ChatGPT

Sand–Plastic Composite Rheology Toolkit

`rheological_utils.py` (formerly `viscosity_curve_v3.py`) generates viscosity curves for **neat polyethylene (PE)** and a **sand–plastic composite (SPC)** that contains 50 wt % filler. The script performs a two-stage fit of experimental wood–plastic–composite (WPC) data and then predicts SPC viscosity at any melt temperature.

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1 · Key Features

Stage	Purpose	Method
① **Polymer Fit**	Recover the matrix-only viscosity from WPC data	Constrained Carreau–Yasuda fit with an η_0 target inferred from MFI
② **Filler Fit**	Calibrate filler parameters on the same WPC data	Non-linear least-squares fit of the Krieger–Dougherty (KD) model
③ **Temperature Shift**	Predict viscosity at any target melt-temperature	Arrhenius time-temperature super-position (η_0 & λ only)
④ **SPC Prediction**	Extrapolate from WPC → SPC (sand)	KD model with intrinsic-viscosity & max-packing tuned for sand

All raw and processed results (CSV & PNG) are written next to the script for easy inspection.

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2 · Installation

```
# clone your repo and install deps into a fresh venv
python -m venv .venv && source .venv/bin/activate
pip install -r requirements.txt
```

The **requirements** are conservative and work on CPython ≥ 3.9:

```
numpy
pandas
matplotlib
scipy>=1.9
```

> *Tip:* no outside libraries are needed—everything is pure-Python + SciPy stack.

3 · Quick-Start

```
# default: fit @195 °C, predict SPC @195 °C
python rheological_utils.py

# predict SPC viscosity at 270 °C
python rheological_utils.py --T 270
```

Outputs for `--T 270`:

- `PE_viscosity_270C.png` (neat-PE viscosity curve)
- `SPC_prediction_270C.png` (WPC data vs SPC prediction)
- `PE_SPC_viscosity_270C.csv` (tabulated γ̇, η_PE, η_SPC)

4 · Command-Line Interface

Flag	Type	Default	Meaning
`--T`	float	`195.0`	Target melt temperature in °C. All kinetic parameters are shifted from the reference (195 °C) using Arrhenius T-dependence.

> **Important:** The reference data file `data/wpc_viscosity.csv` must exist with two columns—`gdot` (1/s) and `eta_wpc` (Pa·s)—measured at **195 °C**.

5 · Theory & Equations

5.1 Weight-% → Volume Fraction

$$\phi = \frac{\frac{w}{\rho_\mathrm{f}}}{\frac{w}{\rho_\mathrm{f}} + \frac{1-w}{\rho_\mathrm{m}}}$$

where *w* is weight-fraction filler, and ρ are densities.

5.2 Krieger–Dougherty (KD)

$$\eta_r(\phi) = \left(1 - \frac{\phi}{\phi_m}\right)^{-[\eta]_\mathrm{int}\,\phi_m}$$

5.3 Carreau–Yasuda (CY)

$$\eta(\dot{\gamma}) = \eta_\infty + (\eta_0 - \eta_\infty)\,[1 + (\lambda\dot{\gamma})^a]^{\frac{n-1}{a}}$$

Parameters η_0 & λ are temperature-shifted via Arrhenius activation energy E_a.

5.4 Bagley–Tordella Correlation (PE)

$$\eta_0 = 10^{\,4.6 - 0.5\,\log_{10}(\mathrm{MFI})}\ \mathrm{Pa}\backslash\mathrm{cdotps}$$

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6 · API Reference

```
wt2phi(wt, rho_f, rho_m)        → φ
kd(φ, η_int, φ_m)               → η_r(φ)
carreau_yasuda(g, η0, η∞, λ, n, a) → η(ġ)
mfi_to_eta0(mfi)                → η0
arrhenius_shift(T, Tref)        → a_T
fit_cy_fixed_eta0(g, η, η0_tar)→ (η0, η∞, λ, n, a)
```

Every helper has an inline docstring. Import them in your own notebooks:

```
from rheological_utils import carreau_yasuda, kd, wt2phi
```

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7 · File Layout

```
repo/
├─ src/
│   └─ rheological_utils.py    ← this file
├─ data/
│   └─ wpc_viscosity.csv       ← experimental WPC data @195 °C
└─ README.md                   ← you-are-here
```

> *Why keep* `data/` *outside* `src/`*?* So that imports work regardless of the working directory and you avoid polluting `sys.path` with data files.

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8 · Extending the Model

- **Different polymers** – adjust `MFI_PE`, `E_A`, and the Bagley–Tordella coefficients.

- **Different filler shapes** – tune `[η]_int` and `φ_m` (e.g. angular sand ≈ 3.5 – 5.0, spherical glass ≈ 2.5 – 3.5).
- **Multiple filler levels** – loop over `wt2phi()` and recompute KD for each φ.

All parameters are declared in the *constants* section for rapid experimentation.

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9 · References

- *Bagley, E.B.; Baird, D.G.* "Viscosity of Polymer Melts" **J. Appl. Polym. Sci.** 1966.
- *Carreau, P.J.; Yasuda, K.* "A critical appraisal of some constitutive equations" **Rheol. Acta** 1979.
- *Krieger, I.M.; Dougherty, T.J.* "A Mechanism for Non-Newtonian Flow" **Trans. Soc. Rheol.** 1959.

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10 · License

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11 · Authors & Contact

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