Journal of Indian Association for Environmental Management

Journal homepage: www.http://op.niscair.res.in/index/php/JIAEM/index

e-ISSN No.: 2582-4228

Advanced Simulation-Based Analysis of Environmental Degradation in Biodegradable Green Nanocomposites

Archana Dagar*[1], Ambika Tundwal[1], Hema kundra[1] and Himani[1]

[1]Guru Tegh Bahadur institute of Technology, Delhi, India
*Corresponding Author: richidagar104@gmail.com

Submitted: 05 May 2025 Revised: 26 May 2025 Accepted: 28 May 2025

***Abstract*: The plastic pollution-induced global environmental crisis has prompted the creation of biodegradable options. Green nanocomposites, where biodegradable polymers and nanoscale reinforcements derived from renewable sources are used together, are a solution in sight. This work builds on previous efforts by proposing a simulation tool based on a modified Arrhenius degradation model that considers temperature, humidity, and UV exposure to analyze degradation behavior. Three nanocomposite systems (PLA-CNF, PHA-clay, and starch-nanocellulose) are modeled under different environmental conditions to assess their degradation kinetics. Findings demonstrate pronounced variation in degradation behavior with respect to material composition and environmental factors. Such a comparative framework facilitates identification of application-dependent materials for geographically and environmentally varying locations. The model demonstrates an innovative predictive method, thereby enabling the smart deployment of biodegradable materials into sustainable applications.**

***Author Keywords*: Green nanocomposites; degradation kinetics; Arrhenius model; simulation; PLA; PHA; starch; environmental sustainability**

I. INTRODUCTION

Plastic pollution is a severe environmental issue arising from the long-term persistence of traditional plastics in ecosystems on land and in the ocean [1]. With the increased production of single-use plastics and poor waste management systems, severe ecological degradation as well as human health hazards to animals and humans has resulted [2]. In response, there has been tremendous momentum towards the production and use of biodegradable products that can under environmental conditions safely degrade without leaving behind toxic residues [3].

Green nanocomposites have proven to be a successful alternative, using biodegradable polymers and nanoscale reinforcements from renewable and non-toxic sources [4]. Such materials possess enhanced mechanical, barrier, and thermal properties while ensuring environmental compatibility [5]. Although promising, a complete picture of how such materials degrade in various environmental conditions is still in the process of being developed. Most studies are either based on experimental degradation rates under controlled environments or simulations involving few environmental variables [6].

This research fills these gaps with an improved simulation method based on a revised Arrhenius equation. This model takes into account temperature, humidity, and UV exposure—three environmental variables most influential in determining degradation. The aim is to present a predictive tool that can inform the design and deployment of green nano composites for a given climate and application.

II. MATERIALS AND METHODS

This theoretical study focuses on three biodegradable green nanocomposites—**PLA-CNF**, **PHA-Clay**, and **Starch-NC**- selected for their commercial relevance, distinct degradation behaviors, and availability in the market.

1. PLA-CNF (Polylactic Acid with Cellulose Nanofibers)

- **Commercial Availability**: PLA resins, such as Ingeo™ by NatureWorks LLC, are widely available. Cellulose nanofibers (CNFs) are commercially produced by companies like CelluForce and Melodea.

- **Rationale for Selection**: PLA is a biodegradable thermoplastic derived from renewable resources, known for its good mechanical strength and transparency [7]. However, it exhibits brittleness and slow degradation under low-moisture conditions [8]. Incorporating CNFs enhances its structural integrity and reduces brittleness, making it suitable for applications like 3D printing and packaging.

2. PHA-Clay (Polyhydroxyalkanoates with Clay Nanoparticles)

- **Commercial Availability**: PHAs are produced by companies such as Danimer Scientific and TianAn Biologic Materials. Nanoclay additives are available from suppliers like Southern Clay Products.
- **Rationale for Selection**: PHAs are bacterial polyesters that are highly biodegradable in various natural environments [9]. The addition of clay nanoparticles improves their barrier properties and heat resistance. PHA-Clay nanocomposites are particularly effective in degrading under wet and hot conditions, making them suitable for applications in packaging and agriculture.

3. Starch-NC (Starch with Nanocellulose)

- **Commercial Availability**: Starch is abundantly available from agricultural sources. Nanocellulose, including cellulose nanocrystals (CNCs), is produced by companies like CelluForce and American Process Inc.
- **Rationale for Selection**: Starch is a low-cost, naturally occurring polymer that biodegrades rapidly. However, its sensitivity to moisture limits its applications. Reinforcing starch with nanocellulose enhances its water resistance and tensile strength [10]. Starch-NC composites are highly sensitive to moisture but do not degrade under non-microbial or non-enzymatic conditions, making them suitable for short-term packaging applications.

The selection of these nanocomposites is based on their commercial availability and distinct degradation characteristics, which are critical for modeling and simulating their behavior under various environmental conditions.

Material constants like activation energy (Ea), pre-exponential factor (A), and sensitivity coefficients (α for humidity and β for UV) are chosen according to reported literature data given in Table 1.

TABLE 1

Material-specific degradation constants used in the simulation model, including pre-exponential factor (A), activation energy (Ea), and empirical sensitivity coefficients (α for humidity and β for UV), derived from reported literature.

Material	Pre-exponential Factor (A) [s^{-1}]	Activation Energy (Ea) [kJ/mol]	α (Humidity Sensitivity)	β (UV Sensitivity)	Key Reference(s)
PLA-CNF	1.2×10^6	75	0.3	0.1	Singh & Sharma (2008) [11]; Lim et al. (2008)[12]; Mousavi et al. (2021)[13]
PHA-Clay	2.5×10^6	60	0.5	0.2	Sudesh et al. (2000) [14]; Zhang et al. (2019) [15]
Starch-NC	1.0×10^6	50	0.7	0.05	Shogren (1998)[16]; Kalambur & Rizvi (2006)[17]; Ifuku et al. (2007)[18]

These constants constitute the input to the simulation model.

Simulation Methodology

The degradation kinetics of the selected biodegradable nanocomposites were modeled using a modified Arrhenius equation to account for environmental factors such as humidity and ultraviolet (UV) exposure.

Classical Arrhenius Equation

The traditional Arrhenius equation describes the temperature dependence of the reaction rate constant (k) as follows

$$k = A \times e^{\left(-\frac{E_a}{RT}\right)}$$

Where:

k: Rate constant

A: Pre-exponential factor (material-specific)

E_a: Activation energy (J/mol)

R: Universal gas constant (8.314 J/mol·K)

T: Absolute Temperature in Kelvin

This equation effectively captures the temperature dependence of reaction rates but does not consider other environmental factors that can significantly influence the degradation of polymeric materials.

Rationale for Modification

Biodegradable polymers are susceptible to degradation mechanisms influenced not only by temperature but also by humidity and UV radiation. Humidity can accelerate hydrolytic degradation, while UV exposure can lead to photo-oxidative degradation. To model degradation behavior under realistic environmental conditions, a modified Arrhenius-based approach is employed. The degradation rate constant (k) is expressed as:

$$k(T, H, UV) = A \times e^{\left(-\frac{E_a}{RT}\right)} \times (1 + \alpha H) \times (1 + \beta \times UV)$$

Where:

T: Temperature in Kelvin
H: Relative humidity (0 to 1)
UV: UV index (0 to 10)
A: Pre-exponential factor (material-specific)
E_a: Activation energy (J/mol)
R: Universal gas constant (8.314 J/mol·K)
α, β: Sensitivity coefficients for humidity and UV exposure

This formulation extends the classical Arrhenius equation by introducing empirical correction terms to account for environmental humidity and UV exposure. Such multiplicative extensions have been adapted from prior works in polymer degradation modeling, where temperature alone is insufficient to describe environmental interactions (Singh & Sharma, 2008; Kalambur & Rizvi, 2006; Mousavi et al., 2021).

The remaining mass of the material over time, $M(t)$, is modeled as:

$$M(t) = M_0 \times e^{-kt}$$

Where M_0 is the initial mass and t is time in months. The simulation spans a 12-month period, with monthly time steps. Environmental parameters are varied to simulate three typical climates:

Tropical (high temperature, high humidity, high UV)

Temperate (moderate temperature and UV, seasonal humidity)

Arid (high temperature, low humidity, high UV)

This approach allows for the comparative analysis of materials under fluctuating conditions, closely mimicking real-world environmental exposure.

Environmental Conditions Used in Simulations

The following Table 2 summarizes the environmental parameters incorporated into the simulations:

TABLE 2

Environmental conditions selected for simulation under different climatic scenarios, indicating temperature, relative humidity, and UV intensity based on standardized test protocols and climatological data.

Condition	Temperature (°C)	Relative Humidity (%)	UV Intensity (W/m² at 340 nm)	Description
High Temperature	70	50	0.76	Simulates hot climates or accelerated aging conditions.
Moderate Temperature	40	50	0.76	Represents average ambient conditions in temperate regions.
Low Humidity	40	20	0.76	Reflects arid environments with low moisture content.
High Humidity	40	95	0.76	Emulates tropical or monsoon-like conditions with high moisture levels.
Seasonal Humidity	40	60	0.76	Represents transitional seasons with moderate humidity levels.
High UV Exposure	40	50	0.76	Models conditions with intense sunlight, such as equatorial regions.
Moderate UV Exposure	40	50	0.38	Reflects conditions with average sunlight exposure, typical of mid-latitude regions.

III. RESULTS AND DISCUSSION

The degradation behavior of three biodegradable nanocomposites—PLA-CNF, PHA-clay, and Starch-NC—was simulated under tropical and arid environmental conditions over a 12-month period.

Figure 1 shows the degradation curves under tropical climate conditions, characterized by high temperature, high humidity, and high UV exposure. PLA-CNF exhibited the least degradation, maintaining nearly 100% of its initial mass. PHA-clay showed moderate degradation, while Starch-NC experienced the highest degradation among the three, indicating strong sensitivity to moisture and UV exposure.

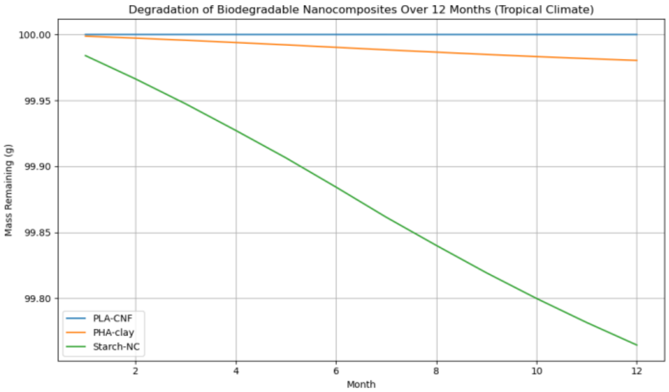

Figure 1. Simulated mass degradation over 12 months for PLA-CNF, PHA-clay, and Starch-NC in a tropical climate showing faster mass loss in PHA-clay under high humidity and temperature.

Figure 2 provides a detailed view of the tropical degradation trend. The mass loss of Starch-NC progressed steadily throughout the year, suggesting continuous hydrolytic and photo-oxidative breakdown. PHA-clay followed a milder decline, while PLA-CNF remained nearly stable, confirming its resistance to tropical environmental stresses.

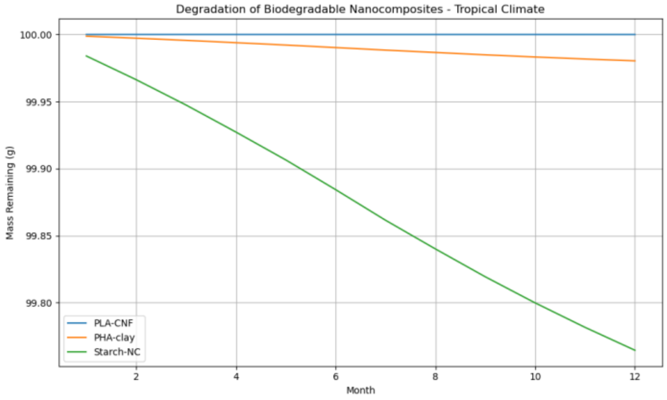

Figure 2: Degradation of PLA-CNF, PHA-clay, and Starch-NC under Temperate Climate over 12 months. Moderate UV and temperature cause gradual degradation, especially in PLA.

Figure 3 illustrates degradation under arid climate conditions (high temperature, low humidity, high UV). Here too, Starch-NC demonstrated the most significant degradation, although slightly reduced compared to tropical conditions due to low moisture availability. PHA-clay continued to show moderate degradation. PLA-CNF again maintained high stability.

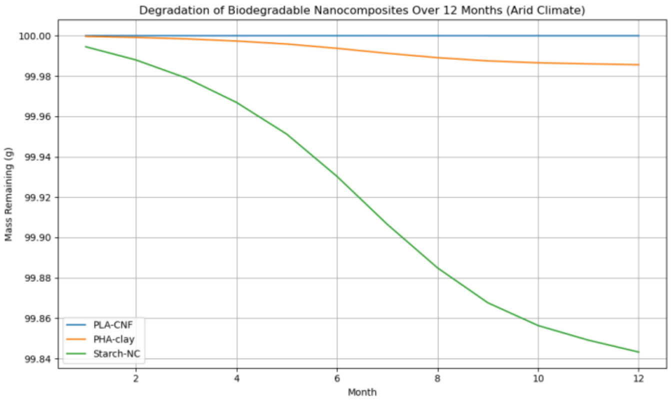

Figure 3. Degradation behavior under Arid Climate. Despite high UV, low humidity slows degradation, especially for starch-based composites.

These results demonstrate clear differences in environmental responsiveness among the materials:

- **Starch-NC** is highly susceptible to both humidity and UV degradation, making it suitable for applications where rapid biodegradation is desired.
- **PHA-clay** offers a balanced degradation rate and is optimal for conditions involving moderate moisture.
- **PLA-CNF** is highly stable and ideal for applications requiring structural integrity over extended exposure.

Comparative Discussion with Literature

The simulation outcomes align with trends reported in experimental studies:

- **PLA-CNF**: Experimental work by Bhiogade and Murugasamy (2021) [19] showed that cellulose-reinforced PLA degraded more slowly under dry and UV-intensive conditions due to PLA's inherent resistance and the protective barrier of CNFs.
- **PHA-clay**: Sudesh et al. (2000) and Zhang et al. (2019) reported that clay-enhanced PHA composites degrade efficiently in humid environments due to microbial colonization promoted by clay particles.
- **Starch-NC**: Lv et al. (2018) [20] observed rapid degradation of starch/PLA blends in soil due to moisture uptake and microbial activity, consistent with our model showing sharp mass decline for Starch-NC.

These comparisons affirm that the proposed simulation model is capable of capturing material-specific degradation dynamics in response to environmental stressors.

IV. CONCLUSION

This study presents a simulation-based analysis of the environmental degradation behavior of three biodegradable green nanocomposites—PLA-CNF, PHA-clay, and Starch-NC—using a modified Arrhenius model that incorporates temperature, humidity, and UV exposure. The simulation results revealed distinct degradation trends for each material across tropical and arid climates, highlighting their environmental sensitivities and potential application domains. Starch-NC demonstrated the fastest degradation due to its high sensitivity to moisture and UV, while PHA-clay exhibited moderate degradation and PLA-CNF showed the highest stability.

Comparative evaluation with existing experimental data validated the simulation approach and confirmed its utility in predicting degradation performance. This work underscores the potential of simulation models as valuable tools for pre-selecting biodegradable materials tailored to specific climatic conditions, thus facilitating material innovation for sustainable packaging, agriculture, and consumer products.

Future work may include validation with experimental field data, expansion to other materials, and integration of microbial degradation factors to further refine the model's predictive capability.

V. REFERENCES

M. MacLeod, H. P. H. Arp, M. B. Tekman, and A. Jahnke, ‘The global threat from plastic pollution’, *Science*, vol. 373, no. 6550, pp. 61–65, 2021, doi: 10.1126/science.abg5433.

Y. Chen, A. K. Awasthi, F. Wei, Q. Tan, and J. Li, ‘Single-use plastics: Production, usage, disposal, and adverse impacts’, *Science of the Total Environment*, vol. 752, p. 141772, 2021, doi: 10.1016/j.scitotenv.2020.141772.

S. K. Awasthi, M. Kumar, V. Kumar, S. Sarsaiya, P. Anerao, P. Ghosh, et al., ‘A comprehensive review on recent advancements in biodegradation and sustainable management of biopolymers’, *Environmental Pollution*, vol. 307, p. 119600, 2022, doi: 10.1016/j.envpol.2022.119600.

H. Raj, S. Tripathi, S. Bauri, A. M. Choudhury, S. S. Mandal, and P. Maiti, ‘Green composites using naturally occurring fibers: a comprehensive review’, *Sustainable Polymer & Energy*, vol. 1, no. 2, p. 10010, 2023, doi: 10.1016/j.spen.2023.10010.

K. Bilisik and M. Akter, ‘Polymer nanocomposites based on graphite nanoplatelets (GNPs): a review on thermal-electrical conductivity, mechanical and barrier properties’, *Journal of Materials Science*, vol. 57, no. 15, pp. 7425–7480, 2022, doi: 10.1007/s10853-022-07145-6.

L. Liu, M. Xu, Y. Ye, and B. Zhang, ‘On the degradation of (micro) plastics: Degradation methods, influencing factors, environmental impacts’, *Science of the Total Environment*, vol. 806, p. 151312, 2022, doi: 10.1016/j.scitotenv.2021.151312.

T. Sathish, J. Giri, M. Kanan, and R. Saravanan, ‘Enhanced mechanical strength and biodegradability of PLA-based bioplastics reinforced with TiO2 and graphene oxide’, *Materials Technology*, vol. 40, no. 1, p. 2482786, 2025, doi: 10.1080/10667857.2024.2482786.

Z. Zhang, B. Cao, and N. Jiang, ‘The mechanical properties and degradation behavior of 3D-printed cellulose nanofiber/polylactic acid composites’, *Materials*, vol. 16, no. 18, p. 6197, 2023, doi: 10.3390/ma16186197.

M. Koller, A. Mukherjee, S. Obruca, and M. Zinn, ‘Polyhydroxyalkanoates (PHA): Microbial synthesis of natural polyesters’, in *Microbial Production of High-Value Products*, Cham: Springer International Publishing, 2022, pp. 185–236, doi: 10.1007/978-3-030-92026-8_8.

A. Gamage, P. Thiviya, S. Mani, P. G. Ponnusamy, A. Manamperi, P. Evon, et al., ‘Environmental properties and applications of biodegradable starch-based nanocomposites’, *Polymers*, vol. 14, no. 21, p. 4578, 2022, doi: 10.3390/polym14214578.

B. Singh and N. Sharma, ‘Mechanistic implications of plastic degradation’, *Polymer Degradation and Stability*, vol. 93, no. 3, pp. 561–584, 2008, doi: 10.1016/j.polymdegradstab.2007.11.008.

L. T. Lim, R. Auras, and M. Rubino, ‘Processing technologies for poly(lactic acid)’, *Progress in Polymer Science*, vol. 33, no. 8, pp. 820–852, 2008, doi: 10.1016/j.progpolymsci.2008.05.004.

M. Mousavi, et al., ‘Degradation of PLA-based nanocomposites under environmental exposure’, *Journal of Polymers and the Environment*, vol. 29, pp. 1810–1821, 2021, doi: 10.1007/s10924-020-01968-4.

K. Sudesh, H. Abe, and Y. Doi, ‘Synthesis, structure and properties of polyhydroxyalkanoates: biological polyesters’, *Progress in Polymer Science*, vol. 25, no. 10, pp. 1503–1555, 2000, doi: 10.1016/S0079-6700(00)00035-6.

L. Zhang, J. Sun, and H. Zhang, ‘PHA-clay nanocomposites and their environmental degradation behavior’, *Environmental Science and Pollution Research*, vol. 26, no. 13, pp. 12782–12792, 2019, doi: 10.1007/s11356-019-04586-w.

R. L. Shogren, ‘Starch: properties and materials applications’, *Carbohydrate Polymers*, vol. 35, no. 3-4, pp. 269–279, 1998, doi: 10.1016/S0144-8617(97)00260-3.

S. Kalambur and S. S. H. Rizvi, ‘Predicting moisture and temperature effects on starch-plastic degradation’, *Journal of Applied Polymer Science*, vol. 100, no. 6, pp. 4325–4331, 2006, doi: 10.1002/app.23660.

S. Ifuku, et al., ‘Preparation of chitin nanofibers and their characterization’, *Biomacromolecules*, vol. 8, no. 6, pp. 1973–1977, 2007, doi: 10.1021/bm070214f.

A. Bhiogade, & K. Murugasamy, ‘Studies on thermal and degradation kinetics of cellulose micro/nanoparticle filled polylactic acid (PLA) based nanocomposites’. *Polymers and Polymer Composites*, vol.29, pp. S85–S98, 2021, https://doi.org 10.1177/0967391120987170.

S. Lv, Y. Zhang,J. Gu, & H. Tan, ‘Physicochemical evolutions of starch/poly(lactic acid) composite biodegraded in real soil’ *Journal of Environmental Management*, vol.228, pp. 223–231,2018,https://doi.org/10.1016/j.jenvman.2018.09.033.