Leveraging Machine Learning for Recyclate Transparency and Circular Material Compliance

Dr. Sara Simon[1*], Dr. Natalie Rudolph[1]

[1] NETZSCH Analyzing & Testing, Selb, Germany

* Dr. Sara Simon *(sara.simon@netzsch.com)*

Keywords: *Recycling, Circular-economy materials technologies, AI, Machine learning, Proteus® Now Quantify*

1. Abstract

Regulatory pressure is accelerating the shift toward circular plastics. The EU will require documented proof of recyclate origin and composition by 2030, while regions such as Canada are advancing recycled-content and labelling rules. These trends make reliable, scalable analysis of recycled materials increasingly essential for compliance and market access. NETZSCH developed Proteus® Now Quantify, a machine-learning–assisted tool designed for estimating polymer-family composition and blend ratios in unknown recyclates. Trained on curated datasets of known polymers and calibrated blends, the model detects characteristic thermal patterns and delivers composition predictions with typical errors of 1–5%. This automated approach enhances recyclate transparency, accelerates quality assessments, and demonstrates how AI can strengthen sustainable materials technologies and circular-economy compliance.

2. Introduction

The transition toward a circular plastics economy is accelerating, driven by regulatory mandates, sustainability targets, and resource constraints. Recyclates are increasingly deployed in structural applications, where material performance requirements are stringent. However, in contrast to virgin polymers - manufactured under tightly controlled conditions with well-defined specifications - recyclates constitute heterogeneous and poorly defined material systems. Their composition is governed by mixed waste streams, additive packages, fillers, contamination, degradation history, and supplier variability, resulting in substantial uncertainty in both material identity and composition [1–3].

This uncertainty represents a fundamental limitation for the scalable and reliable use of recycled materials. Even classifications such as “PP” or “PP mix” can obscure complex multi-component systems, where small compositional variations induce nonlinear effects on crystallization behavior, rheology, and mechanical performance. These effects propagate into processing instabilities and variability in final product properties, often leading to conservative strategies such as overengineering or material downgrading.

At the same time, regulatory frameworks impose increasingly stringent requirements on recycled materials. The European Union's Circular Economy Action Plan, Packaging and Packaging Waste Regulation (PPWR), and Ecodesign for Sustainable Products Regulation (ESPR) introduce mandatory recycled-content targets and require traceable material composition [4–6]. Similar developments in Canada and the United States reinforce the need for accurate identification, quantitative compositional analysis, and standardized reporting [7-9]. These requirements establish quantitative material transparency as a prerequisite for compliance and market access.

Conventional characterization methods such as melt flow index (MFI) and Fourier-transform infrared (FTIR) spectroscopy are widely used but exhibit significant limitations for complex recyclates. These techniques are often qualitative, lack universality, and struggle with heterogeneous or multilayer systems [2–4, 10–11]. Even differential scanning calorimetry (DSC), while capable of detecting polymer phases and thermal transitions, does not directly provide quantitative composition for complex blends due to overlapping signals, unknown material histories, and non-ideal blending behavior. As a result, analysis remains highly dependent on expert interpretation, limiting throughput, introducing operator-dependent variability, and hindering integration into scalable, automated workflows.

From a data-science perspective, recyclate characterization can be formulated as a high-dimensional pattern recognition problem, where thermal signals encode information about polymer identity and composition. Machine learning (ML) enables the extraction of latent features from these signals and their mapping to quantitative descriptors [12-14]. When trained on calibrated datasets, such models can generalize to unknown material systems. Integrating ML into thermal analysis workflows enables the transition from expert-driven interpretation to automated, reproducible, and scalable data evaluation, allowing non-specialists to perform quantitative compositional analysis and enabling deployment in industrial quality-control environments [13-15].

However, a critical constraint remains: DSC-derived features are highly sensitive to measurement conditions. Variations in experimental parameters introduce signal changes that are not separable from compositional effects, making standardized testing conditions a prerequisite for meaningful ML-based analysis.

This work establishes that standardized DSC measurement conditions are required for machine learning-based quantitative compositional analysis of recyclates and introduces an automated framework (Proteus® Now Quantify) for identifying and quantifying polymer fractions in unknown materials.

3. Methods and Procedures

3.1. *Compounding of Calibrated Polymer Blends*

Proteus® Now Quantify is trained on calibrated polymer blends composed of virgin materials with known constituents and defined mass fractions. Virgin polymers provide reproducible thermal fingerprints, while post-consumer recyclates exhibit uncertain compositions and are unsuitable as ground-truth datasets.

The training strategy is based on the observation that variability within a polymer class (polyolefins) exceeds differences between virgin and recycled grades [16]. A diverse set of polyolefins (LLDPE, LDPE, HDPE, PP) from multiple suppliers was used.

Blends were produced via controlled compounding with compositions ranging from trace levels (<5 wt%) to dominant fractions (>80 wt%), reflecting realistic contamination scenarios and dominant phase behavior relevant for model training. Compounding ensured homogeneous, representative materials with realistic phase interactions and crystallization behavior, providing a robust and physically meaningful basis for model training and validation.

3.2. DSC Measurement Conditions and Calibration

Measurements were performed using NETZSCH DSC 214 Polyma or a NETZSCH DSC 300 Caliris. Blend analyses were conducted in AI Concavus® crucibles with pierced lids under a nitrogen atmosphere (e.g., 60 mL/min protective gas and 40 mL/min purge gas for the DSC 300 Caliris). Samples were analyzed from −20 °C to 200 °C with calibrated temperature and heat-flow signals as well as an activated baseline correction (BeFlat®).

To define reproducible conditions for machine learning-based quantification of thermal analysis data, sample mass and heating and cooling rates were systematically varied as shown in Table 1. These settings were established for pure polymer and were confirmed for mixtures / blends. [17].

Table 1: Investigated Test Settings for Defining Standardized Test Conditions.

Test Setting	**Unit**	**Value**
Sample Mass	mg	10, 20
Heating Rate	K/min	5, 10, 20
Cooling Rate	K/min	5, 10, 20

3.3. ML-Based DSC Data Evaluation with Proteus®Now Quantify

Proteus® Now Quantify applies supervised machine learning to map DSC thermograms to polymer composition.

Thermal signals are processed by modular data processing pipelines that automatically elevate the raw measurement data to a higher quality level through calibration, signal reduction, and additional preprocessing steps, before extracting features such as transition temperatures, peak shape, and enthalpy.

The framework incorporates machine learning algorithms, complemented by advanced data-driven approaches to capture non-linear relationships in multi-component systems. Model performance was validated using independent datasets of known composition.

4. Results and Discussions

DSC-derived features are highly sensitive to experimental conditions. From a machine learning perspective, variations in measurement parameters are not separable from compositional differences, as both manifest as changes in the input signal. Therefore, strictly standardized testing conditions are essential, and in this section the optimal parameters are determined.

4.1. *Sample Mass*

Sample mass affects peak resolution and signal quality. Higher mass (20 mg) increases thermal gradients within the specimen and between the sample and sensor, causing thermal lag, peak broadening, and reduced separability of overlapping transitions. This effect is shown in Figure 1 for a polyolefin blend (HDPE, LDPE, LLDPE). Lower mass (10 mg) improves peak resolution, but reducing the mass below 10 mg can decrease signal intensity, increase baseline noise, and introduce greater measurement uncertainty.

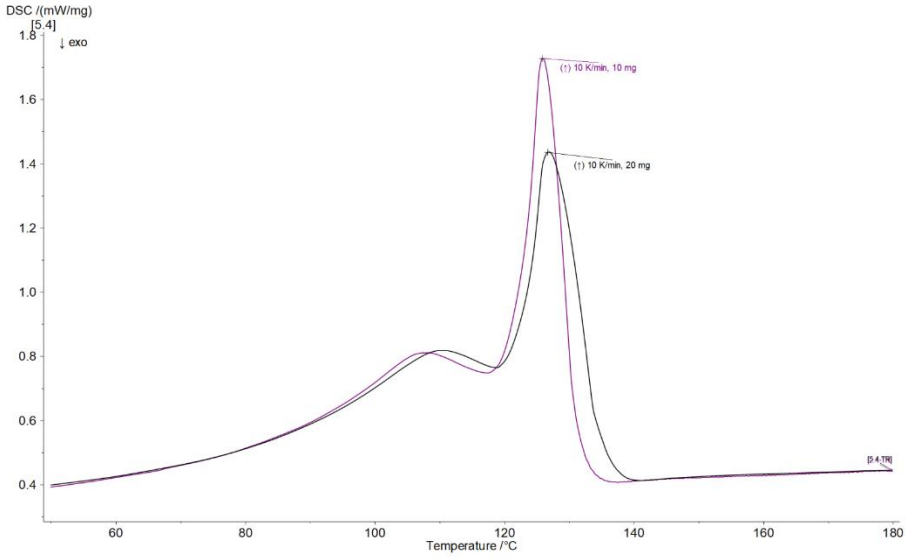

Figure 1: Effect of sample mass (10 mg, 20 mg) at 10 K/min heating rate for a polymer blend of HDPE, LDPE, and LLDPE (33.3% each).

Considering these effects, a mass of 10 mg ± 1 mg defines an optimal operating point, ensuring consistent feature representation for machine learning.

4.2. *Heating and Cooling Rates*

Heating and cooling rates influence peak position and morphology. Higher heating rates shift transitions to higher temperatures (thermal lag, broadens peaks, reducing the resolution of closely spaced events; Figure 2), while higher cooling rates alter crystallization behavior (Figure 3). Crystallization is shifted to lower temperatures and influence peak morphology and apparent crystallinity through kinetic effects, including changes in nucleation and crystal growth behavior. As a result, even identical materials exhibit systematic variations in DSC signals when measured under different rates.

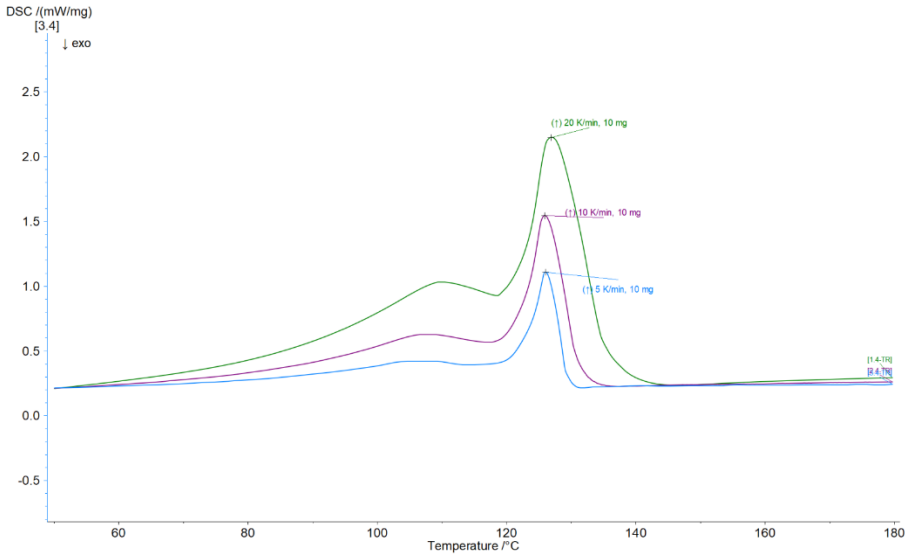

Figure 2: Effect of the heating rate (5, 10, 20 K/min) for a 10-mg sample of a blend containing HDPE, LDPE, and LLDPE (33.3 % each).

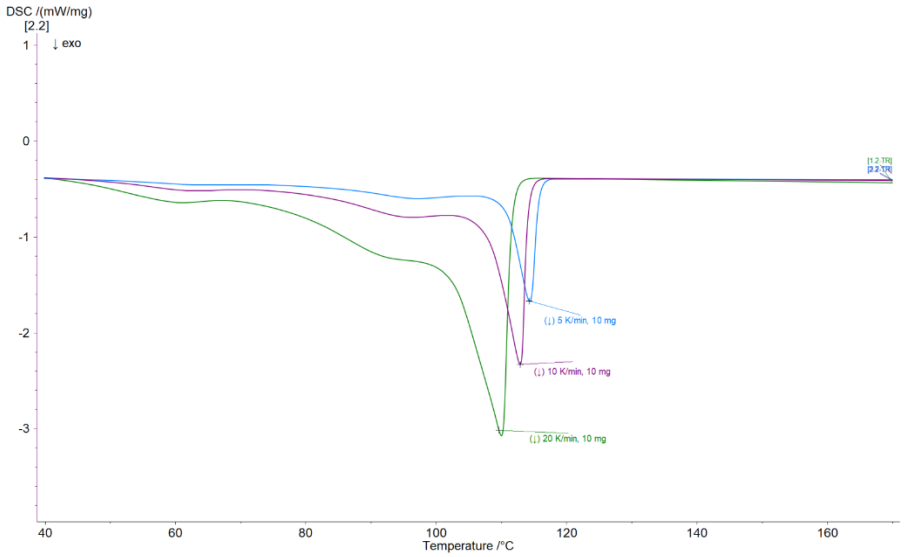

Figure 3: Effect of the cooling rate (5, 10, 20 K/min) for a 10-mg sample of a blend with HDPE, LDPE, and LLDPE (33.3% each).

A rate of 10 K/min was selected to ensure consistent and reproducible feature extraction, as rate-dependent changes in transition temperature, peak shape, and enthalpy can introduce systematic deviations in the feature space and reduce prediction accuracy if not strictly standardized.

4.3. *Validation with Known Recyclate*

Using these standardized test conditions, calibrated blends were analyzed under identical parameters to generate a consistent reference databank. Model performance was validated using a

known recyclate sample with defined composition (Figure 4, Table 2). Low deviations between predicted and target compositions confirm robust performance. Accuracy is quantified using the root mean square error (RMSE), which reflects the deviation between predicted and actual compositions and depends on the amount and quality of training data for each polymer class.

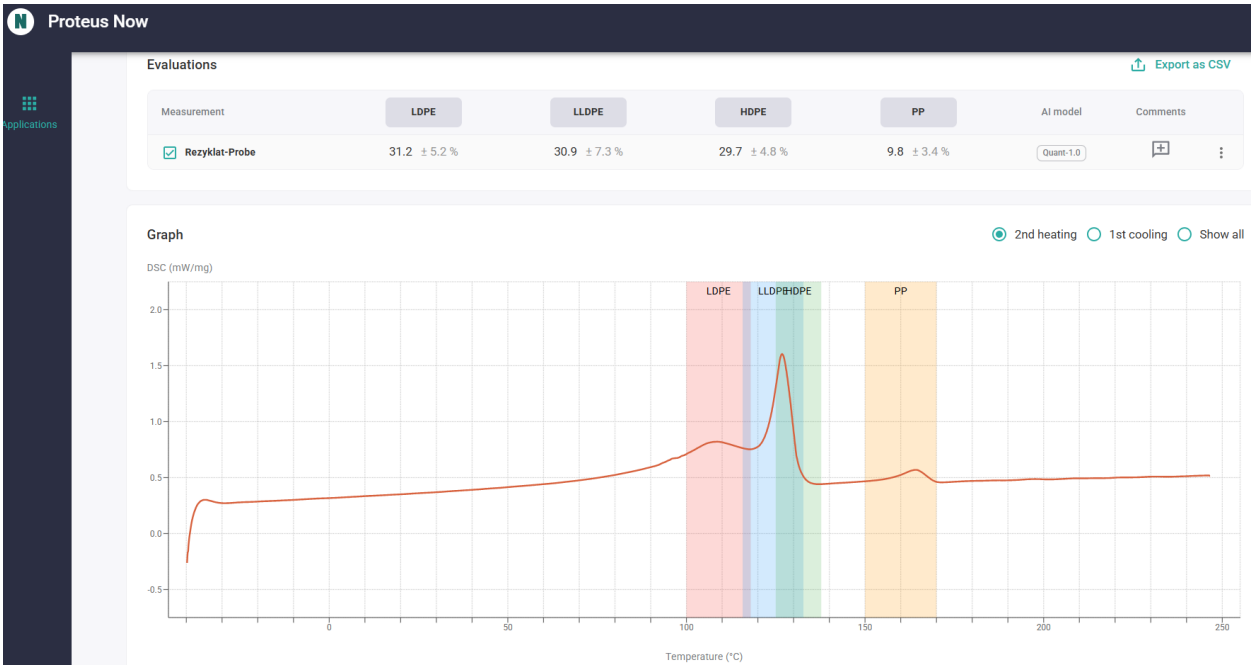

Figure 4: Proteus® Now Quantify interface showing DSC-based identification and quantification of polymer fractions in a recyclate sample, including the corresponding thermal signal and assigned transition regions.

Table 2: Comparison between target and predicted polymer concentrations for a known recyclate sample using Proteus® Now Quantify. The prediction is assessed via RMSE (%) & deviation (%).

Identified Material [-]	Target Quantity [%]	Predicted Quantity [%]	RMSE [%]	Deviation [%]
LDPE	30	31.2	5.2	1.2
LLDPE	30	30.9	7.3	0.9
HDPE	30	29.7	4.8	0.3
PP	10	9.8	3.4	0.2

5. Conclusions and Future Work

This work establishes that machine learning–based quantitative compositional analysis of recyclates is fundamentally dependent on standardized DSC measurement conditions. Variations in sample mass and thermal rates introduce signal changes that cannot be separated from compositional effects, directly affecting prediction accuracy. By enforcing standardized conditions (Sample mass: 10 mg ± 1 mg, Heating and Cooling Rate:10 K/min), a consistent feature space was

achieved, enabling robust, reproducible, and scalable quantification of polymer composition. Under these conditions, machine learning–assisted DSC analysis enables scalable and operator-independent characterization of complex recyclate systems.

A key finding is that data consistency and label accuracy outweigh dataset size. Inconsistent training data directly degrade model performance. This underscores that standardized measurement protocols and reliable ground truth are essential prerequisites for deploying AI in materials analysis.

Future work will extend the material databank beyond polyolefins to include PET, PA, ABS, HIPS, PC, PUR, and engineered materials. This expansion is required to capture the complexity of real-world recycling streams and ensure reliable model performance across heterogeneous industrial recyclates.

6. References

[1] J. Hopewell, R. Dvorak and E. Kosior. “Plastics recycling: challenges and opportunities”. Philosophical Transactions of the Royal Society B, Vol. 364, No. 1526, pp. 2115–2126, 2009.
[2] F. Vilaplana and S. Karlsson. “Quality concepts for the improved use of recycled polymeric materials”. Macromolecular Materials and Engineering, Vol. 293, No. 4, pp. 274–297, 2008.
[3] K. Ragaert, L. Delva and K. Van Geem. “Mechanical and chemical recycling of solid plastic waste”. Waste Management, Vol. 69, pp. 24–58, 2017.
[4] European Commission. “A new Circular Economy Action Plan for a cleaner and more competitive Europe”. European Commission, 2020.
[5] European Commission. “Proposal for a Regulation on Packaging and Packaging Waste (PPWR)”. European Commission, 2022.
[6] European Commission. “Ecodesign for Sustainable Products Regulation (ESPR)”. European Commission, 2022.
[7] Government of Canada. “Proposed Regulations Respecting Minimum Recycled Content in Plastic Products and Labelling of Plastic Products”. Environment and Climate Change Canada, 2023.
[8] California State Legislature. “Senate Bill No. 343 – Environmental advertising: recycling symbol”. State of California, 2021.
[9] California State Legislature. “Assembly Bill No. 793 – Plastic beverage containers: minimum recycled content”. State of California, 2020.
[10] M. Schyns and M. P. Shaver. “Mechanical recycling of packaging plastics: A review”. Macromolecular Rapid Communications, Vol. 42, No. 3, 2000415, 2021.
[11] S. Serranti, G. Bonifazi and S. Luciani. “Application of infrared spectroscopy for the identification of polymers in waste recycling”. Waste Management, Vol. 31, No. 11, pp. 2217–2227, 2011.
[12] L. Himanen, A. Geurts, A. Foster and P. Rinke. “Data-driven materials science: status, challenges, and perspectives”. Advanced Science, Vol. 6, No. 21, 1900808, 2019.
[13] K. T. Butler, D. W. Davies, H. Cartwright, O. Isayev and A. Walsh. “Machine learning for molecular and materials science”. Nature, Vol. 559, No. 7715, pp. 547–555, 2018.

[14] R. Ramprasad, R. Batra, G. Pilania, C. Mannodi-Kanakkithodi and C. Kim. "Machine learning in materials informatics: recent applications and prospects". npj Computational Materials, Vol. 3, No. 54, 2017.

[15] J. Gräßler and A. Höhne. "Machine learning in thermal analysis: a review of recent developments and applications". Journal of Thermal Analysis and Calorimetry, Vol. 143, No. 4, pp. 2765–2783, 2021.

[16] N. Rudolph. "DSC Measurements on Recycling Materials: Objective Interpretation with Proteus® Now Quantify — Why training on virgin data works: The natural grade-to-grade spread is larger than the shifts caused by degradation". NETZSCH-Gerätebau GmbH, Application Note, 2025. Available: https://analyzing-testing.netzsch.com/en/application-literature/dsc-measurements-on-recycling-materials-objective-interpretation-with-proteus-now-quantify.

[17] G. W. Ehrenstein, G. Riedel and P. Trawiel. "Thermal Analysis of Plastics – Theory and Practice". Carl Hanser Verlag GmbH & Co. KG, 2004.