

COMSOL Simulation Application for Thermoplastics Viscosity Measurement

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Abstract: Present study discusses a new method of how to apply COMSOL-Multiphysics® numerical simulation to improve the accuracy of polymer melts viscosity measurements. The main emphasis is placed on to evaluate the effects of entrance and exit geometry of a capillary rheometer on viscosity measurement. By combining experimental and COMSOL® simulation results, an accurate Bagley correction factor was found for a low density polyethylene (LDPE) - a stable power-law polymer melt. The results showed the Bagley correction factor based on COMSOL simulation was different from the experimental results. The method which combines experimental and simulation data can give an optimized value for Bagley correction factor for other thermoplastics. And it will be used to precisely predict polymer melt viscosity for online rheometers attached to an extrusion line.

Keywords: Capillary rheometer, shear viscosity, numerical simulation, viscous heating, Comsol.

1. Introduction

Most important characteristic of polymers vis-à-vis processability in extrusion is their viscosity behavior. The viscosity of a polymer melt is sensitive to both temperature and shear rate, which makes it a non-Newtonian fluid. For most of thermoplastic polymers, how to accurately measure viscosity is extremely important [1-6].

Many facilities rely on off-line viscosity measurements. However, off-line methods can't provide accurate real-time data because viscosity is directly affected by temperature, shear rate and other variables that can be different off-line from what they are in production. Therefore, in-situ viscosity measurement is crucial as it helps in making right decision on processability and to ensure consistent quality. That is why in-situ viscosity measurement is widely used in industry.

In-situ viscosity measurements are usually done either with capillary rheometer or slit die rheometer. Capillary rheometers are widely used because of following advantages over slit: i) they are economical to build and simple to operate; ii) provide closed-channel flows with no free surface in the test region, hence cast no edge effect as is the case with slit die rheometer; iii) can reduce errors caused by multiple pressure transduces. However, the raw data obtained from capillary rheometers includes entrance and exit losses, which need corrections introduced by Bagley to determine "true" as opposed to the "apparent" material functions i.e. shear stress, shear rate and shear viscosity [2-3]. The calculated Bagley correction factor only based on the experimental data always has some errors.

In order to accurately find Bagley correction factor to get the precise viscosity data of thermoplastic polymer melts, we used experimental data from a capillary rheometer and combined with COMSOL simulation to improve the accuracy of polymer viscosity.

2. Model Description

2.1 Geometry

A 3D geometry of custom-designed capillary rheometer was created in Autodesk Inventor® 2014, and imported to COMSOL® for simulation. The cap-face feature of COMSOL® was employed to create separate domains for cavities including the flow channel of capillary die, which is 5 mm in diameter and 150 mm long. The capillary die comprises of three stages i.e. stage1, L/D=10, stage2, L/D=20 and stage3, L/D=30, as shown in Fig. 1.

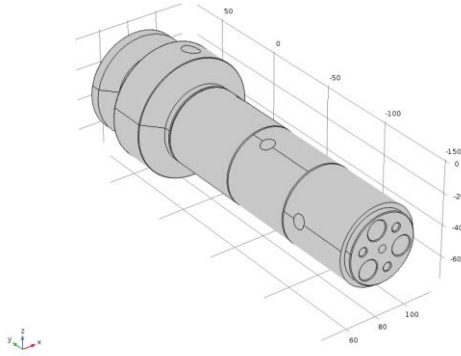


Figure 1: Geometry of Capillary Rheometer

2.2 Physics and boundary conditions

The Physics employed to simulate the experimental process conditions include: i) conjugate heat transfer to incorporate heat transfer both in solids and liquids by conduction, convection and radiation, ii) laminar flow interface to describe the velocity and pressure fields for the flow of a single-phase non-Newtonian polymer melt that obeys power law viscosity model, and iii) the events interface to maintain the process temperature near to the setting temperature at the thermocouple control points. This allows reaching a steady state condition at solid-fluid interface representing the process condition employed during experiment. In this regard COMSOL® Integration Operators are coupled with events interface. The Multiphysics coupling to couple the heat transfer interface and the laminar flow interface was non-isothermal flow. Under the study node a stationary, fluid study step was introduced to obtain consistent initial conditions followed by a time-dependent study. No slip condition was employed to the stationary solid wall representing the fluid-solid interface. The solver uses finite element method to solve equation of continuity, momentum and energy along with power law viscosity model. A finer mesh as shown in Fig. 2 with free tetrahedral elements was employed to domains of capillary cavity and solid geometry ensuring accuracy of results.

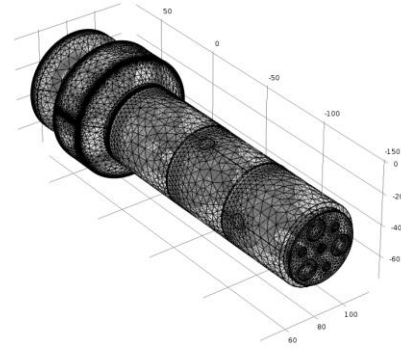


Figure 2: Tetrahedral mesh defined for fluid and solid domains

2.3 Governing equations

Listed below are the governing equations used to model the heat transfer and laminar flow. The constitutive equations representing material functions such as shear viscosity based on power law viscosity model are also presented.

Energy Equation for solid and fluid:

$$\rho C_p \frac{\partial T}{\partial t} + \rho C_p \mathbf{u} \cdot \nabla T + \nabla \cdot \mathbf{q} = Q + Q_{ted}$$

$$\rho C_p \frac{\partial T}{\partial t} + \rho C_p \mathbf{u} \cdot \nabla T + \nabla \cdot \mathbf{q} = Q + Q_p + Q_{vd}$$

Conduction heat flux:

$$\mathbf{q} = -k \nabla T$$

Convective heat flux:

$$q_0 = h \cdot (T_{ext} - T)$$

Momentum Equation:

$$\rho \frac{\partial \mathbf{u}}{\partial t} + \rho (\mathbf{u} \cdot \nabla) \mathbf{u} = \nabla \cdot \left[-p \mathbf{I} + \mu (\nabla \mathbf{u} + (\nabla \mathbf{u})^T) - \frac{2}{3} \mu (\nabla \cdot \mathbf{u}) \mathbf{I} \right] + \mathbf{F}$$

Continuity Equation

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u})$$

Power Law Viscosity Model:

$$\mu = m \dot{\gamma}^{(n-1)}$$

Where ρ is the density, C_p the heat capacity at constant pressure, k the thermal conductivity,

u the velocity field, Q the heat source, Q_{ted} the thermoelastic damping, Q_p the pressure work, Q_{vd} viscous dissipation, μ the dynamic viscosity of fluid, n the power law index, and $\dot{\gamma}$ the shear rate.

3. Methods and experimental setup

Our new method is introduced in this research study that involves use of experimental viscosity data measured on a capillary rheometer to run the simulation. A flow chart detailing the iterative method is shown in Fig. 3.

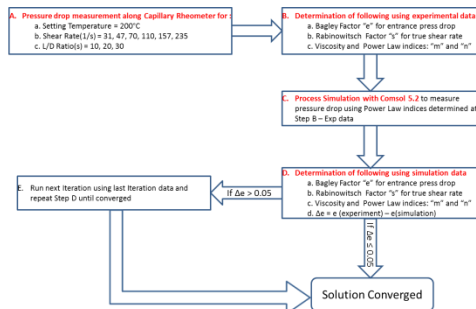
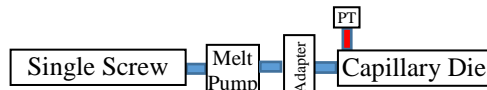


Figure 3. Flow chart detailing iterative method

The experimental viscosity data was obtained from pressure drop measurements of capillary rheometer mounted to an experimental setup that is shown in Fig. 4. A low density polyethylene (LDPE) grade was tested for its viscosity at setting temperatures of 190°C and 200°C and shear rates ranging from 44(1/s) to 340 (1/s) corresponding to a melt pump speed of 4rpm to 30rpm respectively. The melt pump delivers the polymer melt at a mass flow rate of 0.0117 lbs/rpm. The material properties are provided in Table 1. As explained earlier, for polymer melt viscosity measurement the use of capillary rheometer involves two types of end corrections: Bagley and Rabinowitsch. The former calculates the entrance pressure drop on L/D axis and determines the true wall stress, whereas the later determines true shear rate at wall.



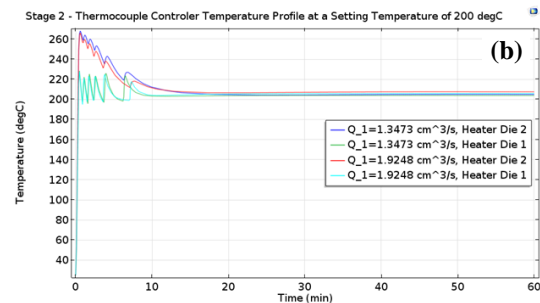
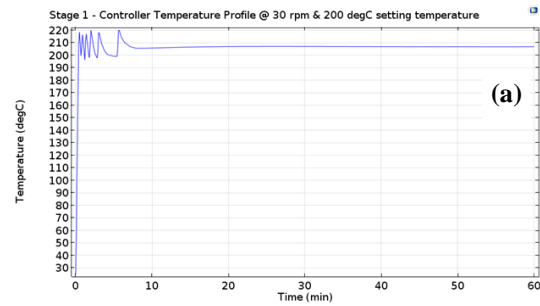
PT - Pressure transducer

Figure 4: Viscosity measurement system

4. Results and Discussion

Presented below in Figure 5(a) to 5(c) are the temperature profiles at thermocouple controller points for stage 1(L/D=10), stage 2(L/D=20) and stage 3(L/D=30) respectively. These profiles clearly indicate that after around 20 minutes of heating, a thermal equilibrium reached and the temperatures perfectly represented process setting temperature of 200°C.

Figure 6 and Figure 7 show Bagley Plots representing simulation (iteration-4) and experiment results respectively. It is evident from simulation Bagley plot [1,2,3] that the entrance correction factor (e) for the shear rates (melt pump speeds) reached a converged value of -3.42 on L/D axis after iteration-4 (Fig. 8). In other words, entrance correction factor “e” reported by simulation is more accurate compared with experiment. Which is why the viscosity curve obtained from simulation is 10% to 14% lower than that calculated by experimental data. This is reflected in Fig. 9, where shear thinning behavior of LDPE can also be observed with power law coefficients: $m=9700$, $n=0.3827$.



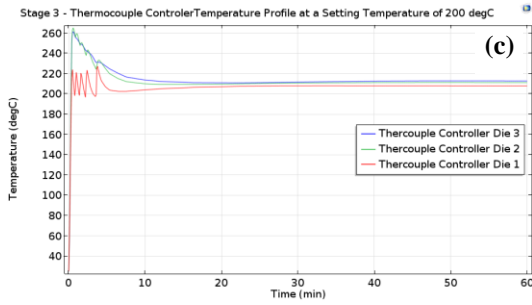


Figure 5. Temperature profile at thermocouple controller points: a) Stage-1, b) Stage-2 and c) Stage-3

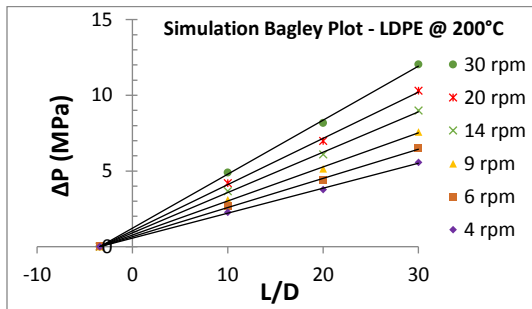


Figure 6. End Correction “e” – Simulation iter4

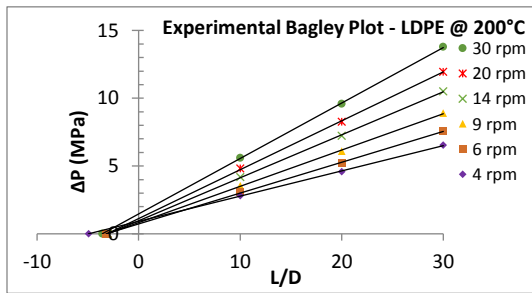


Figure 7. End Correction “e” – Experimental

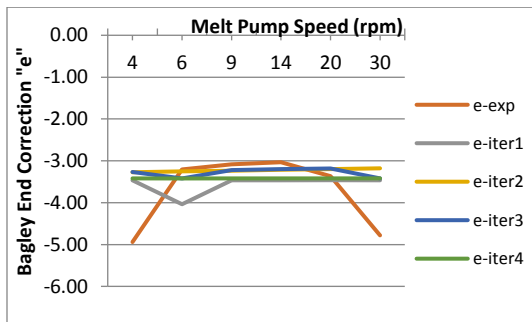


Figure 8. End Correction “e” – Exp. vs Sim.

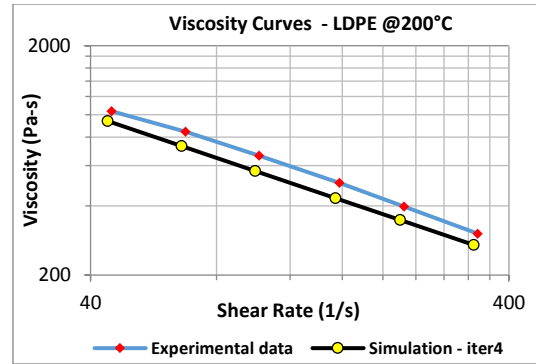


Figure 9. Viscosity Curves – Simulation vs Experimental Results

Table 1. Thermal and physical properties of LDPE

| Property | Nominal Value | Test Method |
|---|----------------------|-------------|
| Melt Flow Index (g/10min) | 0.33 (190°C/2.16 kg) | ISO 1133 |
| Density (g/cm ³) | 0.921 | ASTM D792 |
| Thermal Conductivity (W/m.K) | 0.18 | |
| Heat Capacity at constant pressure (J/kg.K) | 2604 | |

5. Conclusions

Study reveals that viscosity measurement of polymer melts using our new method can precisely and successfully obtain a converged value for Bagley correction factor and viscosity.

Accuracy in viscosity measurements can further be improved by incorporating viscous heating effects in viscosity calculation. Experimental data can't consider this part, but COMSOL simulation could. That will more precisely separate the contribution to viscosity change by temperature and shear rate.

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