Michigan Technological University
Department of Mechanical Engineering – Engineering Mechanics

John O. Hallquist Endowed Chair in Computational Mechanics

2023 Annual Report

Gregory M. Odegard

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Introduction

The purpose of this report is to detail the research activities that were performed with support from the endowed position titled "John O. Hallquist Endowed Chair in Computational Mechanics" in the year 2023. This position has been held since February 4, 2021 by Prof. Gregory M. Odegard of the Department of Mechanical Engineering – Engineering Mechanics (MEEM) at Michigan Technological University. Prof. Odegard is the Director of Research in the department and the Director of the NASA Space Technology Research Institute (STRI) for Ultra-Strong Composite Materials by Computational Design (US-COMP).

Prof. Odegard would sincerely like to thank the Hallquist family for their generous gift. Their continuous support for the MEEM department has made a difference in raising our profile among ME department around the country and has played an important role in improving the educational experience of both undergraduate and graduate students in our department.

Supported students

Khatereh Kashmari was supported by the fund in summer and fall semesters of 2023. Khatereh is a PhD student in the MEEM department, and she is in the final 2 years of her PhD. The Hallquist funds are ideal for a student like Khatereh, who can't participate in my other sponsored projects because she is not a U.S. Citizen. However, she is conducting excellent research, and deserves our financial support.

Resulting research accomplishments

In 2023, Khatereh completed the first phase of her PhD work using the Hallquist funds, and the work resulted in the following publications:

- Kashmari, K., H. Al Mahmud, S.U. Patil, W.A. Pisani, P. Deshpande, M. Maiaru, G.M. Odegard, "Multiscale Process Modeling of Semi-Crystalline PEEK for Tailored Thermo-Mechanical Properties", *ACS Applied Engineering Materials*, Vol. 1, no. 11, pp. 3167–3177 (2023)
- Kashmari, K., H. Al Mahmud, S.U. Patil, W.A. Pisani, P. Deshpande, M. Maiaru, and G.M. Odegard, "Molecular Dynamics Modeling of PEEK Resin Properties for Processing Modeling", *38th American Society for Composites Conference*, Boston, MA, September 18-20, 2023

Research abstract: Poly ether ether ketone (PEEK) is a semi-crystalline thermoplastic that is used in high-performance composites for a wide range of applications. Because the crystalline phase has a higher mass density than the amorphous phase, the evolution of the crystalline phase during high-temperature annealing processing steps results in the formation of residual stresses and laminate deformations, which can adversely affect composite laminate performance. Multiscale process modeling, utilizing molecular dynamics, micromechanics, and phenomenological PEEK crystal kinetics laws, is used to

predict the evolution of volumetric shrinkage, elastic properties, and thermal properties as a function of crystalline phase evolution, and thus annealing time, in the 306 – 328° C temperature range. The results indicate that lower annealing temperatures in this range result in a faster evolution of thermo-mechanical properties and shrinkage toward the pure crystalline values. Therefore, from the perspective of composite processing, it may be more advantageous to choose the higher annealing rates in this range to slow down the volumetric shrinkage and allow PEEK stress-relaxation mechanisms more time to relax internal residual stresses in PEEK composite laminates and structures.

Technical details: The workflow for this project is shown in Figure 1. The project utilizes techniques such as molecular dynamics (MD) simulation and micromechanics modeling. As a result, molecular- and micro-scale information is used to predict the properties of PEEK as a function of processing conditions. With this information, improved PEEK components can be manufactured with optimizal processing parameters.

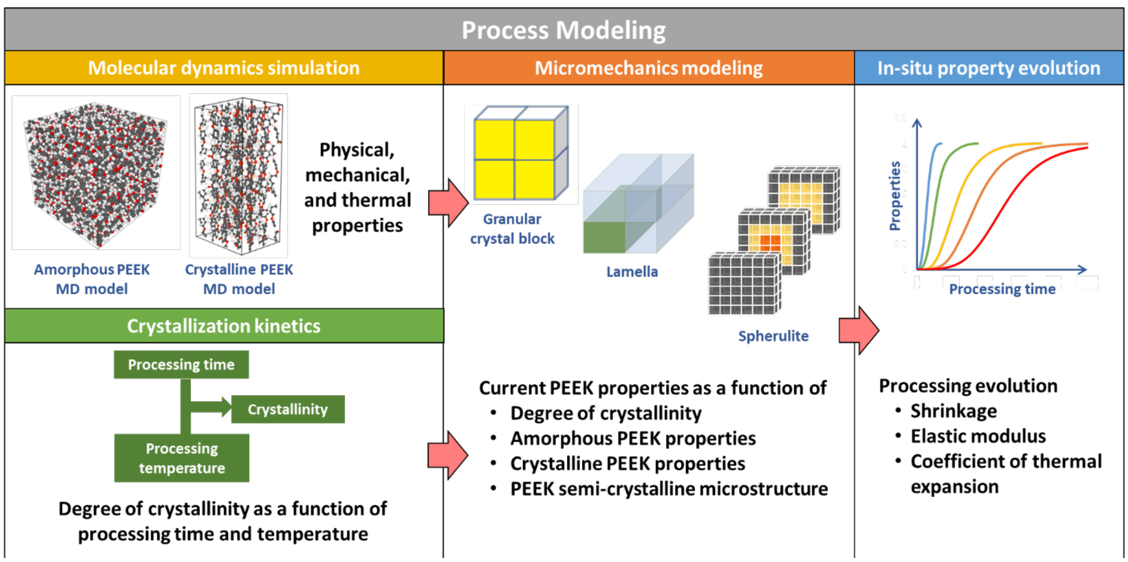

Figure 1. Multiscale modeling workflow for semicrystalline PEEK

For example, Figure 2 shows how shrinkage, Young's modulus, Poisson's ratio, shear modulus, and coefficient of thermal expansion (below and above the glass transition temperature) vary with processing time and processing temperature. These results are important to be able to optimize the desired properties by adjusting the processing conditions. Specifically, it is desired to have the volumetric shrinkage increase as slowly as possible during processing so that viscoelastic relaxation can reduce the residual stresses in the polymer and thus increase the overall strength. The results show that higher processing temperatures result in a slower evolution of shrinkage, thus indicating that strength can be maximized with higher processing temperatures. The rest of the data in Figure 2 demonstrates that the elastic/thermal properties all eventually converge to the same level, regardless of the processing time. The slower drop in coefficient of thermal expansion at higher processing temperatures may be advantage in further reducing residual stresses in manufactured composites, thus further improving the overall composite structural strength.

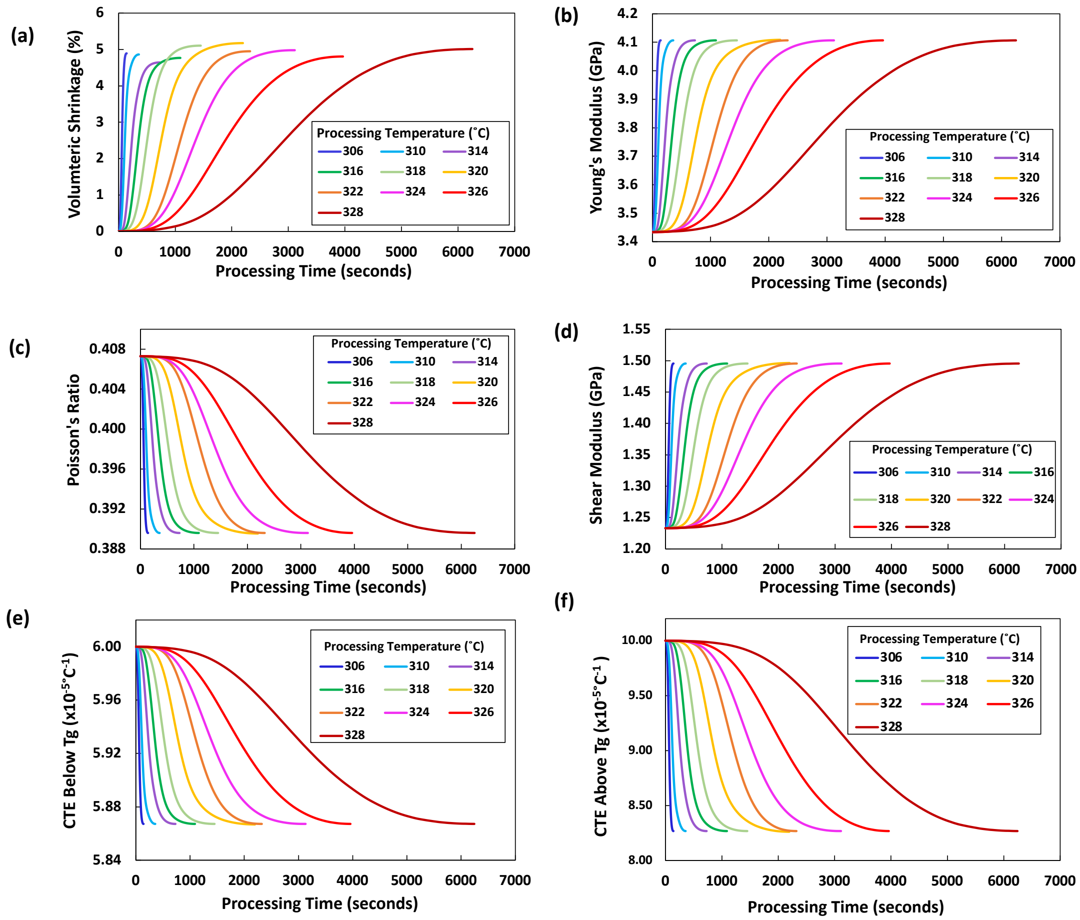

Figure 2. Evolution of (a) volumetric shrinkage, (b) Young's modulus, (c) Poisson's ratio, (d) shear modulus, (e) and (f) coefficient of thermal expansion as a function of processing time for varying processing temperatures.

Importance of Hallquist funding

The Hallquist funds were crucial for our research group to finish the above-described process modeling research. This achievement serves two important roles:

1. The publication will further solidify Michigan Tech as a global leader in process modeling research
2. The publication will open the door for optimization of material manufacturing process research for more advanced composite material systems. Specifically, this work will provide computational tooling for upcoming NASA and DoD projects that will be funded in 2024. Thus, the Hallquist funds have served as a critical seed grant for these efforts.