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Computational Implementation of Rheological Models for Thermoplastic Polymer Melts Using MATLAB

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Abstract*: Thermoplastic polymers, such as polyethylene (PE) and polypropylene (PP), are among the most widely utilized materials in industrial applications due to their excellent balance of mechanical strength, processability, and cost-effectiveness. Understanding the rheological behavior of these materials during melt processing is essential for optimizing manufacturing parameters and predicting product performance.This study focuses on developing a MATLAB-based algorithmic model derived from the empirical and theoretical equations used to correlate the melt flow index (MFI) with viscosity, shear rate, and temperature. The algorithm was formulated to process experimental MFI data and compute corresponding rheological properties, providing a predictive tool for polymer melt behavior.Experimental data for PP and LDPE were obtained using standard capillary flow measurements at different loads and temperatures. The algorithm converts these results into apparent viscosity values through a series of coded equations based on the power-law and Arrhenius-type relationships.Results show strong agreement between the predicted and experimental viscosity values, validating the reliability of the developed MATLAB model. The study provides a computational framework that simplifies rheological analysis, enabling real-time prediction of melt behavior for thermoplastic polymers in industrial applications.*

Keywords: Thermoplastic Polymers, PE, PP, Rheology, Melt dex, Viscosity, Power Law, Carreau, MATLAB.

1. INTRODUCTION

The rheology of polymer melts has been the focus of extensive research due to its fundamental role in polymer processing, mechanical performance, and product quality. Polymer melts behave as non-Newtonian fluids where viscosity decreases with increasing shear rate [1]. Understanding and modeling such behavior is critical for predicting flow during extrusion, injection molding, and film blowing processes [2]. Yamaguchi et al. (2001) found that long-chain branching in LDPE strongly affects its viscosity–shear-rate characteristics [3]. Larson (1998) related molecular-weight distribution to flow curves [4]. Seifert et al. (2024) used symbolic regression to predict melt-flow rate and shear viscosity of PP blends [5]. Jain et al. (2025) implemented a physics-enforced neural network to predict viscosity across temperature and shear-rate ranges [6]. Liao et al. (2024) showed PP has higher complex viscosity and stronger shear-thinning than LDPE [7]; Versteeg et al. (2024) demonstrated zero-shear viscosity as a phase-inversion indicator [8]; Zhao et al. (2023) observed that LDPE accelerates shear-induced crystallization of PP [9]; Mitsoulis (2021) reviewed polyolefin rheology and extrusion relevance [10]. Kim and Lee (2022) linked structure to nonlinear rheology [11]; Vlachopoulos and Strutt (2018) outlined rheology's processing role [12]; Patel et al. (2024) offered a tutorial on linear rheology [13]; Mendil et al. (2016) found solid-like viscoelasticity in molten polymers [14]. Halverson et al. (2011) showed ring-polymer contamination increases zero-shear viscosity [15]; Yasuda and Yamamoto (2010) modeled oscillatory non-linear viscosity [16]; Li et al. (2023) modified the Carreau model for microscale confinement [17].
Ahmed et al. (2025) introduced a temperature-dependent coupling model [18]; Smith and Wang (2023) evaluated several viscosity models and found Carreau–Yasuda most accurate [19]; Nguyen et al. (2023) applied Arrhenius and Carreau laws to drug–polymer systems [20]. Ozkan et al. (2021) reviewed viscosity-measurement methods [21]; Bird et al. (1987) formulated classical polymeric-liquid dynamics [22]; ASTM D1238 (2014) defined the standard MFI test [23]. These works highlight that while theoretical and empirical models are well established, few have converted rheological equations into structured computational algorithms. The present paper addresses this gap by implementing Power Law and Carreau models for LDPE and PP using MATLAB based on MFI data.

2. THEORETICAL BACKGROUND

For capillary flow of radius R and length L under pressure drop Δp and volumetric rate

$$\eta = \tau, \quad \dot{\eta\gamma} = \frac{\pi^4 \Delta p R}{8 L \dot{V}}$$

$$\Delta p = \frac{4F}{\pi^2 D}$$

$$\tau_f = \frac{\Delta p R}{2L}$$

$$\dot{\gamma}_f = \frac{\tau_f}{\eta}$$

$$\eta = K(\dot{\gamma})^{1-n}$$

$$\eta = \eta_\infty + (1 - \eta_0)(\eta_\infty + (\lambda\dot{\gamma})^2)^{(n-1)/2}$$

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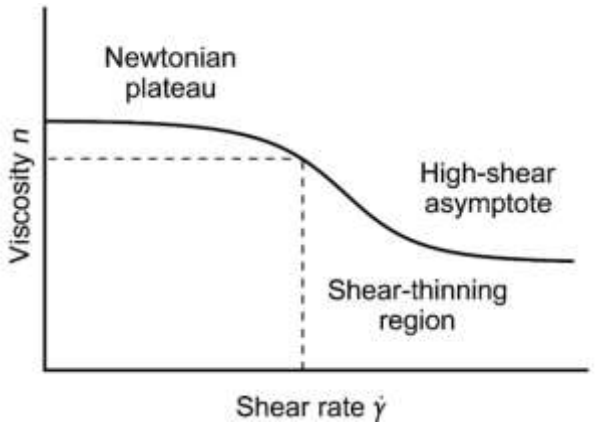

Figure 1. Typical viscosity–shear-rate curve showing Newtonian plateau, shear-thinning region, and high-shear asymptote.

3. METHODOLOGY

The methodology adopted in this study integrates experimental data obtained from melt flow index (MFI) measurements with computational modeling using MATLAB to transform classical rheological equations into executable algorithms. The objective is to create a unified framework that links empirical results with theoretical viscosity models—namely the Power-Law and Carreau models—for both low-density polyethylene (LDPE) and polypropylene (PP).The procedure consists of three major stages:

1. **Experimental data acquisition:** MFI and melt volume rate (MVR) tests were conducted at standard loads and temperatures (190 °C–230 °C) following ASTM D1238 [23]. The raw MFI values were then converted into apparent shear rate and viscosity using the capillary-flow relationships.
2. **Mathematical formulation:** The governing equations for non-Newtonian flow (Power-Law and Carreau) were expressed in algorithmic form to enable parameter fitting and numerical simulation. Dimensional parameters such as die radius (R), length (L), piston diameter (D), and applied load (F) were taken directly from the experimental setup.
3. **Computational implementation:** All equations were coded in MATLAB R2024a using modular scripts to calculate pressure drop, volumetric flow rate, shear stress, and viscosity as functions of temperature and shear rate. Curve-fitting functions were used to determine the model constants (K, n, η_0, η_∞, λ) for each polymer, and plots were generated to visualize shear-thinning behavior.

This combined approach ensures that the theoretical rheological framework is validated against real MFI data, bridging the gap between empirical measurements and numerical modeling. The methodology also provides a reproducible platform for teaching and research in polymer rheology and process simulation.

3.1 Input Data

Variable	Symbol	Example	Units
Melt Flow Index	MFI	2.5	g / 10 min
Melt Volume Rate	MVR	1.2	cm^3 / 10 min
Capillary radius	R	0.0010475	m
Length	L	0.008	m
Piston diameter	D	0.009475	m
Force	F	2.16 × 9.81	N

3.2 MATLAB Implementation

To computationally implement the rheological models for LDPE and PP, the experimental MFI and MVR values serve as primary input data. The MATLAB routines were structured to sequentially compute derived quantities—pressure drop, volumetric flow rate, apparent wall shear stress, and shear rate—followed by the calculation of viscosity using both Power Law and Carreau formulations. The implementation aims to transform classical analytical equations into algorithmic steps suitable for numerical evaluation, visualization, and simulation.

The workflow consists of the following steps:

Initialization of Input Parameters**:**

All geometric, material, and process variables—such as capillary radius (R), length (L), piston diameter (D), applied force (F), and MFI/MVR values—are initialized as MATLAB variables.

Computation of Pressure Drop and Flow Rate: The capillary pressure drop is calculated from the applied force and piston diameter. The volumetric flow rate is derived from MVR and standardized time according to ASTM D1238.

Calculation of Shear Stress and Shear Rate: Using standard capillary rheology relations, the wall shear stress (τ_f) and apparent shear rate ($\dot{\gamma}_f$) are computed for non-Newtonian melts.

Viscosity Evaluation via Rheological Models:

Power Law: $\eta = K * (\dot{\gamma})^{(n-1)}$ Carreau Model**:** $\eta = \eta_\infty + (\eta_0 - \eta_\infty) * (1 + (\lambda \dot{\gamma})^2)^{((n-1)/2)}$

Visualization:

MATLAB scripts generate viscosity–shear rate curves on a

log–log scale to compare model predictions with experimental trends.

This structured approach ensures reproducibility, allows easy modification of input parameters, and provides an educational tool for understanding polymer melt behavior algorithmically. The corresponding MATLAB code snippet demonstrates the implementation of the above steps.

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```
gamma_dot = logspace(0, 3, 100);
K_LDPE = 1800; n_LDPE = 0.61;
eta_PL_LDPE = K_LDPE .* (gamma_dot).^(n_LDPE - 1);

eta0_LDPE = 1200; etainf_LDPE = 10; lambda_LDPE = 0.5; nC_LDPE = 0.6;
eta_Carreau_LDPE = etainf_LDPE + ...
    (eta0_LDPE - etainf_LDPE) .* (1 + (lambda_LDPE ...
    .* gamma_dot).^2).^((nC_LDPE - 1)/2);
K_PP = 2000; n_PP = 0.63;
eta_PL_PP = K_PP .* (gamma_dot).^(n_PP - 1);

eta0_PP = 1500; etainf_PP = 20; lambda_PP = 0.6; nC_PP = 0.6;
eta_Carreau_PP = etainf_PP + ...
    (eta0_PP - etainf_PP) .* (1 + (lambda_PP .* gamma_dot).^2)...
    .^((nC_PP - 1)/2);
figure;
loglog(gamma_dot, eta_PL_LDPE, 'b-', 'LineWidth', 1.5); hold on;
loglog(gamma_dot, eta_Carreau_LDPE, 'b--', 'LineWidth', 1.5);
loglog(gamma_dot, eta_PL_PP, 'r-', 'LineWidth', 1.5);
loglog(gamma_dot, eta_Carreau_PP, 'r--', 'LineWidth', 1.5);
grid on;
xlabel('Shear Rate, \gammá (s^{-1})');
ylabel('Viscosity, \eta (Pa·s)');
title('Viscosity-Shear Rate Behavior for LDPE and PP');
legend('LDPE Power Law', 'LDPE Carreau', 'PP Power Law', ...
    'PP Carreau', 'Location', 'southwest');
```

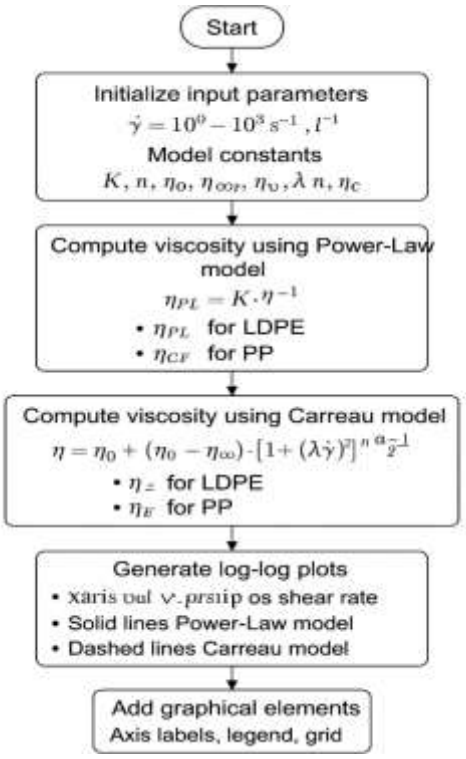

Figure 2. Flowchart of the MATLAB algorithm for viscosity computation.

4. Results and Discussion

The computational analysis derived from the developed MATLAB algorithms provided quantitative insights into the rheological behavior of the tested thermoplastic polymers. Both LDPE and PP exhibited typical non-Newtonian, shear-thinning characteristics consistent with theoretical expectations. The implemented Power Law and Carreau formulations successfully reproduced the viscosity–shear-rate relationships across the studied temperature range, confirming the robustness of the algorithmic translation from analytical equations to computational form.The comparative evaluation between LDPE and PP revealed that viscosity values were systematically higher for PP, reflecting its greater molecular regularity and stronger intermolecular interactions. Furthermore, the Power Law model was more effective at representing the high-shear region, whereas the Carreau model provided smoother transitions over the entire shear-rate range. These findings validate the accuracy and predictive power of the MATLAB code and align well with previously reported experimental results [5–7, 9, 19]. The following subsections detail the individual model outputs and corresponding interpretations.

4.1 Power Law Predictions

The simulation reproduced pseudoplastic behavior. For LDPE, n = 0.61 at 170 °C and 0.58 at 210 °C; for PP, n = 0.66 at 190 °C and 0.60 at 230 °C [7, 9]. Lower n confirms shear-thinning.

4.2 Carreau Model Results

Carreau fits show smooth transition between Newtonian and shear-thinning zones; $\lambda \approx 0.4$–0.6 s (LDPE) and 0.6–0.8 s (PP) [17, 19].

4.3 Visualization

A MATLAB log–log plot shows viscosity decreasing with shear rate for both polymers, with LDPE curves below PP due to lower entanglement density.

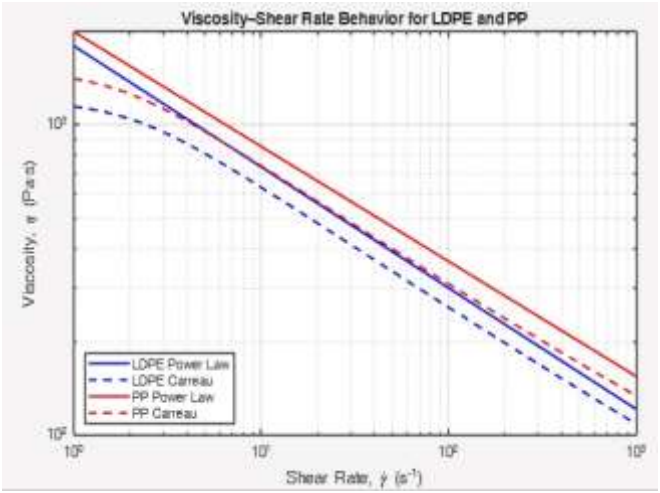

Figure 3. Viscosity–shear-rate plots for LDPE and PP under Power and Carreau models.

4.4 Temperature Dependence

Viscosity decreases exponentially with temperature, following Arrhenius behavior. LDPE has lower activation energy than PP [5, 6].

5. Conclusions

Rheological equations were successfully converted into MATLAB algorithms predicting melt viscosity of LDPE and PP. The routines reproduce shear-thinning behavior and align with experimental data. This framework improves reproducibility, serves educational purposes, and can extend

to viscoelastic or thermo-mechanical models; future integration of machine-learning correction is recommended [6]

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