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MODELING THE PYROLYSIS BEHAVIOUR OF PLASTIC MIXTURES USING ARTIFICAL NEURAL NETWORK

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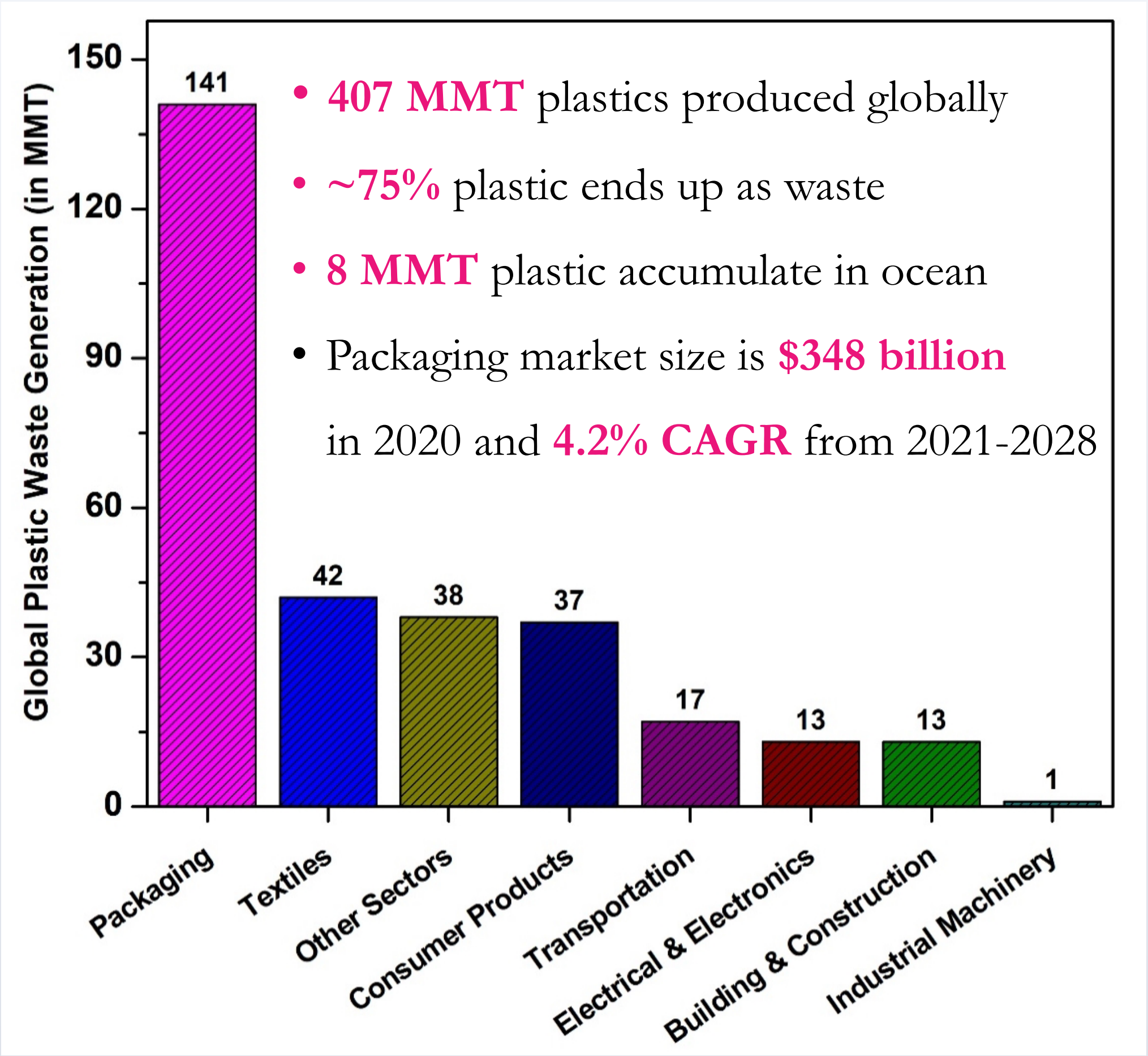
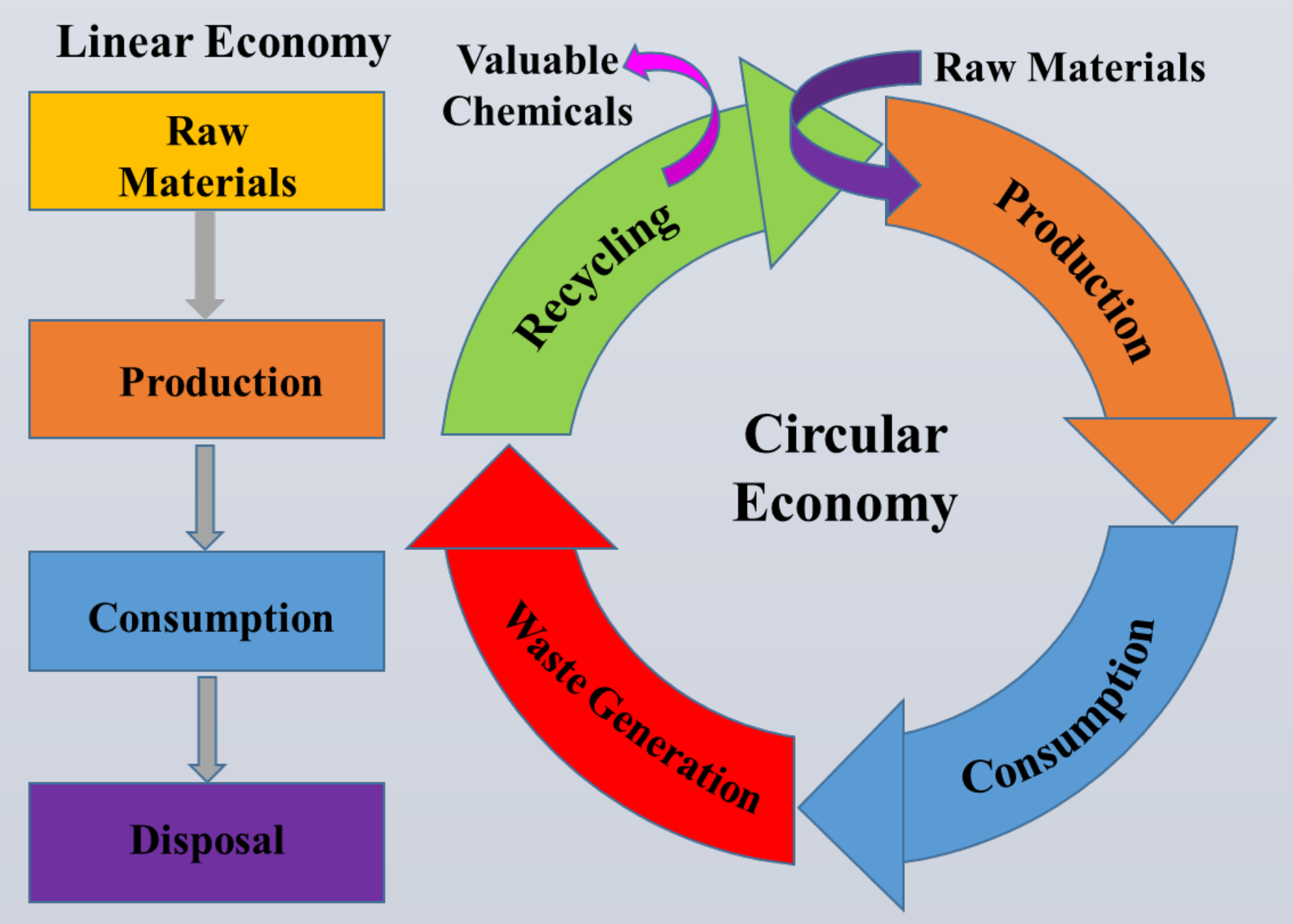
INTRODUCTION



- **407 MMT** plastics produced globally
- **~75%** plastic ends up as waste
- **8 MMT** plastic accumulate in ocean
- Packaging market size is **$348 billion** in 2020 and **4.2% CAGR** from 2021-2028

Linear versus Circular Economy



Plastic Waste Management

OBJECTIVES

- To study the pyrolysis behaviour of Polyethylene Terephthalate (PET) and Polyamide 6 (PA6) in different mixture ratios
- To evaluate the kinetic and statistical parameters and model the PET-PA6 mass loss behaviour using artificial neural network (ANN)
- To test the efficacy of ANN model on new dataset

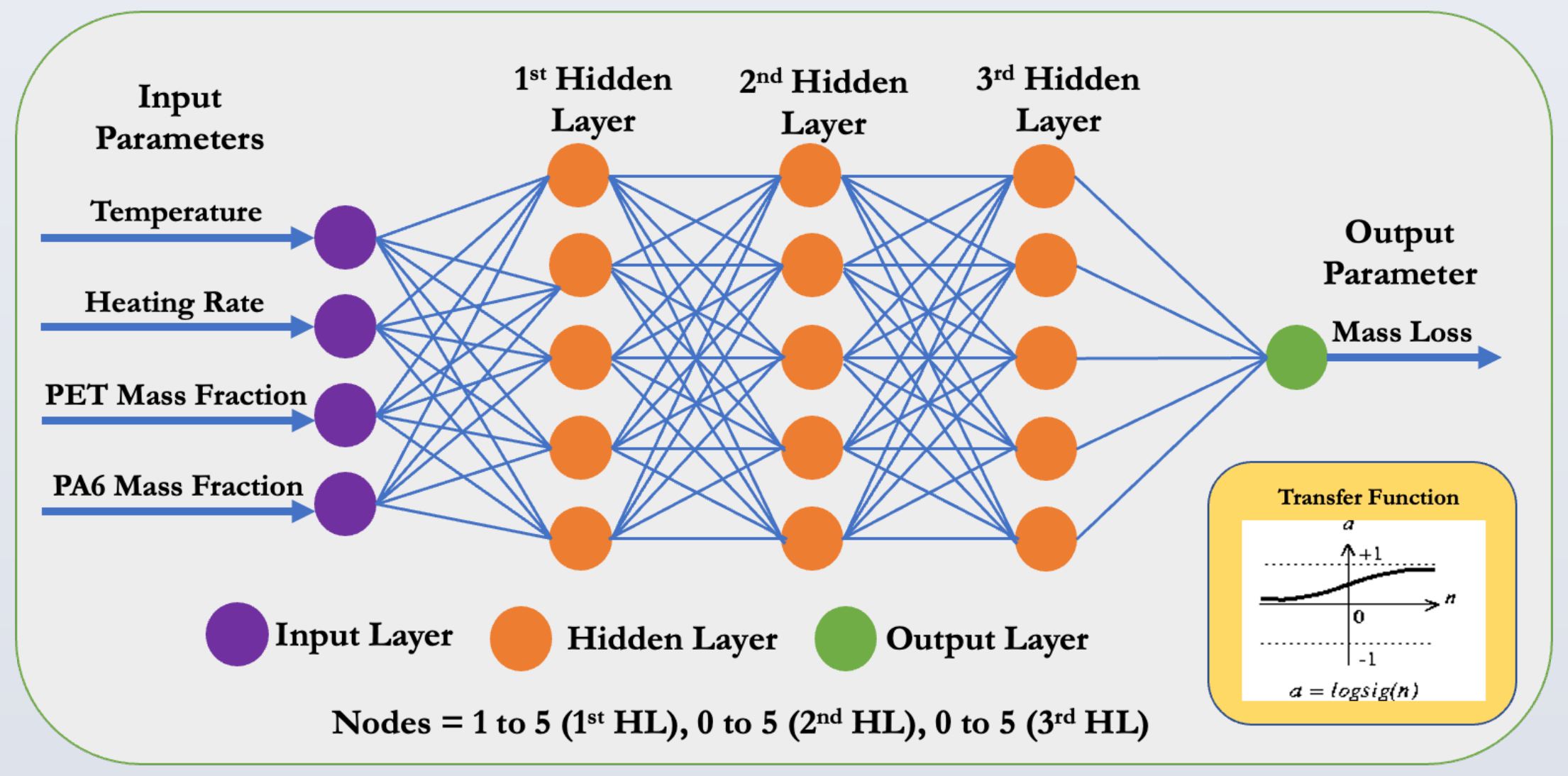
MATERIAL & METHODS

Samples: PET: PA6 in 1:0, 0:1, 1:1, 1:3, 3:1

TGA Experimental Conditions:

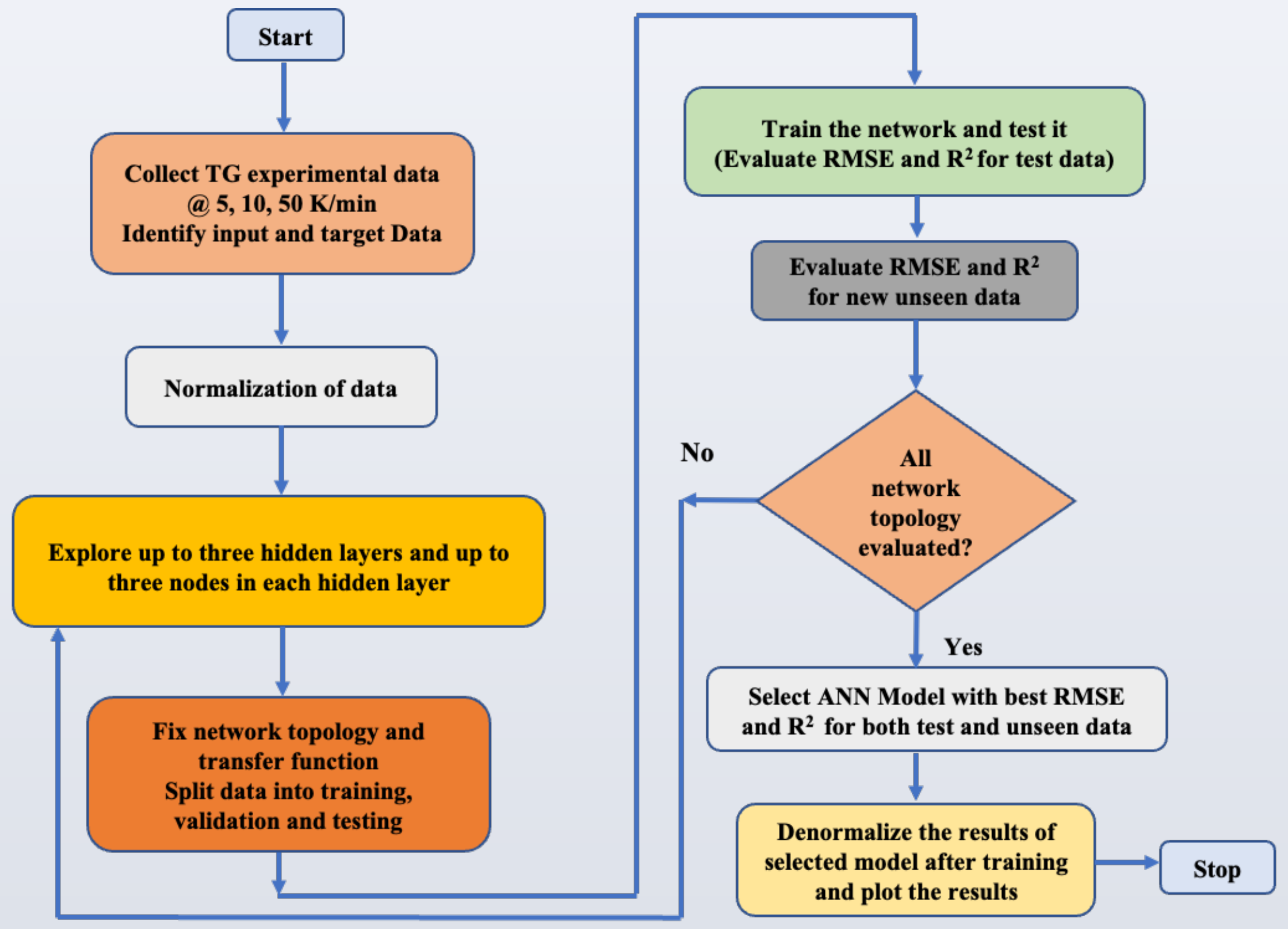
- **Heating rate = 10 K/min; Sample mass = 7 mg**
- **Nitrogen ambience (100 mL/min); T = 25-700 °C**

ANN topology for PET-PA6 mixtures



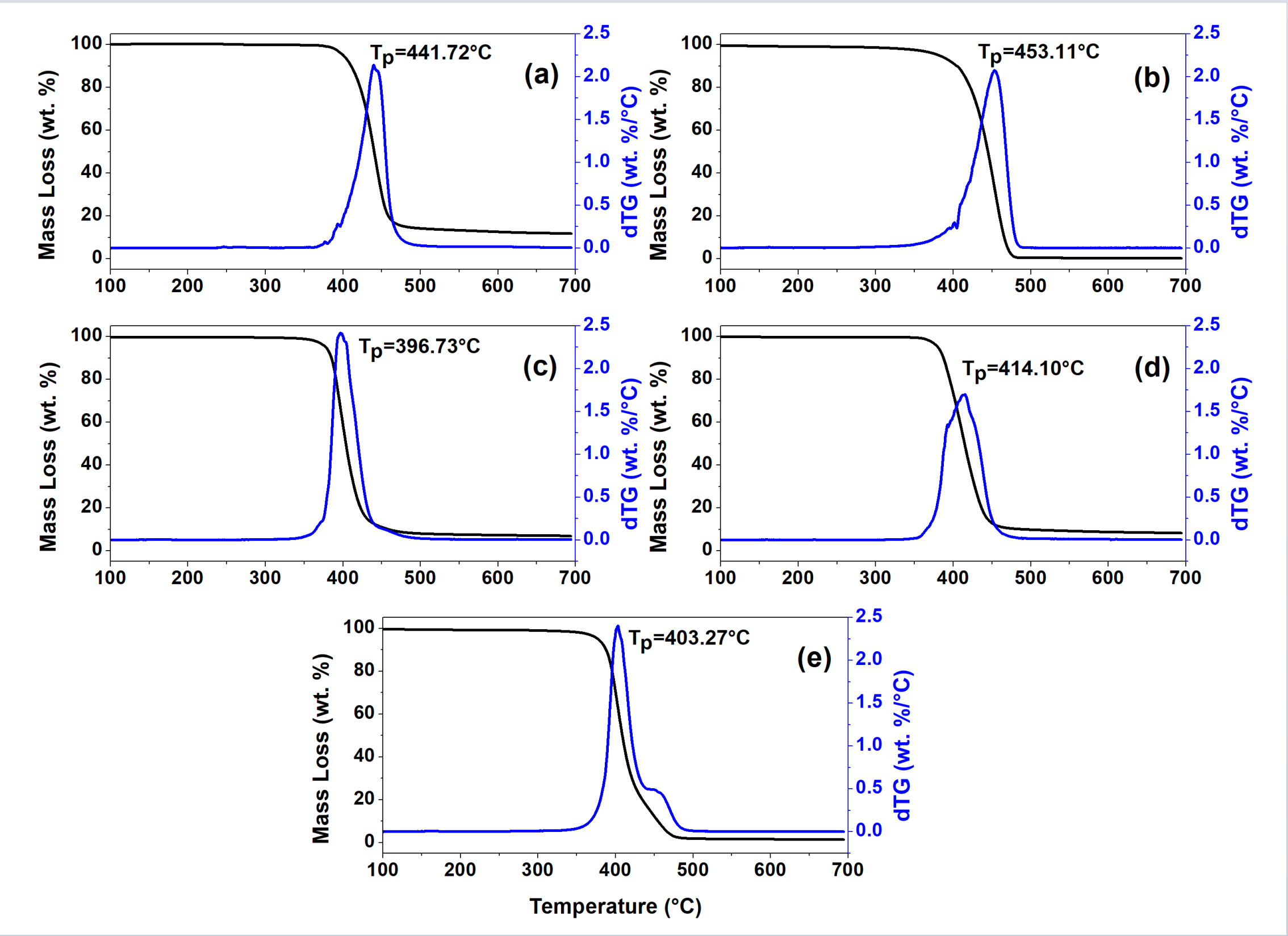
Nodes = 1 to 5 (1st HL), 0 to 5 (2nd HL), 0 to 5 (3rd HL)

Flowchart for algorithm of ANN modeling

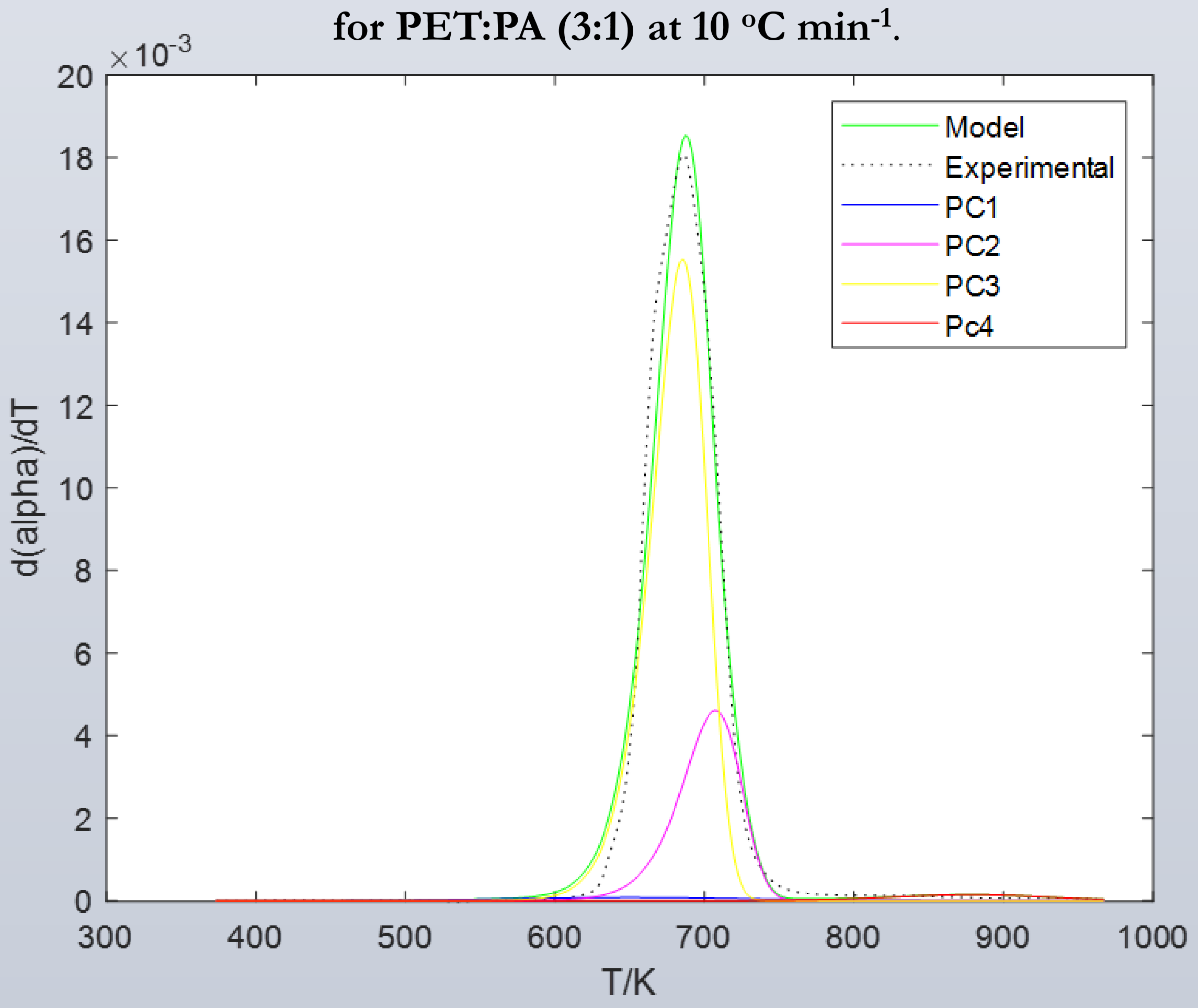


RESULTS

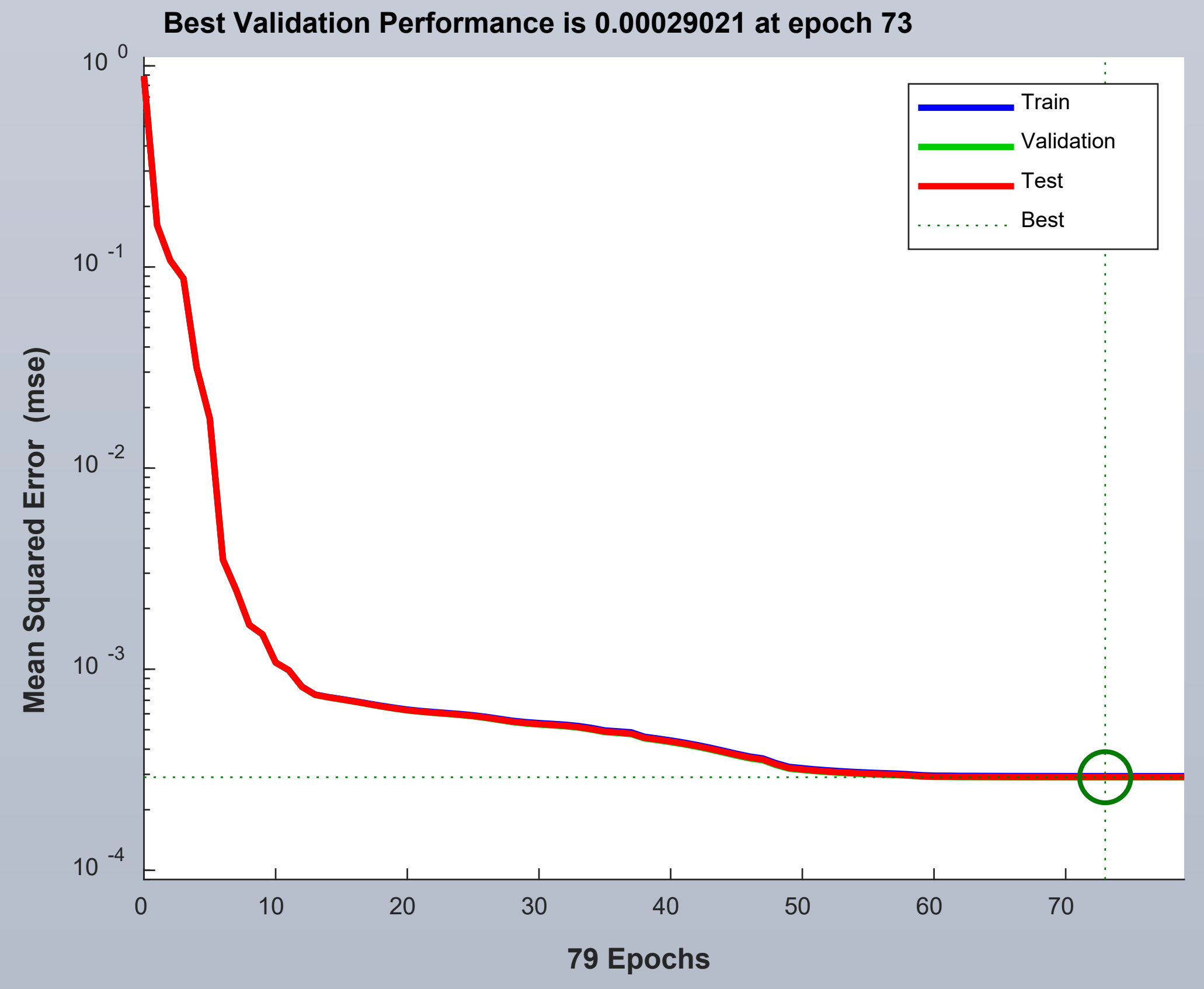
Experimental TG data for PET:PA6 (a) 1:0, (b) 0:1, (c) 1:1, (d) 3:1, (e) 1:3.



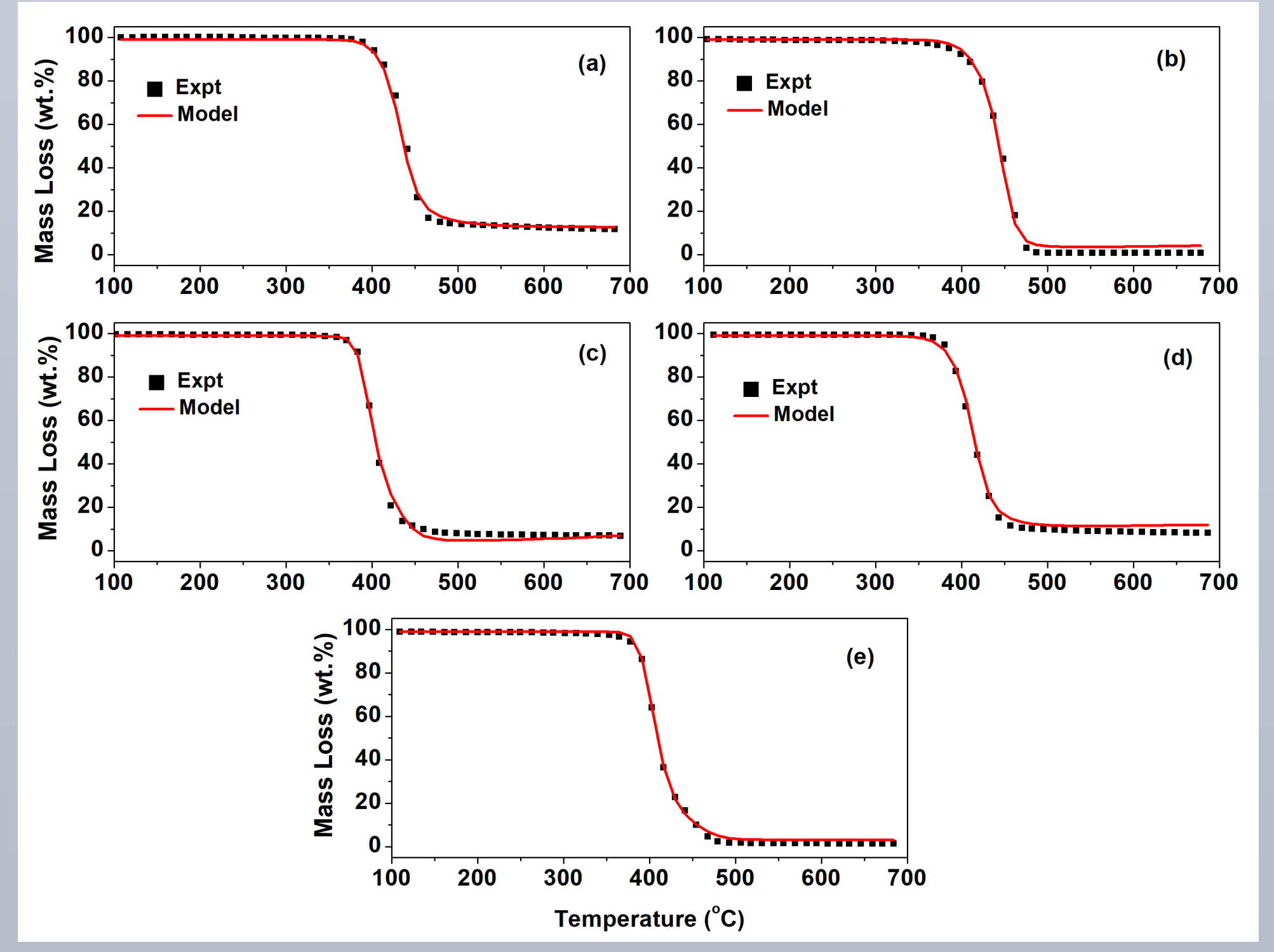
Experimental and simulated DTG profile for PET:PA (3:1) at 10 °C min^{-1}.



Performance plot of ANN511 model. The training, validation and testing plots overlap with each other.



Experimental versus predicted TG curves on testing data at 10 °C/min using ANN511 for PET:PA6 mixtures (a) 1:0, (b) 0:1, (c) 1:1, (d) 3:1, and (e) 1:3.



CONCLUSIONS

- The TGA results confirm that there are **significant interactions** among PET and PA6 mixtures.
- The kinetic study was carried out using isoconversional methods such as Kissinger-Akahira-Sunose (KAS) and Flynn-Wall-Ozawa (FWO), and a **multi-Gaussian distributed activation energy model** (DAEM).
- The average activation energy (E_a) obtained by KAS and FWO methods was in the range of **168-194 kJ mol^{-1}**, which is in good agreement with the value obtained by the DAEM model.
- The mass loss profiles of PET-PA6 mixtures were modelled using **Artificial Neural Network** (ANN).
- The model **ANN511** predicted the experimental mass loss behaviour reasonably well for both test data and new data at interpolated conditions of PET:PA6 in different ratios with root mean square error (RMSE) less than **3%.**

REFERENCES

1. Ni, Z., Bi, H., Jiang, C., Wang, C., Tian, J., Zhou, W., & Lin, Q. (2021). Investigation of the co-pyrolysis of coal slime and coffee industry residue based on machine learning methods and TG-FTIR: Synergistic effect, kinetics and thermodynamic. Fuel, 305, 121527.
2. Al-Yaari, M., & Dubdub, I. (2020). Application of Artificial Neural Networks to Predict the Catalytic Pyrolysis of HDPE Using Non-Isothermal TGA Data. Polymers, 12(8), 1813.
3. Sun, H., Bi, H., Jiang, C., Ni, Z., Tian, J., Zhou, W., ... & Lin, Q. (2022). Experimental study of the co-pyrolysis of sewage sludge and wet waste via TG-FTIR-GC and artificial neural network model: Synergistic effect, pyrolysis kinetics and gas products. *Renewable Energy*, *184*, 1-14.
4. Özveren, U., Kartal, F., Sezer, S., & Özdoğan, Z. S. (2022). Investigation of steam gasification in thermogravimetric analysis by means of evolved gas analysis and machine learning. *Energy*, *239*, 122232.
5. Wilamowski, B. M., & Yu, H. (2010). Improved computation for Levenberg–Marquardt training. *IEEE transactions on neural networks*, *21*(6), 930-937.

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