Матеріали XXV Міжнародної науково-практичної конференції
«Екологія. Людина. Суспільство»
пам'яті д-ра Дмитра СТЕФАНИШИНА
(12 червня 2025 р., м. Київ, Україна)

Proceedings of the XXV International Science Conference
«Ecology. Human. Society»
dedicated to the memory of Dr. Dmytro STEFANYSHYN
(June 12 2025, Kyiv, Ukraine)

ISSN (Online) 2710-3315
https://doi.org/10.20535/ehs2710-3315.2025.330316

MATHEMATICAL MODULAR MODELING METHODS FOR SIMULATING MATERIAL – ENVIRONMENT INTERACTIONS (MEI)

Andrejs KRAUKLIS
Latvia University of Life Sciences and Technologies,
MEI Core Group
Akadēmijas Street 19, Jelgava, LV-3001, Latvia
e-mail: andrejs.krauklis@lbtu.lv

Abstract
Material-environment interactions (MEI) significantly impact the durability and performance of various engineered materials, creating uncertainties that complicate the prediction of their service lifetimes, as well as affect the environment by the release of chemicals and ions. The duality of lifetime prediction lies in the definitions of failure criteria and end-of-life scenarios. Similar modeling methodologies can be applied, whether prioritizing "safety," "decomposition" of the material, or environmental pollution. Conventional experimental approaches are costly and time-consuming, presenting a substantial hurdle to innovation. Mathematical modeling methods offer a cost-effective and efficient alternative by combining accelerated testing data and simulations based on fundamental scientific principles of MEI. This paper presents a modular and multiscale modeling framework, illustrating how environmental factors such as chemical composition, temperature, acidity, and mechanical stresses influence material degradation. This framework, applicable to a wide variety of materials and environments, provides essential tools for predicting service lifetimes, contributing to both academia and industrial applications.

Keywords: *mathematical modeling methods, environment, modular methods, multiscale modeling, material-environment interactions.*

1. Introduction

Materials interact continuously with their environments, leading not only to their gradual degradation and eventual failure but also to environmental pollution through chemical and ionic releases. Traditional experimental approaches, involving extensive long-term testing, are costly and time-intensive, restricting the rapid assessment and innovation in materials design. Thus, reliable, accurate, and economically viable MEI modeling methods are urgently required to better predict both material lifespan and environmental impacts [1].

This paper proposes a modular, multiscale modeling framework based on fundamental physical and chemical principles. The framework incorporates accelerated testing and predictive modeling, bridging short-term data with long-term predictions, facilitating cost reduction, and streamlining the innovation process. Given the multicomponent nature of many engineered materials, the approach also considers each component individually, addressing their unique interaction pathways and environmental consequences [2]. The multiscale nature of MEI simulations is shown in Figure 1.

2. Methods

2.1. Modular Concept

The modular modeling framework integrates processes across multiple scales, from atomic-level chemical interactions to macroscopic responses. Each module is developed separately, addressing specific degradation mechanisms such as chemical reactions, diffusion, and mechanical stress-induced failures. The modular approach also explicitly accounts for chemical releases into the environment, thus enabling comprehensive lifetime predictions from both safety and environmental perspectives [4]. The modular approach (as an example for composite materials) is schematically shown in Figure 2. The methodology of the “red” (meaning theoreticized) quantitative structure-property relationship (QSPR) module was recently developed and described in [5].

2.2. MEI Simulations of Matrix Constituents

Matrix materials commonly undergo degradation through various mechanisms such as hydrolysis, and oxidation. The modeling methods employed here incorporate degradation rate kinetics, empirical correlations, and advanced simulations to capture these complex processes accurately. Diffusion-driven processes such as moisture absorption and chemical leaching are modeled using advanced diffusion equations, enabling assessment of both the structural integrity loss and the environmental impact due to chemical releases.

Quantitative Structure-Property Relationship (QSPR) modeling is particularly highlighted for its ability to correlate molecular properties with macroscale performance, bridging molecular interactions and large-scale structural responses effectively [6].

2.3. MEI Simulations of Reinforcing Constituents

Reinforcing elements, including fibers and particulates, exhibit diverse environmental degradation pathways such as chemical dissolution, corrosion, and stress-corrosion cracking. Predictive kinetic models and micromechanical approaches quantify the degradation rates and associated chemical emissions. These models facilitate predictions concerning both mechanical performance deterioration and potential environmental pollution resulting from constituent breakdown.

Advanced analytical tools are employed to evaluate interactions at the microstructural level, further linking these micro-level changes to macro-scale material behaviors and environmental impact scenarios.

An analytical toolbox consisting of seven modeling modules was presented in a recent work (2021) on the Modular Paradigm for composite GFRPs [7]. The seven developed modules of the Reinforcement Modular Group within the Modular Paradigm are shown in Figure 3.

Models that predict mass loss and radius reduction are the Contracting Cylinder model [8], the Shrinking Cylinder model [9] and the Dissolving Cylinder Zero-Order Kinetic (DCZOK) model [10].

The crack growth evolution can be modelled by micromechanical models [11]. The link between the dissolution kinetics (DCZOK model) and the hydrolytic crack growth is described in [12].

As shown in Figure 2, modules are divided in four sections that relate to the overall composite configuration and modeling of environmental degradation of individual micro-constituents (polymer, fibers and interphase).

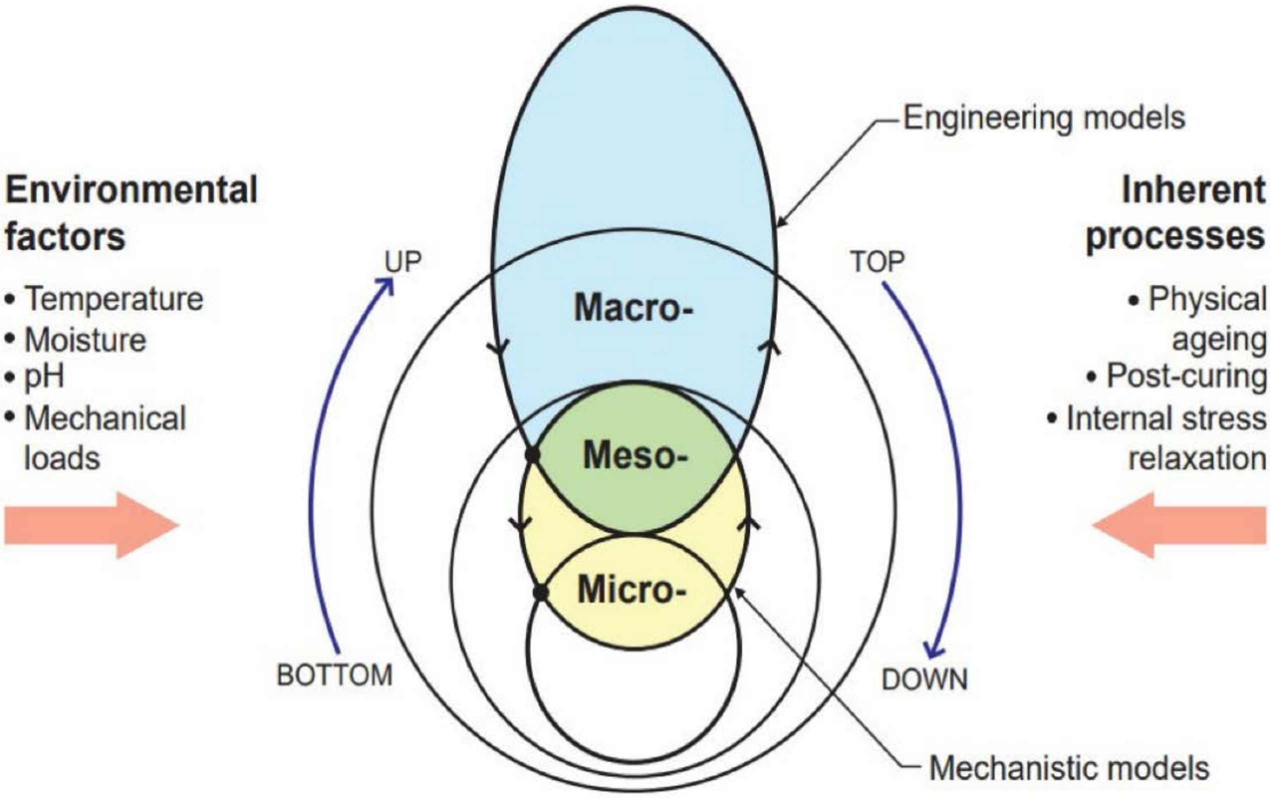

Figure 1. *Multitude of scales involved in MEI Modeling [3]*

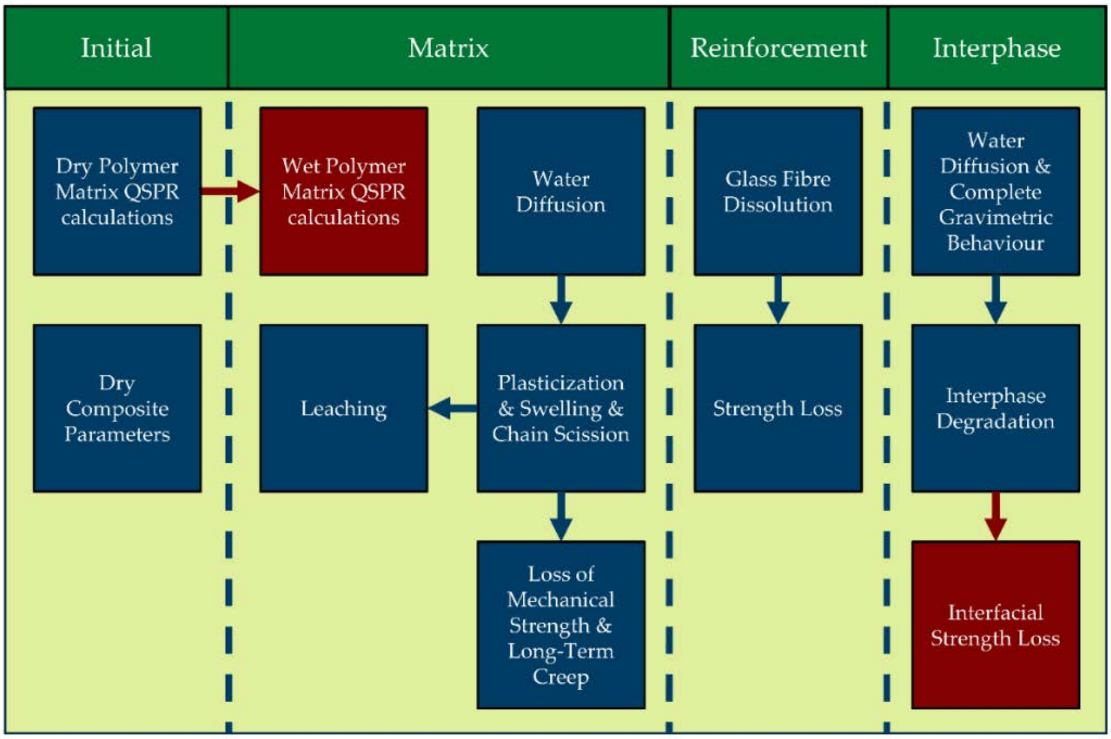

Figure 2. *Modular MEI framework for composite materials [6]*

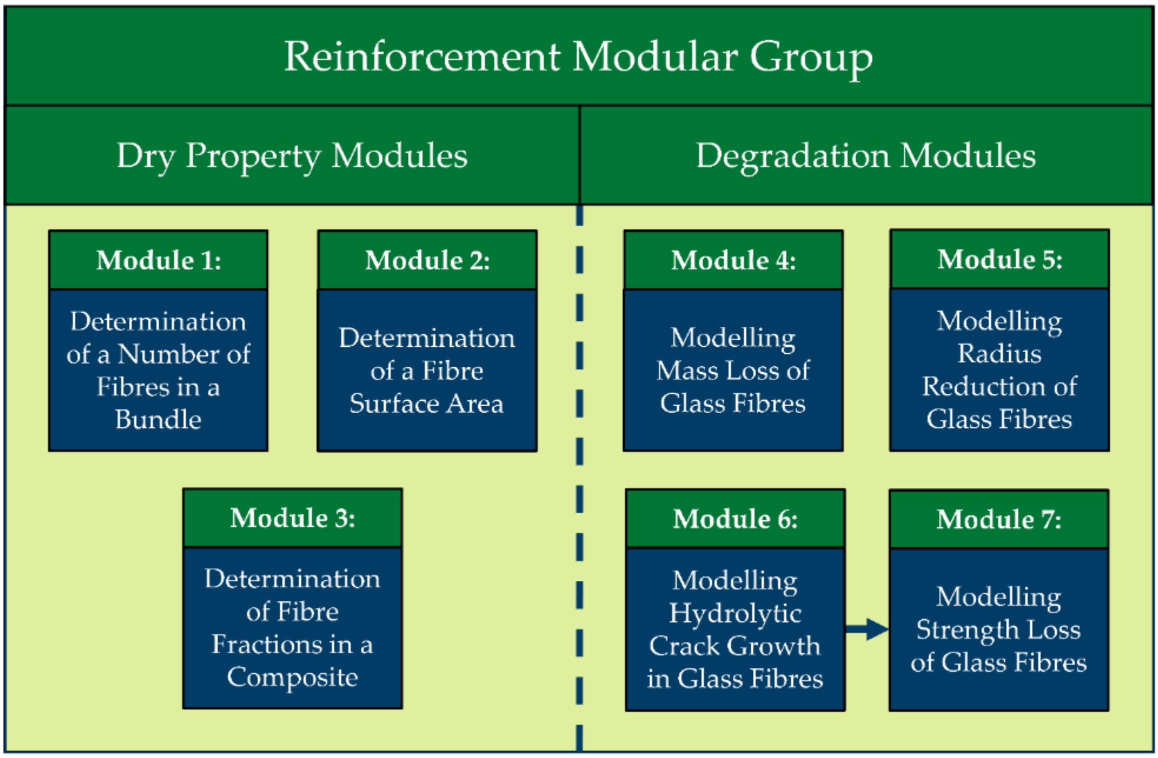

Figure 3. *The seven modules for Reinforcement within the Modular Modeling Concept [7]*

2.4. MEI Simulations of Interphase Constituents

Interphase degradation between the reinforcement and matrix phases significantly affects both structural integrity and the potential for environmental contamination through chemical release. Mass balance and kinetic modeling approaches characterize the degradation processes, enabling accurate predictions of both mechanical property loss and chemical leaching [13-15].

Improved models linking interphase degradation to global structural and environmental impacts are still evolving and represent a critical area for further research to enhance predictive capabilities comprehensively [13-15].

3. Discussion

The predictive modeling of material lifetimes involves clearly defining failure criteria and end-of-life scenarios, which directly impacts both safety management and environmental considerations. Similar degradation processes and modeling techniques apply irrespective of whether the primary objective is structural reliability or minimizing environmental pollution.

Future improvements should focus on enhancing the precision of individual modeling modules, expanding the integration of modules, and explicitly incorporating environmental release and pollution metrics into lifetime prediction models.

4. Conclusions

The presented modular and multiscale mathematical modeling framework effectively predicts material-environment interactions (MEI) and advances multiscale modelling frameworks by connecting molecular degradation processes to macroscopic mechanical behaviour, encompassing both structural integrity and environmental impacts.

The modular design of this framework allows for the integration of additional experimental and computational tools, enhancing its versatility for different material systems and aging conditions.

The methodology significantly reduces reliance on extensive physical testing, thereby enabling efficient and accurate lifetime and pollution predictions. By offering on-site, non-destructive solution for structural health monitoring, this methodology has broad potential applications across various industries. By offering on-site, non-destructive solution for structural health monitoring, this methodology has broad potential applications across various industries.

This approach supports sustainable material design and enhances reliability predictions, significantly benefiting both academia and industry.

Acknowledgments: The author acknowledges TEN4 funding. Andrey is especially grateful to Oksana for her support.

References

1. A. E. Krauklis. *Environmental Aging of Constituent Materials in Fiber-Reinforced Polymer Composites*. Ph.D. Thesis, NTNU, Trondheim, 2019.
2. A. E. Krauklis, C. W. Karl, I. B. C. M. Rocha, J. Burlakovs, R. Ozola-Davidane, A. I. Gagani, and O. Starkova. Modelling of Environmental Ageing of Polymers and Polymer Composites—Modular and Multiscale Methods. *Polymers*, 14:216-259, 2022.
3. O. Starkova, A. I. Gagani, C. W. Karl, I. B. C. M. Rocha, J. Burlakovs, and A. E. Krauklis. Modelling of Environmental Ageing of Polymers and Polymer Composites—Durability Prediction Methods. *Polymers*, 14:907-942, 2022.
4. A. T. Echtermeyer, A. I. Gagani, A. E. Krauklis and T. Mazan. Multiscale Modelling of Environmental Degradation—First Steps. In Durability of Composites in a Marine Environment, vol 2, pages 135-149, Springer, Berlin, 2018.
5. E. Krauklis, F. Verceux, S. Grammatikos. Rapid Non-Destructive Polymer Degradation Degree Evaluation Method Using Quantitative Structure-Property Relationship. *Mechanics of Composite Materials*, 2025 (*accepted for publication*).
6. A. E. Krauklis. Environmental Durability of Composite Materials: Analytical Modelling Toolbox. In *Proceedings of the Aachen Reinforced! Symposium*, Aachen, pages 62–70, 2021.
7. A. E. Krauklis. Modular Paradigm for Composites: Modeling Hydrothermal Degradation of Glass Fibers. *Fibers* 9, 83-94, 2021.
8. A. Khawam and D. R. Flanagan. Solid-State Kinetic Models: Basics and Mathematical Fundamentals. *J. Phys. Chem. B* 110, 17315–17328, 2006.
9. S. T. Bashir, L. Yang, J. J. Liggat and J. L. Thomason. Kinetics of dissolution of glass fiber in hot alkaline solution. *J. Mater. Sci.* 53, 1710–1722, 2018.
10. A. E. Krauklis and A. T. Echtermeyer. Long-Term Dissolution of Glass Fibers in Water Described by Dissolving Cylinder Zero-Order Kinetic Model: Mass Loss and Radius Reduction. *Open Chem.* 16, 1189–1199, 2018.
11. H. Sekine and P. W. Beaumont. A physically based micromechanical theory of macroscopic stress-corrosion cracking in aligned continuous glass-fibre-reinforced polymer laminates. *Compos. Sci. Technol.* 58, 1659–1665, 1998.
12. A. T. Echtermeyer, A. E. Krauklis, A. I. Gagani, and E. Sæter. Zero Stress Aging of Glass and Carbon Fibers in Water and Oil—Strength Reduction Explained by Dissolution Kinetics. *Fibers* 7, 107-120, 2019.
13. A. E. Krauklis, O. Starkova, D. Gibhardt, G. Kalinka, H. A. Aouissi, J. Burlakovs, A. Sabalina and B. Fiedler. Reversible and irreversible effects on the epoxy GFRP fiber-matrix interphase due to hydrothermal aging. *Composites Part C: Open Access* 12, 100395-100403, 2023.

14. A. E. Krauklis, A. I. Gagani and A. T. Echtermeyer. Long-Term Hydrolytic Degradation of the Sizing-Rich Composite Interphase. Coatings 9, 263-286, 2019.

15. R. Plonka, E. Mäder, S. Gao, C. Bellmann, V. Dutschk and S. Zhandarov. Adhesion of epoxy/glass fibre composites influenced by aging effects on sizings. *Compos. Part A Appl. Sci. Manuf.* 35, 1207–1216, 2004.

МАТЕМАТИЧНІ МЕТОДИ МОДУЛЬНОГО МОДЕЛЮВАННЯ ДЛЯ ІМІТАЦІЇ ВЗАЄМОДІЇ МАТЕРІАЛІВ ІЗ ДОВКІЛЛЯМ

Андрейс КРАУКЛІС
Латвійський університет наук про життя і технологій
Akadēmijas Street 19, Jelgava, LV-3001, Латвія
https://orcid.org/0000-0003-2380-4450

Анотація

Взаємодія матеріалів із довкіллям суттєво впливає на довговічність і експлуатаційні характеристики різних інженерних матеріалів, створюючи невизначеності, які ускладнюють прогнозування їхнього строку служби, а також спричиняючи забруднення довкілля через виділення хімічних речовин та іонів. Подвійність у прогнозуванні строку служби полягає у визначенні критеріїв відмови та сценаріїв завершення експлуатації. Схожі методи моделювання можуть бути застосовані незалежно від того, що ставиться в пріоритет — «безпека», «розклад» матеріалу чи забруднення довкілля. Традиційні експериментальні підходи є затратними за часом і коштами, що створює значні перешкоди для впровадження інновацій. Натомість математичні методи моделювання пропонують економічно вигідну та ефективну альтернативу, поєднуючи дані прискорених випробувань із симуляціями, заснованими на фундаментальних наукових принципах моделювання взаємодії. У цій роботі представлено модульний багатомасштабний підхід до моделювання, який ілюструє, як чинники довкілля — хімічний склад, температура, кислотність і механічні навантаження — впливають на деградацію матеріалів. Цей підхід, що застосовується до широкого спектра матеріалів і середовищ, забезпечує важливі інструменти для прогнозування строків служби, сприяючи як академічним дослідженням, так і промисловому використанню.

Ключові слова: *методи математичного моделювання, навколишнє середовище, модульні методи, багатофакторне моделювання, взаємодія матеріал-середовище.*