ViscoPINN: Viscosity Prediction Software

Overview

ViscoPINN is a MATLAB-based software package for predicting temperature-dependent viscosity of multicomponent aqueous mixtures using a **Physics-Informed Neural Network (PINN)** framework. The software supports mixtures of up to **17 pure components** and enables both direct PINN inference and optional **Vogel–Fulcher–Tammann (VFT)** extrapolation toward the glass transition regime.

The package is distributed in two complementary forms:

1. **Standalone Windows executable (.exe)** for plug-and-play use without MATLAB
2. **MATLAB function-based interface** for scripting, automation, and reproducibility

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Package Contents

The repository/package folder contains the following files:

Core Files

- **ViscosityPredictor.m**
  Main MATLAB function implementing the PINN-based viscosity prediction. This function performs input normalization, network inference, optional VFT fitting, and output formatting.
- **PINN.mat**
  Trained Physics-Informed Neural Network model required for all predictions.
- **mixture_data.mat**
  Supporting mixture property data used internally by the model.
- **Tg_fitted_VFT.mat**
  Pre-fitted parameters used for VFT extrapolation when enabled.

Example and Output Files

- **Example.m**
  Demonstration MATLAB script showing how to call ViscosityPredictor programmatically, define mixture composition, specify temperature range, and visualize results.

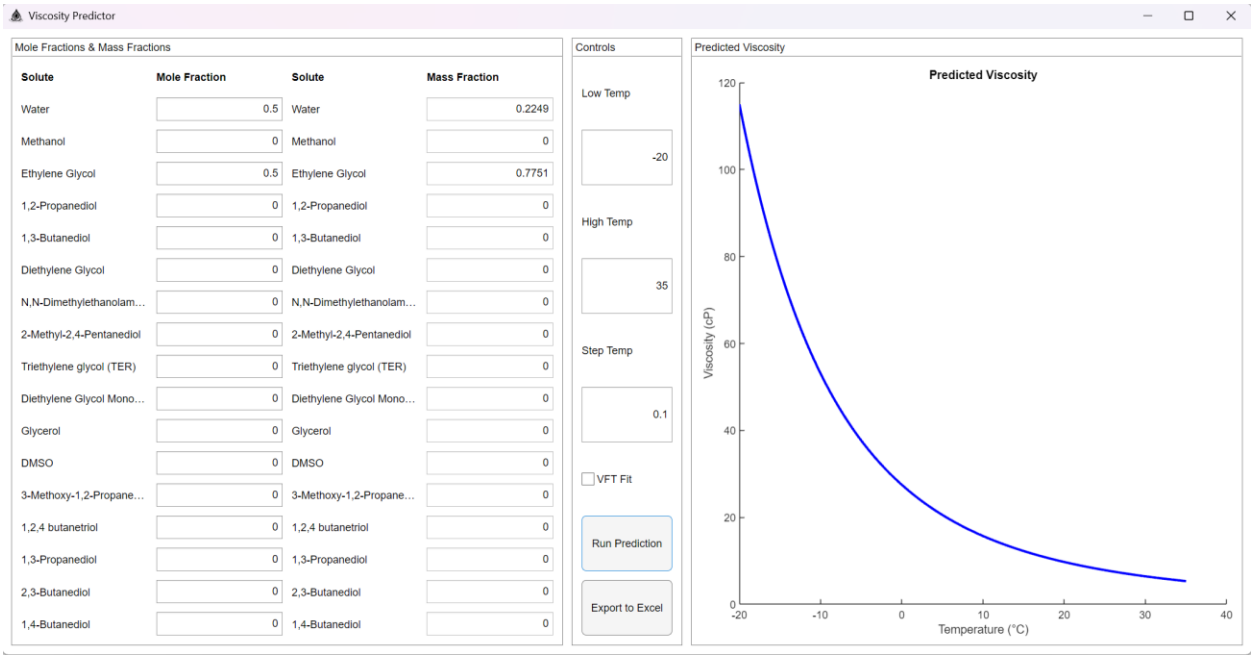
- **MyResults.xlsx**
  Example output file generated by the software when exporting predicted viscosity–temperature data.

Standalone Application

- **MyAppInstaller_web.exe**
  A standalone Windows executable providing a **graphical user interface (GUI)** for viscosity prediction.
  This version does **not require MATLAB** and is intended for user-friendly, interactive use.

Standalone GUI Application (No MATLAB Required)

The ViscoPINN GUI provides a plug-and-play interface for viscosity prediction and is suitable for users without programming experience.



GUI Structure

The interface consists of three main panels:

1. Input Panel

- Users define mixture composition using **mole fractions or mass fractions**

- Supports up to **17 components**
- Fractions are internally normalized by the software

2. Control Panel

- Temperature range specification:
    - Lower bound (°C)
    - Upper bound (°C)
    - Step size (°C)
- **VFT Fit option**:
    - **Unchecked (default):** Direct PINN inference
        - Highest accuracy within the training range: **−20 °C to 35 °C**
    - **Checked:** PINN + VFT fitting
        - Enables theoretical extrapolation toward the glass transition temperature
- Buttons:
    - **Run Prediction**
    - **Export to Excel**

3. Output Panel

- Displays predicted viscosity as a continuous function of temperature
- Output units: **centipoise (cP)**
- Provides immediate visualization of non-linear temperature and composition effects

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MATLAB Function Usage

Advanced users may directly call the prediction engine from MATLAB for scripting, batch processing, or integration with other models.

Basic Usage

finalResults = ViscosityPredictor(...

moleFractions, ...

LowT, StepT, HighT, ...

useVFT, ...

outputFile);

Input Arguments

Argument	Description
moleFractions	1×17 vector of mole fractions (must sum to 1)
LowT	Lower temperature bound (°C)
StepT	Temperature increment (°C)
HighT	Upper temperature bound (°C)
useVFT	Logical flag (true / false) for VFT fitting
outputFile	Excel filename for exported results

Example MATLAB Script

```
clc; clear; close all;

% Initialize mole fractions
myMoleFractions = zeros(1,17);
myMoleFractions(1) = 0.5;  % Water
myMoleFractions(2) = 0.5;  % Methanol

% Temperature range
LowT  = -20;
HighT = 35;
StepT = 0.5;
```

```
% Enable VFT extrapolation
useVFT = true;

% Output file
outputFile = 'MyResults.xlsx';

% Run prediction
finalResults = ViscosityPredictor( ...
   myMoleFractions, LowT, StepT, HighT, useVFT, outputFile );

% Extract results
Temperature = finalResults.Temperature;
Viscosity   = finalResults.Viscosity;

% Plot
figure;
plot(Temperature, Viscosity, 'b-', 'LineWidth', 2);
grid on;
xlabel('Temperature (°C)');
ylabel('Viscosity (cP)');
title('Predicted Viscosity vs Temperature');
```

Notes on Model Validity

- Direct PINN predictions are most accurate within **−20 °C to 35 °C**

- VFT extrapolation enables extension toward lower temperatures but should be interpreted as **theoretical extrapolation**
- The model is trained on experimentally validated multicomponent datasets described in the accompanying publication

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Citation

If you use this software, please cite:

Kavian *et al.*, *[Journal Name]*, Year.
ViscoPINN: Physics-Informed Neural Network for Multicomponent Viscosity Prediction.

(Full citation provided in the manuscript.)