https://doi.org/10.56452/2022-11-005

ISSN: 0974-5823 Vol. 7 No. 11 November, 2022

International Journal of Mechanical Engineering

Kinetic Investigation and Parameters Estimation of Polymer

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Abstract:

Thermo-gravimetric analyzer (TGA) is an approach to understand the thermal degradation of any biomass or polymer. In TGA, the thermal decomposition of any thermally degradable item can be degraded with a specific heating rate and in the presence of nitrogen. Municipal solid waste (MSW) consists of lingo-cellulosic and various polymers constitutes which are thermally degradable. To convert all such MSW constitutes into energy using either incineration, pyrolysis, or gasification, the first step is to design a reactor. For this purpose, the estimation of kinetic parameters is necessary. The focus of the present work is to estimate the kinetic parameters of polythene, polystyrene, and polyester. So in general, various polymers have a heating rate of 10 ^{0}C/min in a nitrogen atmosphere.

Keywords: Kinetic Parameters, Municipal Solid Waste, Polymer, Thermo-gravimetric analyzer.

1. Introduction

The ability to convert waste into energy is crucial to meeting the needs of a growing global population. Waste-to-energy (WTE) refers to a group of processes that may turn almost any type of garbage into usable heat, fuel, or electricity. By avoiding the use of fossil fuels to generate electricity, waste-to-energy reduces carbon dioxide (CO2) emissions; by preventing methane (CH4) from being released from landfills during combustion, waste-to-energy prevents future methane emissions; and by recovering nonferrous and ferrous metals, waste-to-energy reduces greenhouse gas emissions.

Aparna Sarkar et al [1] studied on pyrolysis and kinetic of Newspaper wasteusing specially design reactor on nitrogen atmosphere. **Samy Yousef et al [2]** focused on estimation of kinetic parameter metalized food related packaging plastics waste utilizing independent parallel processes. **Botagoz Kuspangaliyeva et al [3]** aimed to investigate the thermal transformation and combustion properties of refuse derived solid fuel (RDF) materials and its constituent compounds were gathered from MSW landfills in Nur-Sultan's. Newspapers can be repurposed as a gaseous fuel by a process called pyrolysis, which **M. N. A. Bhuiyan et al [4]** studied extensively. **V. Chhabra et al [5]** reviewed by various researchers on kinetics of pyrolysis of mixed MSW. Thermo gravimetric analysis in nitrogen across the temperature range of 450-900 K at heating rates of 1, 2, and 5 K/ min with two phases of degradation was reported by **Chao-Hsiung Wu et al [6]**.

Data on the pyrolysis properties and chemical kinetics of MSW's most essential components was the primary focus of **L. Sorum et al [7]**. Based on a number of TGA studies with cardboard, **C. David et al [8]** talked about the pyrolysis phenomenon. In this study, we calculate the kinetic parameters for cardboard. **Julia Molto [9]** zeroed in A kinetic model has been created and tested to describe the actions of all the runs conducted in the degradation of old cotton fibers. **R. Miranda [10]** used thermo gravimetric and semi-batch pyrolysis to investigate the thermal responses of textile waste at several heating rates. From an engineering standpoint, **Ujwala Hujuri et al [11]** presented their work correlating and/or predicting the thermal decomposition kinetics of binary and ternary mixes of PE, PP, and PET polymers.

Samit Kumar Singh et al [12] focused on thermal degradation behavior of Newspaper and Glossy paper using thermo gravimetric method. **Samit Kumar Singh et al [13]** carried out experimental analysis of to understand thermal decomposition of cardboard and glossy paper for estimation kinematic parameters. **Samit Kumar Singh et al [14]** studied micro and macro degradation behavior of cotton waste at heating rate of 10^0C/min. **Samit Kumar Singh et al [15]** conducted thermal degradation studies on cotton polythene mixture at heating rate of 10 ^{0}C/min in which degradation occurs in three stages. **Samit Kumar Singh et al [16]** evaluated thermal degradation behavior of cardboard waste at 5, 10, and 15 °C/min heating rate and also ash obtained during decomposition of cardboard analyzed using Scanning Electron Microscope (SEM).

2. Kinetic Model

The model is commonly known as the kinetic model, and it outlines the stoichiometric alterations and the rates at which they occur in the reactor. Using the following model, we developed a technique to determine the activation energy from a single set of dynamic TGA data **[17, 18].**

$$\int_0^{\alpha} \frac{d\alpha}{f(\alpha)} = \frac{\mathrm{A}}{\beta} \int_0^{T} \exp\left(\frac{-E}{RT}\right) dT$$

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Since there is no unique answer to this equation, the **Flynn-Wall-Ozawa [19]** approximation method has been used to get close.

$$\log \beta = \log[AE / g(a)R] - 2.315 - 0.457E / RT \quad \text{Flynn - Wall - Ozawa}$$

In case of polymers thermal degradation, the Flynn-Wall-Ozawa method has been utilized for determination of kinetic constants as five different heating rates are used.

3. Experimental Procedure

TGA testing was performed on fragments of polymer ingredients which were cut into tiny pieces of 2-3 mm of municipal solid waste (polythene, polystyrene, polyester) procured from a local market. Using a Mettler Toledo TGA/SDTA 851e thermal system, we performed both thermal gravimetric and differential thermal gravimetric analysis. The samples were heated in a nitrogen gas medium at atmospheric pressure and a flow rate of 50 ml/min, and the temperature range covered was from ambient to 600 °C at a heating rate of (β) 5, 7, 10, 15, 20 ^{0}C/min. For 15 minutes, the nitrogen was completely eliminated. Studies examining the impact of the sample weight and heating rate informed the decision to use a maximum of 6 mg of sample **[7, 20]**.

4. Result and Discussion

Polymers such as polythene, polystyrene, and polyester, which are biodegradable and may be utilized as energy sources, are the second most abundant component of MSW composition. Thermoplastics can undergo a phase transition to a viscous state (a polymer melt) without a corresponding chemical reaction. The polymer melt separates into small liquid or gaseous pieces when heated further. If these shards of liquid are heated enough, they will disintegrate and evaporate. Chain scission is the most typical reaction mechanism for basic thermoplastics like polyethylene, which involves the breaking of bonds in the primary polymer chain. It is generally assumed that reactions may be represented by a first-order Arrhenius formula. Degradation of polythene, polystyrene, and polyester occurs in a single step.

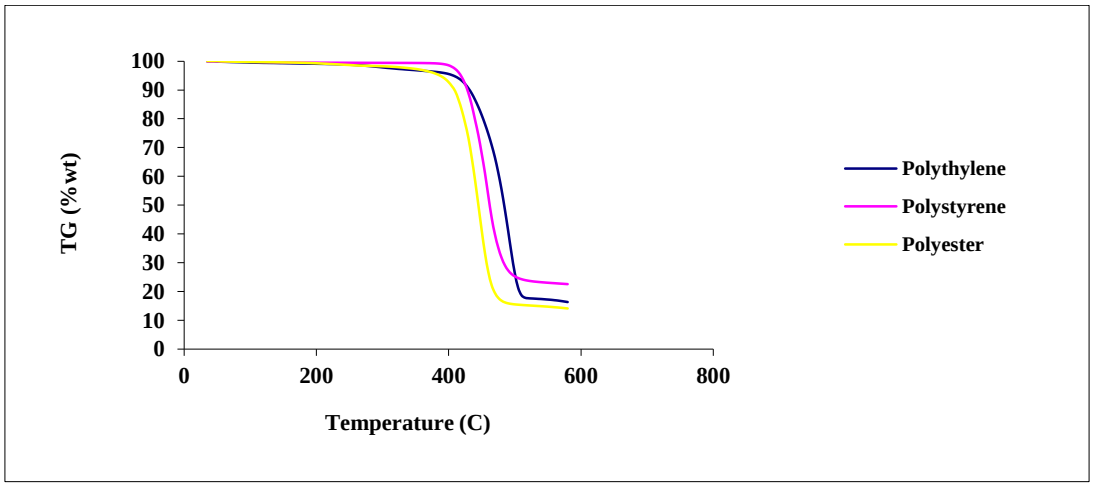

Fig. 1 Comparative Study between Polythene, Polystyrene and Polyester

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Figure 1 indicates comparative decomposition of polythene, polystyrene and polyester whereas Figure 2 includes DTG curves at a heating rate (β) 10 ^{0}C/min.

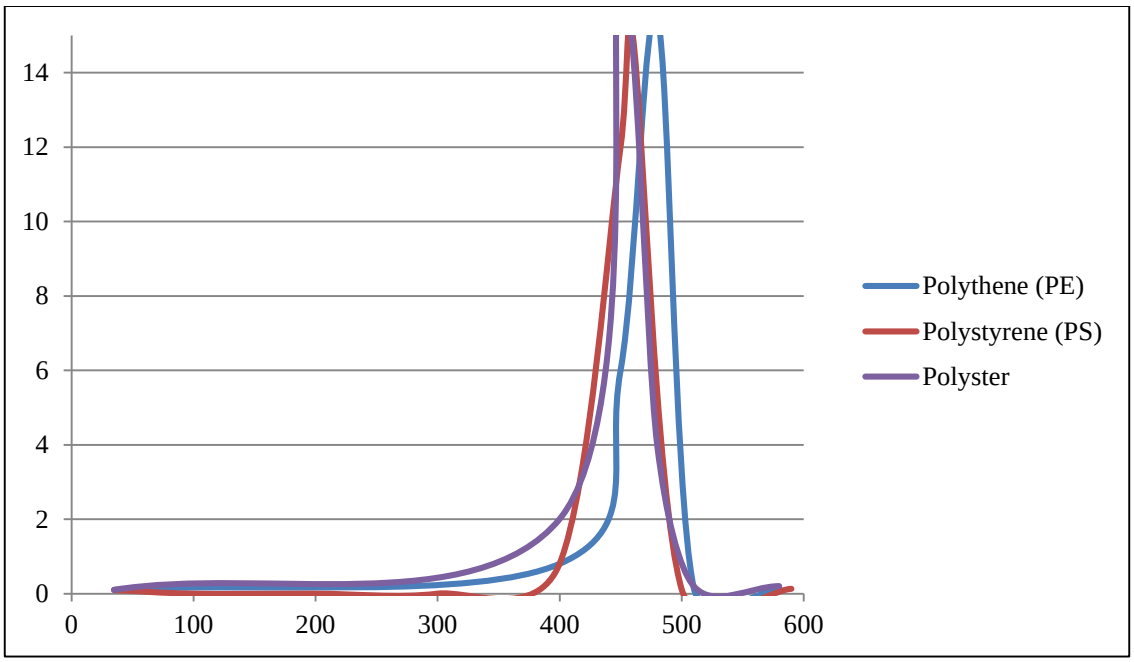

Fig. 2 DTG Curves

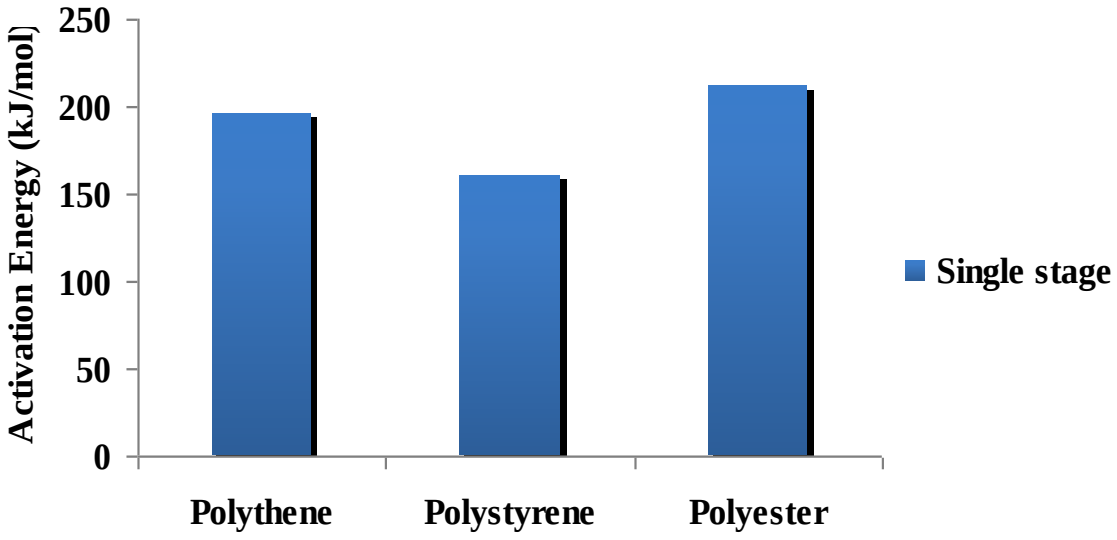

Fig. 3 Activation Energy for Polymer Composition

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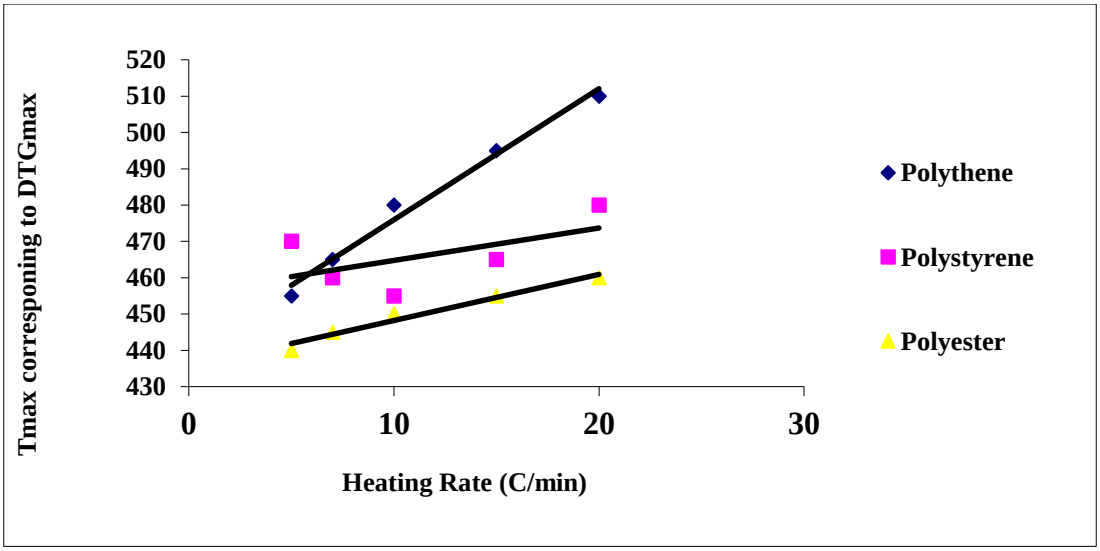

Fig 4. T_{max} Corresponding to DTG_{max} Polymer Composition

Figure 3 show values of activation energy for polymer whereas Figure 4 shows the maximum temperature corresponding to maximum decomposition rate for polythene, polystyrene and polyester at different heating rates.

It is interesting to observe from these results that the degradation occurs in single stage as also reported by L. Sorum et.al **[7]** and corresponding temperature ranges are 395-525 ^{0}C, 410-505 ^{0}C and 400-500 ^{0}C for polythene, polystyrene and polyester, respectively. It can be seen from Figure 1 that in case of polythene the decomposition occurs at faster rate compared to polystyrene and polyester, respectively, which may be related to bond energy level **[21, 23]**. Figure 2 represents the weight loss characteristics and DTG curves at heating rate (β) 10 ^{0}C/min **[7, 21, 22]**. The value of activation energy increases with increases in degree of transformation and the mean values of activation energy in case of polythene, polystyrene and polyester are 195.96, 160.98 and 212.26 kJ/mol, respectively. The results show similar trend and values as reported by J.M. Encinar **[21]**. The decomposition increases with increase in heating in case of polythene, polystyrene and polyester. Compared to other plastic, in case of PVC the more amounts of residues remain irrespective of heating rate while in case of polythene, polystyrene and polyester after degradation more residues remain in case of polyester **[23]**.

5. Conclusion

1. In case of plastics, decomposition takes place in single stage.
2. The polythene decomposes at a faster rate as compared to PVC at a heating rate of 5 ^{0}C/min to 20 ^{0}C/min.
3. The activation energy corresponding to heating rate of 5 ^{0}C/min to 20 ^{0}C/min is 195.96 kJ/mol, 160.98 kJ/mol and 212.26 kJ/mol for Polythene, Polystyrene and Polyester, respectively.

References:

1. Aparna Sarkar, Sudip De Sarkar, Michael Langanki, and Ranjana Chowdhury, Studies on Pyrolysis Kinetic of Newspaper Wastes in a Packed Bed Reactor: Experiments, Modeling, and Product Characterization, Volume 1, 2015.
2. Samy Yousef, Justas Eimontas, Nerijus Striuugas and Mohammed Ali Abdelnaby, Modeling of Metalized Food Packaging PlasticsPyrolysis Kinetics Using an Independent ParallelReactions Kinetic Model, Polymers, Volume 12, 2020.
3. Botagoz Kuspangaliyeva , Botakoz Suleimenova, Dhawal Shah and Yerbol Sarbassov, Thermogravimetric Study of Refuse Derived Fuel Produced from Municipal Solid Waste of Kazakhstan, Appl. Sci. Volume , 11, 2021.
4. M. N. A. Bhuiyan , M. Ota , K. Murakami and H. Yoshida, Pyrolysis Kinetics of Newspaper and Its Gasification, Energy Sources, Part A,, Volume 32, 2010.
5. V. Chhabra,, Y. Shastri, S. Bhattacharya, Kinetics of Pyrolysis of Mixed Municipal Solid Waste- A Review, Procedia Environmental Sciences, Volume 35, 2016.
6. Chao-Hsiung Wu , Ching-Yuan Chang , Jyh-Ping Lin ,Jiann-Yuan Hwang, Pyrolysis kinetics of paper mixture in municipal solid waste, Fuel, Volume 76, 1997.
7. L. Sorum, M.G. Gronli, J.E.Hustad, Pyrolysis Characteristics and Kinetics of Municipal Solid Waste, Fuel, Volume 80, 2001.
8. C. David, S. Salvador, J.L. Dirion, M., Determination of a reaction scheme for cardboard thermal degradation using thermal gravimetric analysis, J. Anal. Appl. Pyrolysis, Volume 67, 2003.
9. J. Molto, R. Font, A. Conesa, I. Martı´n-Gullo´n, Thermogravimetric analysis during the decomposition of cotton fabrics in an inert and air environment, J. Anal. Appl. Pyrolysis (2005) (Article in Press).
10. R. Miranda, C. Sosa_Blanco, D. Bustos-Martı´nez, C. Vasile, Pyrolysis of textile wastes kinetics and yields, J. Anal. Appl. Pyrolysis, Volume 80, 2007
11. U. Hujuri, K.Aloke S. G. Ghoshal, Modeling pyrolysis kinetics of plastic mixtures, Polymer Degradation and Stability, Volume 93, 2008.
12. Samit Kumar Singh and Dr. Sadanand A. Namjoshi, Comparative Thermal Degradation Evaluation of Newspaper and Glossy Paper Constituents, Asian Journal of Organic & Medicinal Chemistry, Volume 7, 2022.
13. Samit Kumar Singh, Dr. Sadanand A. Namjoshi, Comparative Thermal Decomposition Studies of Newspaper, Cardboard and Glossy paper, International Journal of Mechanical Engineering, Volume 6, 2021.
14. Samit Kumar Singh; Dr. Sadanand A. Namjoshi, Anand Patel, Micro and Macro Thermal Degradation Behavior of Cotton Waste, Revista Geintec, Volume 11, 2021.
15. Samit Kumar Singh and Dr. Sadanand A. Namjoshi, Kinetic Parameter Estimation of Cotton Polythene Mixture, Journal of Emerging Technologies and Innovative Research, Volume 6, 2019.
16. Samit Kumar Singh and Dr. Sadanand A. Namjoshi, Evaluation of Thermal Degradation Behavior of Cardboard Waste, Algorithms for Intelligent Systems - Intelligent Energy Management Technologies - ICAEM 2019 (Springer), 2019.

17. Sema Yourlmaz, Investigation of emissions and combustion kinetics of waste wood samples with thermal and spectral methods, PG Dissertation, Middle East Technical University, Beirut, 2006.
18. Zhenhai Liu, Handbook of Thermal Analysis, John Willy & Sons, 1998.
19. J. H. Flynn, L. A. Wall, Polymer Science Part B, Polymer Letters Volume 4, 1966.
20. W. K. Buah, A. M. Cunliffe and P. T. Williams, Characterization of products from the pyrolysis of MSW, Process Safety and Environmental Protection, Volume 85, 2007.
21. J.M. Encinar, J.F. González, Pyrolysis of synthetic polymers and plastic wastes kinetic study, Fuel Processing Technology, Volume 89, 2008.
22. K. Aboulkas, El harfi, A. El bouadili, M. Nadifiyine, M. Benchanaa, A. Mokhlisse, Pyrolysis kinetics of olive residue/plastic mixtures by non-isothermal thermogravimetry, Fuel Processing Technology (2009) (Article in Press).
23. P. Grammelis, P. Basinas, A. Malliopoulou, G. Sakellaropoulos, Pyrolysis kinetics and combustion characteristics of waste recovered fuels, Fuel, Volume 88, 2009.