Cadence

A Computational Architecture for Degradation Engineering with Controlled Expiration

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August 15, 2025

Abstract

The accumulation of persistent plastic waste represents a fundamental mismatch between transient use-cases and the near-permanent chemical nature of conventional polymers. This paper introduces a predictive computational model that treats material lifespan as a programmable engineering parameter. Our multi-factor framework integrates intrinsic material properties, environmental conditions, and an autocatalytic[1] feedback term to predict polymer degradation trajectories. The model successfully reproduces characteristic S-shaped degradation curves observed in biodegradable polymers and provides quantitative predictions for time-to-degradation. We present both theoretical validation through simulation and outline a comprehensive experimental framework for empirical validation using established biodegradable polymers. This approach enables the *ab initio*[2] design of materials with predetermined lifespans.

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[1]A process in which a product of a reaction serves as a catalyst for that same reaction, creating a self-accelerating feedback loop.

[2]Latin, lit. "from the beginning." In a scientific context, this refers to models or calculations derived from first principles, without reliance on experimental data.

Nomenclature

Symbol	Description	Units
$M_w(t)$	Molecular weight at time t	Da
M_{w0}	Initial molecular weight	Da
f_c	Fraction of cleavable bonds	dimensionless
k_{base}	Intrinsic base degradation rate	day^{-1}
env_factor	Environmental harshness scalar	dimensionless
ϵ, t_0	Environmental impact scaling parameters	dimensionless, days
$S(t)$	Sigmoid autocatalytic factor	dimensionless
s, t_s	Autocatalytic shape and timing parameters	day^{-1}, days
γ	Autocatalytic strength factor	dimensionless
α, β	Scission-to-decay coupling constants	dimensionless
M_b	Average molecular weight of cleavable units	Da
θ	Degradation threshold fraction	dimensionless
t_d	Degradation time	days

1 Introduction

1.1 The Challenge of Material Permanence

Modern polymer chemistry has achieved remarkable success in creating durable materials, yet this very durability has become an environmental liability. Conventional polymers like PET and HDPE persist for centuries, accumulating in ecosystems where they fragment into harmful microplastics [1, 2]. Current mitigation strategies—recycling, cleanup, and waste management—address symptoms rather than the fundamental cause: materials designed without consideration of their end-of-life.

1.2 Existing Approaches and Limitations

Current biodegradable polymer research focuses primarily on identifying materials that degrade under specific conditions, with limited ability to predict or control degradation timelines [3]. Existing models typically address single degradation mechanisms (e.g., hydrolysis, enzymatic action) without integrating the complex interplay of environmental factors and autocatalytic processes that govern real-world degradation [4].

1.3 A New Approach: Programmable Material Lifespans

We propose treating material lifespan as a primary engineering parameter, analogous to how mechanical properties are currently designed. This requires a predictive framework capable of relating molecular structure to degradation kinetics across varying environmental conditions. Our model addresses this need by providing a quantitative framework for predicting degradation trajectories based on fundamental material and environmental parameters.

2 Theoretical Framework

2.1 Variables and Assumptions

Our model predicts the temporal evolution of average molecular weight ($M_w(t)$) as a proxy for polymer degradation. The framework incorporates material-specific parameters (initial molecular weight, fraction of cleavable bonds), environmental factors (temperature, moisture, pH), and autocatalytic feedback mechanisms that arise from degradation products.

2.2 Environmental and Autocatalytic Effects

Environmental conditions (e.g., temperature, moisture) influence degradation through a time-dependent rate constant, $k(t)$. We propose a logarithmic functional form as a first approximation to model effects that may saturate over time, such as microbial colonization or moisture penetration:

$$k(t) = k_{\text{base}} \cdot \text{env\_factor} \cdot \left(1 + \epsilon \cdot \ln \left(1 + \frac{t}{t_0} \right) \right) \tag{1}$$

The choice of a logarithmic function is a simplifying assumption; alternative forms (e.g., power-law) may prove more accurate for specific polymer-environment systems upon experimental validation.

Autocatalytic effects are modeled using a time-dependent sigmoid function, $S(t)$. This function serves as a proxy for the concentration of degradation byproducts (e.g., acidic monomers) that catalyze further chain scission:

$$S(t) = \frac{1}{1 + e^{-s(t-t_s)}} \tag{2}$$

This time-based formulation is a key simplification. A more physically rigorous model would define S as a function of the extent of reaction. However, for many systems where degradation proceeds predictably, a time-dependent sigmoid can effectively approximate the autocatalytic feedback loop.

2.3 Unified Predictive Equation

The complete model integrates these effects. The constants α and β are empirical coupling factors that translate the probability of bond cleavage into a macroscopic change in molecular weight; their values must be determined experimentally for a given polymer system:

$$M_w(t) = M_{w0} \cdot \exp \left[-\beta \cdot \alpha \cdot \frac{M_{w0}}{M_b} \cdot \min \left(P_{\text{eff}}(t), 0.99 \right) \right] \tag{3}$$

$$P_{\text{eff}}(t) = P(t) \cdot (1 + \gamma \cdot S(t) \cdot P(t)) \tag{4}$$

$$P(t) = f_c \left(1 - e^{-k(t) \cdot t} \right) \tag{5}$$

The degradation time (t_d) is defined as the time to reach a user-defined threshold, θ. This threshold represents the point at which the material has lost its functional integrity, which is application-specific (e.g., 95% molecular weight loss for packaging vs. 80% for a mulch film):

$$t_d = \min\{t : M_w(t) \leq (1 - \theta) \cdot M_{w0}\} \tag{6}$$

3 Model Validation

3.1 Computational Demonstration and Analysis

To demonstrate the model's behavior and explore its dynamics, we conducted a series of computational simulations, summarized in Figure 1.

3.1.1 Core Model Behavior (Panel A)

First, we simulated a baseline scenario representing a hypothetical polymer under industrial composting conditions. The parameters for this baseline case are detailed in Table 1. The simulation predicted that the polymer would reach the 95% molecular weight loss threshold in **50.2 days**. As shown in Figure 1A, the model successfully reproduces the characteristic S-shaped degradation curve observed in experimental studies, confirming the framework's mathematical coherence.

Table 1: Baseline parameters for the computational demonstration.

Parameter	Value	Description
M_{w0}	100,000 Da	Initial Molecular Weight
f_c	0.8	Fraction of Cleavable Bonds
k_{base}	0.001 day^{-1}	Base Degradation Rate
env_factor	3.0	Environmental Harshness
γ	50.0	Autocatalytic Strength
t_s	80 days	Autocatalysis Midpoint
θ	0.95	MW Loss Threshold (95%)

3.1.2 Sensitivity Analysis (Panel B)

To understand the relative impact of key parameters, we conducted a sensitivity analysis (Figure 1B). We compared the baseline case to two variations: one with a lower fraction of cleavable bonds ($f_c = 0.4$) and another in a milder environment (env_factor $= 1.0$). The results clearly show that the degradation time is highly sensitive to both intrinsic material properties and external conditions. Halving the cleavable bond fraction, for instance, significantly extends the material's lifespan, as does reducing the environmental harshness. This analysis highlights the primary levers available to chemists for tuning a material's lifespan.

3.1.3 Environmental Model Comparison (Panel C)

To address the simplifying assumption of the logarithmic environmental factor, we compared its output to two other plausible models: a linear model (representing steady environmental impact) and a power-law model (representing accelerating impact). As seen in Figure 1C, the choice of functional form has a profound impact on the initial degradation rate. While all models converge, the initial kinetics vary significantly, underscoring the need for experimental data to select the most appropriate environmental model for a given polymer-environment system.
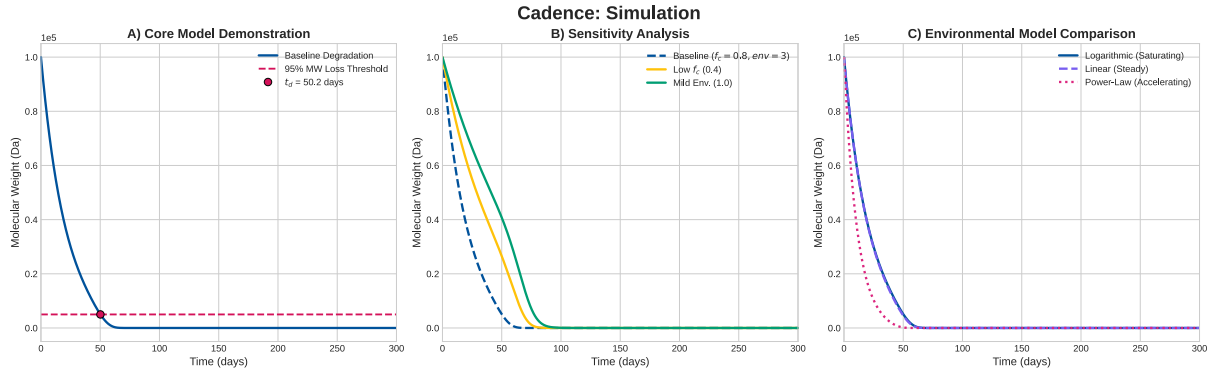
Figure 1: Computational analysis of the cadence model. **A)** Demonstration of the core model for a baseline scenario, predicting a degradation time of 50.2 days. **B)** Sensitivity analysis showing how degradation time is affected by changes in material properties (f_c) and environmental harshness. **C)** Comparison of different functional forms for the environmental factor, demonstrating their impact on degradation kinetics.

4 Applications

4.1 Reverse Engineering Material Design

The validated model enables inverse design: specifying target degradation time and environmental conditions to determine required polymer properties. This approach could accelerate development of:

- Agricultural mulch films with crop-cycle lifespans

- Medical implants with patient-specific degradation profiles

- Packaging materials optimized for supply chain timelines

4.2 Environmental Assessment and Regulatory Framework

Quantitative degradation predictions enable:

- Life cycle analysis with precise end-of-life modeling

- Environmental risk assessment for new materials

- Regulatory framework development for biodegradable claims

- Design of materials that match use-case duration exactly

5 Limitations and Future Work

5.1 Current Limitations

This framework is presented as a foundational model with clear limitations that provide avenues for future research:

- **Model Simplifications:** The time-based autocatalysis and logarithmic environmental factor are key simplifications. Future work should aim to replace these with physically-grounded terms dependent on reactant concentration and specific environmental variables (e.g., temperature via an Arrhenius relationship).

- **Parameter Empiricism:** The coupling constants (α, β) are currently empirical. A key research goal is to link these parameters to fundamental chemical properties, reducing the model's reliance on experimental fitting.

- **Degradation Metric:** The model is limited to molecular weight as the primary degradation metric. Future iterations should incorporate metrics for mass loss, mechanical property decay, and ecotoxicity of degradation byproducts.

- **Calibration Requirements:** Model requires experimental calibration for each polymer class and environmental condition.

5.2 Future Directions

Future directions include:

- Integration with molecular dynamics simulations for *ab initio* parameter prediction

- Extension to multi-component polymer systems

- Development of real-time degradation monitoring techniques to accelerate validation

- Machine learning approaches for parameter optimization across polymer families

- Incorporation of mechanical property evolution alongside molecular weight changes

6 Conclusion

We have presented a comprehensive theoretical framework for predicting polymer degradation as a foundation for designing materials with programmable lifespans. The model successfully captures complex degradation dynamics, including environmental dependence and autocatalytic acceleration. The computational demonstration confirms the framework's mathematical viability and reproduces characteristic S-shaped degradation curves observed in experimental studies.

While this computational validation demonstrates the framework's potential, experimental validation using established biodegradable polymers represents the critical next step. The outlined three-phase experimental program provides a clear pathway toward full empirical validation and practical implementation.

This approach has the potential to transform material design from empirical trial-and-error to predictive engineering, enabling the creation of materials that fulfill their function and then disappear on schedule. Such capability addresses the plastic pollution crisis at its source: the fundamental design of materials themselves, creating a future where material persistence matches intended use duration.

Author Contributions

Author[3]: Conceptualization, Investigation, Methodology, Project Administration.

Data Availability

The Python code used to generate the simulations and figures presented in this study, along with the full source for this paper, is openly available in the following GitHub repository: https://github.com/tylaperryer.

Conflicts of Interest

The authors declare no conflicts of interest.

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