Support Information for

A Nearly Zero-cost Lot-by-lot Inspection of Recycled Plastics: Prediction of Mechanical Properties from Viscosity Evolution during Melt Kneading

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Captions for Supplementary Data 1-2

Other Supplementary Materials for this manuscript include the following:

Data 1-2 are attached in csv format.

Supplementary Figures and Tables

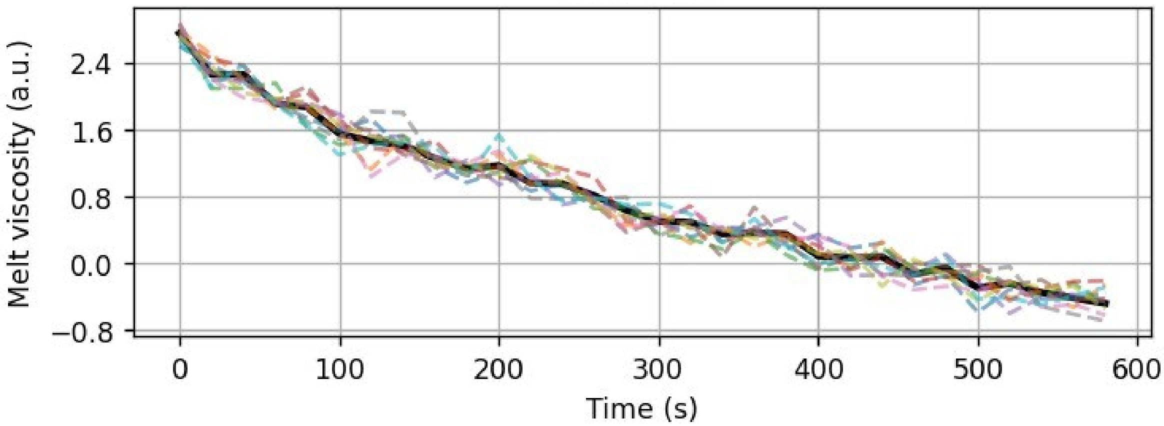

Fig. S1. Data augmentation by adding Gauss noise with standard deviation of 0.15 to the original curve (black bold curve).

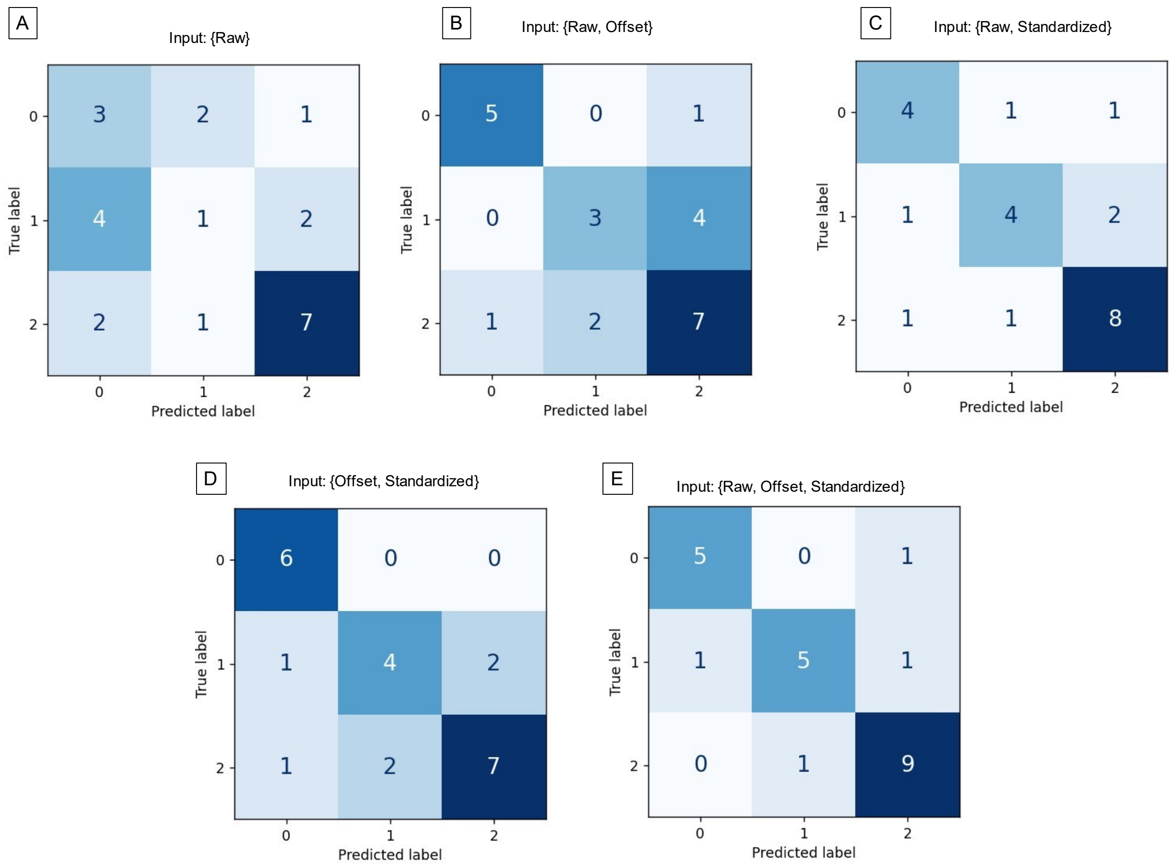

Fig. S2. Confusion matrices representing the results of tensile predictions based on (A) raw data, (B) raw and mean-zero offset data, (C) raw and standardized data, (D) mean-zero offset and standardized data, and (E) all three data.

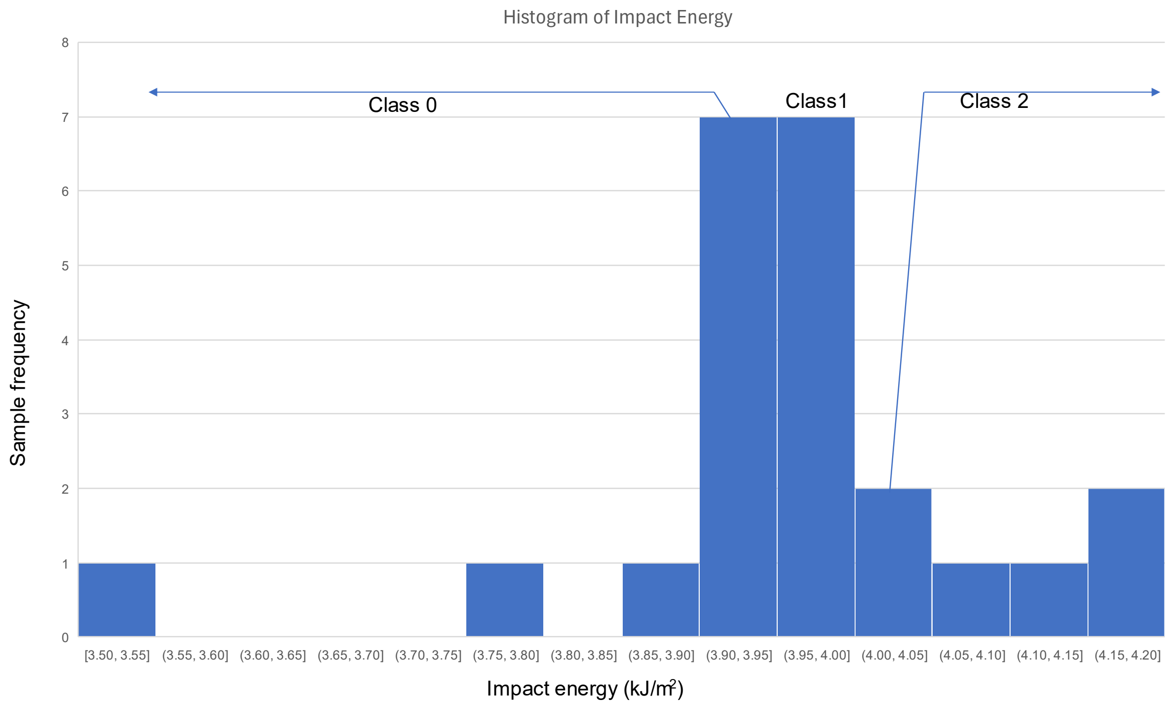

Fig. S3. Distribution of averaged Charpy impact energies from five trials for each sample. See Table S1 for the numerical data. With a standard deviation of 0.07–0.1 kJ/m² across five trials, splitting classes at 3.95 kJ/m² appears arbitrary. Initially, samples with impact energies of 3.90–3.95 kJ/m² were labeled as Class 1, but this led to an imbalanced class distribution: Class 0: 3, Class 1: 14, Class 2: 6. This class imbalance caused prediction errors, as the small size of Class 0 (only 3 members) made feature extraction unreliable. Therefeore, we reclassified the seven samples with impact energies of 3.90–3.95 kJ/m² as Class 0. This adjustment resulted in a more balanced dataset: Class 0: 10, Class 1: 7, Class 2: 6. Although this reclassification may introduce mislabeling due to the relatively large standard deviation, soft labeling mitigated this uncertainty. The soft label for Class 0, defined as [0.75, 0.2, 0.05], reflects the possibility that Class 0 samples could actually belong to Class 1 with a 0.2 probability or to Class 2 with a 0.05 probability.

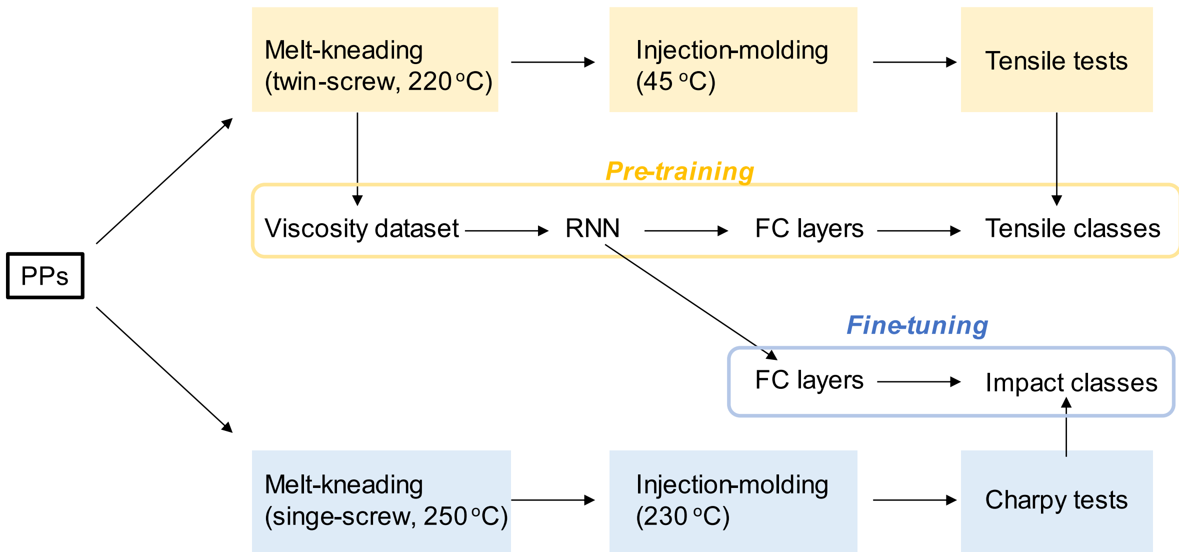

Fig. S4. Flowchart illustrating the relationship between viscosity data, tensile classes, and impact classes. During LOOCV, test data for both tensile and impact classes remained unlabeled and were never used for training. Despite differences in conditions between viscosity acquisition and the preparation of Charpy test specimens, transfer learning from tensile prediction to impact prediction enabled sufficiently accurate predictions, as shown in Fig. 5D. In practical applications, the top orange process represents pelletization, where viscosity data is acquired, while the bottom teal process corresponds to the customer's final product manufacturing. The target property—herein corresponding to Charpy impact energy but not limited to it—can be predicted from viscosity data obtained during pelletization, allowing customers to select pellets optimized for their specific applications.

Table S1. Numerical data of the 23 recycled PP samples used in this study, including tensile properties (averaged values over two trials), impact energy per unit area (averaged values over five trials), and assigned classes.

Sample code	Elastic modulus [MPa]	Yield stress [MPa]	Breaking strain[%]	Impact energy per area [kJ/m^2]	Tensile class	Impact class
PP0	915.40	26.53	186.84	3.50	2	0
PP1	942.05	26.78	289.16	3.80	1	0
PP2	958.77	27.55	192.96	3.88	2	0
PP3	937.35	26.97	359.59	3.92	1	0
PP4	969.02	27.63	191.70	3.92	2	0
PP5	936.67	27.22	250.98	3.92	1	0
PP6	960.34	27.43	186.12	3.93	2	0
PP7	930.52	27.28	263.77	3.93	1	0
PP8	881.30	25.51	303.96	3.93	0	0
PP9	776.46	23.06	414.71	3.93	0	0
PP10	808.41	23.17	368.00	3.95	0	1
PP11	867.59	25.07	304.73	3.96	0	1
PP12	930.38	27.22	250.87	3.98	1	1
PP13	1017.57	27.64	183.46	3.98	2	1
PP14	995.45	28.05	139.34	3.98	2	1
PP15	967.64	27.40	270.55	3.99	1	1
PP16	838.39	24.21	307.27	3.99	0	1
PP17	955.64	27.62	270.81	4.01	1	2
PP18	1050.54	28.41	183.39	4.02	2	2
PP19	976.28	27.42	191.89	4.06	2	2
PP20	1012.12	27.57	63.25	4.15	2	2
PP21	810.15	23.42	330.78	4.18	0	2
PP22	1012.28	27.25	191.41	4.20	2	2

Tensile classes were determined through hierarchical clustering based on the three tensile properties (Fig. 2), while impact classes were assigned by thresholding at 3.95 and 4.0 kJ/m^2

(Fig. S3). The standard deviations of impact energy across five trials ranged from 0.07 to 0.1 kJ/m^2, introducing uncertainty in impact class labeling. This uncertainty was addressed through the application of soft labeling and label distribution learning (see main text).

Caption for Data S1.

The dataset includes melt viscosity measurements and tensile test results from two trials for each sample. The tensile data, comprising absolute strain (mm) and force (N), can be converted to relative strain (%) and stress (MPa) using the specimen dimensions (width: 5.08 mm, depth: 2.04 mm, length: 52.3 mm).

Caption for Data S2.

Python source code for model implementation using the PyTorch package.