) MIXING SECTION

UNION CARBIDE FLUTED MIXING SECTION



MIXING AND SHEAR MECHANISMS IN FLUTED MIXING SECTION



CHALLENGES:

SOLID PARTICLES TRANSPORT

(pellets, size, properties, powders, difficult to describe mathematically particle flow)

- MELTING OF THE PACKED BED OF SOLID PARTICLES (how do solid particle properties affect the melting rate?)
- COMPLEX SCREW GEOMETRY (barrier screws, screws with various types of mixing elements)

Our present modeling approach



MODULAR, EASY TO UPGRADE MODELS FOR EACH SECTION



DARNELL AND MOL (1956) MODEL



BALANCE OF FORCES AND TORQUES

MELTING (Tadmor's Model)

In the late 50's, Bruce Maddock did experiments, pulling the screw and examining what happened. The conclusion was that MELTING REALLY OCCURS IN A FILM BETWEEN BARREL AND SOLID BED. A MELT POOL FORMS IN FRONT OF THE REAR FLIGHT, as shown:



Metering section: We decided to use the Hele – Shaw flow approximation layer – by – layer 2.5D analysis with 3D geometry **Because our objective is screw design** which means, simulation for a starting geometry, geometry upgrade.....till satisfactory results obtained. 50 or more runs maybe need. "trial – and – error on the computer

screen".

3-D NAVIER – STOKES for creeping non – Newtonian flow

$$0 = -\nabla P + \nabla \cdot \overline{\tau} \qquad \nabla \cdot \overline{V} = 0$$
$$e_{ij} = \frac{1}{2} \left(\frac{\partial V_i}{\partial x_j} + \frac{\partial V_j}{\partial x_i} \right) \qquad \tau_{ij} = f(e_{ij}) \qquad i, j = 1, 2, 3$$

ENERGY: $\rho C_P \overline{V} \cdot \nabla T = k \nabla^2 T + \overline{\tau} : \nabla \overline{V}$

HELE – SHAW FLOW APPROXIMATION

$$\frac{\partial}{\partial x} \left(S \frac{\partial P}{\partial x} \right) + \frac{\partial}{\partial y} \left(S \frac{\partial P}{\partial y} \right) = 0 \qquad S(x, y) = \int_{o}^{h} \frac{z^{2} du}{\eta(x, y, z)}$$
$$\overline{V_{x}} = -\frac{S}{h} \frac{\partial P}{\partial x} \quad \overline{V_{y}} = -\frac{S}{h} \frac{\partial P}{\partial y} \qquad V_{y}(z) = -\frac{\partial P}{\partial y} \int_{0}^{h} \frac{z' dz'}{\eta(z')} \quad V_{x}(z) = -\frac{\partial P}{\partial x} \int_{0}^{h} \frac{z' dz'}{\eta(z')}$$

ENERGY: $\rho C_P \overline{V} \cdot \nabla T = k \nabla^2 T + \overline{\tau} : \nabla \overline{V}$ 3D

PLABOR JAPAN EXPERIMENTS

Barrel Diameter = 40 mm



 give measured value of pressure at both ends as boundary condition.
 predict pressure distribution / temperature distribution / extruder output

Material : LDPE, Power-law approximation







McMaster University Experiments - Single flighted screw, no mixing element - D=38 mm, L/D=24

Material: HDPE (80 RPM)

- FLOW RATE
- Measured: 13.34 kg/hr
- Predicted: 13.67 kg/hr
- PEAK PRESSURE
- Measured: 29.75 MPa
- Predicted: 27.21 MPa

Somewhat better results for LDPE

BRAMPTON ENGINEERING/McMASTER UNIVERSITY EXPERIMENTS CANADA



- L/D=30, Diameter (D)= 88.9mm
- 4 different screw designs
- LDPE MI 0.3
- LLDPE MI 1

Experimental conditions

- 16 runs performed: 4 screws x 2 polymers x 2 output rates
- Pressures measured at 8 locations along screw, plus at end of screw
 values recorded once per second
- Melt temperature measured at end of screw

L/D=30, Diameter (D)= 88.9mm Barrier screw with Maddock







Lagrangian melting particle simulation HDPE (Diameter of the initial solid particles: 5 mm)



Lagrangian melting particle simulation HDPE (Diameter of the initial solid particles: 5 mm)



Lagrangian melting particle simulation HDPE (Diameter of the initial solid particles: 2.5 mm)



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THANKS Q&A