

Supplementary Information – Machine Learning of Polyurethane Prepolymer Viscosity: A Comparison of Chemical and Physicochemical Approaches

A.1: Full Chemical Model Results

Table A.1 Full modeling results for the RF and GPR chemical models.

<i>Regresso r</i>	<i>Data</i>	<i>R² Train</i>	<i>RMSE Train (Pa·s)</i>	<i>R² Test</i>	<i>RMSE Test (Pa·s)</i>
RF	All	0.91	9.13	0.57	20.82
-	>25 Pa·s	0.70	27.51	-1.31	62.70
-	<25 Pa·s	0.94	1.39	0.39	3.53
-	>60 °C	0.91	3.01	0.35	4.27
-	<60 °C	0.93	9.02	0.12	46.98
-	Iso-Only	0.57	24.50	0.16	36.64
-	Poly-Only	0.57	24.68	0.33	32.78
GPR	All	0.76	14.63	0.71	17.27
-	>25 Pa·s	1.00	0.01	-0.61	52.35
-	<25 Pa·s	0.81	2.42	0.68	2.54
-	>60 °C	0.86	3.75	0.31	4.39
-	<60 °C	0.91	10.04	0.29	42.24
-	Iso-Only	0.35	30.33	0.20	35.66
-	Poly-Only	0.36	30.02	0.35	32.19

A.2: Full Physical Model Results for Predicting $\eta(T)$

Table A.2 Full modeling results for the RF and GPR physical models for predicting raw viscosity with temperature.

<i>Regresso r</i>	<i>Data</i>	<i>R² Train</i>	<i>RMSE Train (Pa·s)</i>	<i>R² Test</i>	<i>RMSE Test (Pa·s)</i>
RF	All	0.92	8.25	0.60	20.12
-	Sparse Feature Set	0.92	8.72	0.54	21.54
GPR	All	0.83	12.20	0.73	16.50
-	Sparse Feature Set	0.74	15.12	0.73	16.58

A.3: Full Physical Model Results for Predicting B

Table A.3 Full modeling results for the RF and GPR physical models for predicting the Andrade B activation parameter.

<i>Regresso r</i>	<i>Data</i>	<i>R² Train</i>	<i>RMSE Train (Pa·s)</i>	<i>R² Validation</i>	<i>RMSE Validation (Pa·s)</i>
RF	All	0.98	17.65	0.75	89.18
-	Sparse Feature Set	0.98	15.71	0.78	83.53
GPR	All	0.98	18.24	0.59	113.41
-	Sparse Feature Set	0.96	24.76	0.86	65.89

A.4: SHAP Feature Importance for Physicochemical Viscosity Model

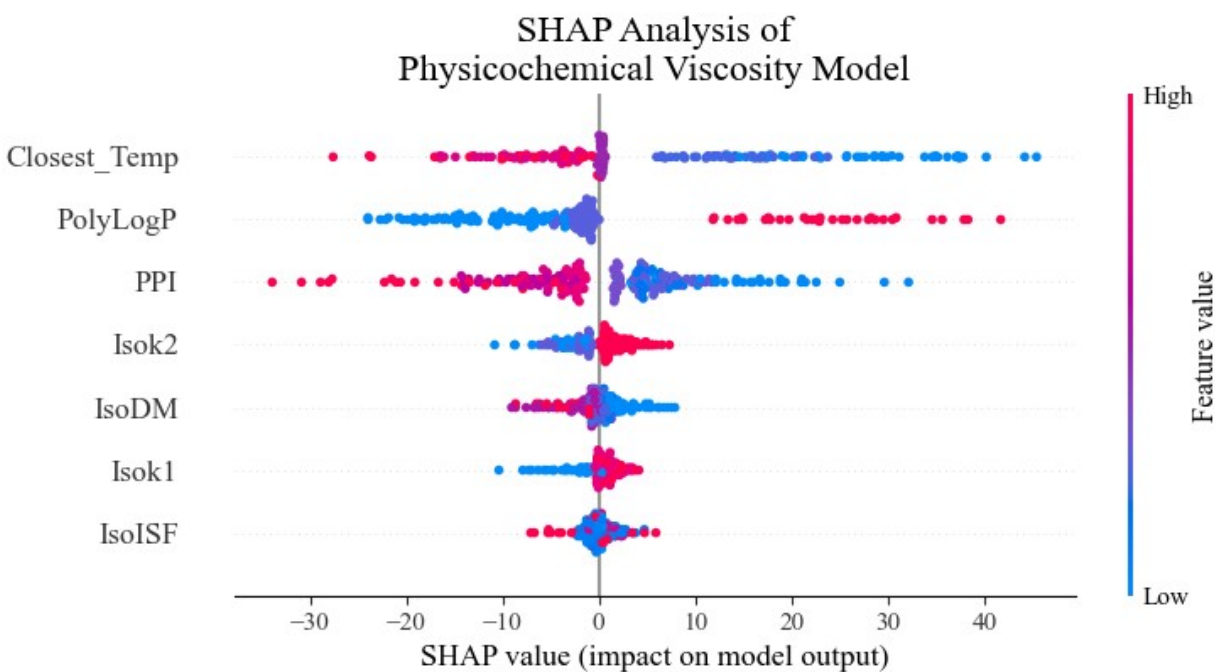


Figure A.1 SHAP analysis beeswarm plot for the GPR physical model for predicting raw viscosity with temperature.