UNDERSTANDING MATERIAL-PROCESS-MICROSTRUCTURE-PERFORMANCE RELATIONSHIPS OF THERMOPLASTIC OLEFINS FOAMS

UNIVERSITY OF DELAWARE | CENTER FOR COMPOSITE MATERIALS

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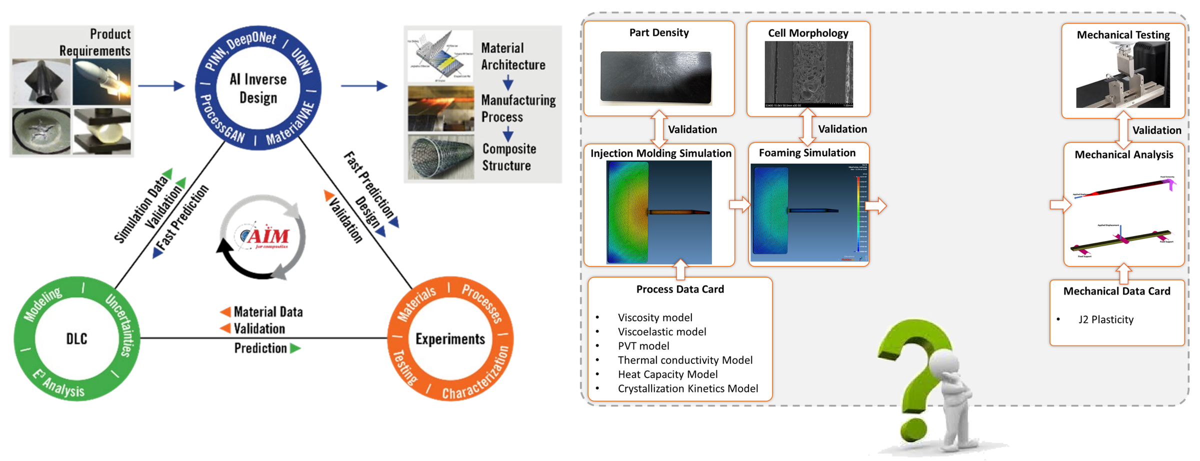
Introduction

- The mission of this EFRC is to build an AI-enabled inverse design approach for fundamental understanding and integrated material-manufacturing design of advanced polymer composites.
- While uncovering these fundamental insights, this EFRC also aims to build Inverse Design Software (InDeS) tools that accelerate the discovery of advanced polymer composites for improved performance and energy- efficient manufacturing, thereby enabling a smaller carbon footprint, lower structural weight, and lower cost."

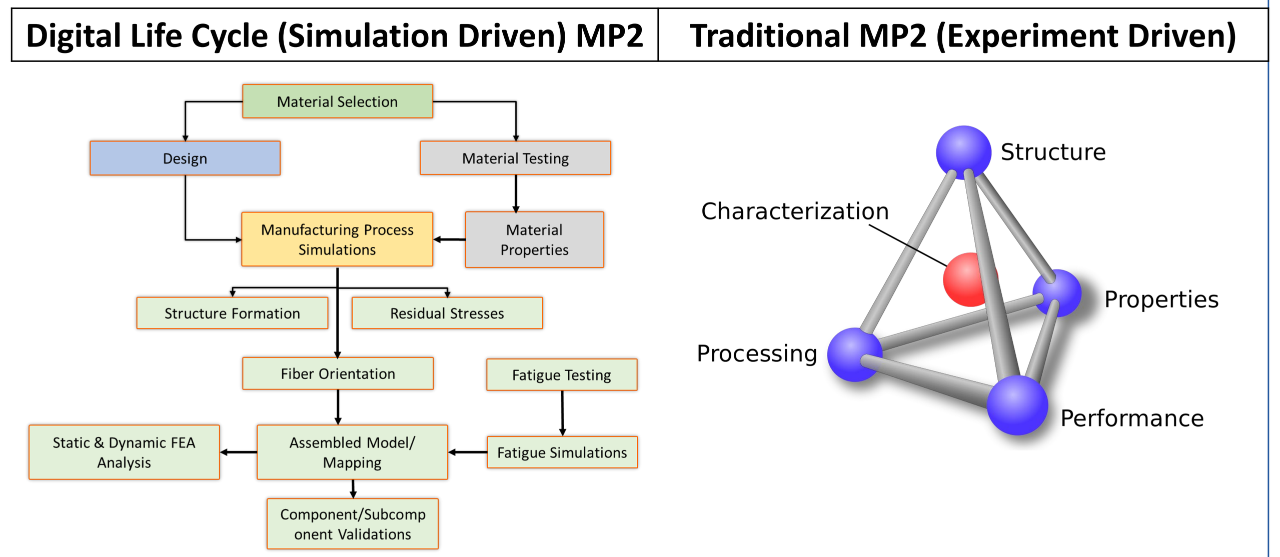


- The work focuses on experimental data generation in Thrust III and validating process simulations DLC Models in Thrust II.

Work	Process	Cell Structure	Tensile	Flexural	Impact	Modelling Approach
Guo et al. [2007]	IM	✓	✓	×	×	-
Santoni et al. [2007]	IM	✓	✓	×	×	-
Peyda et al. [2016]	IM	✓	✓	×	×	-
Wong et al. [2008]	IM	✓	✓	×	×	Ashley Gibson
Kim et al. [2010]	Batch	✓	✓	×	×	-
Kim et al. [2011]	Batch + IM	✓	✓	×	×	Batch foaming model

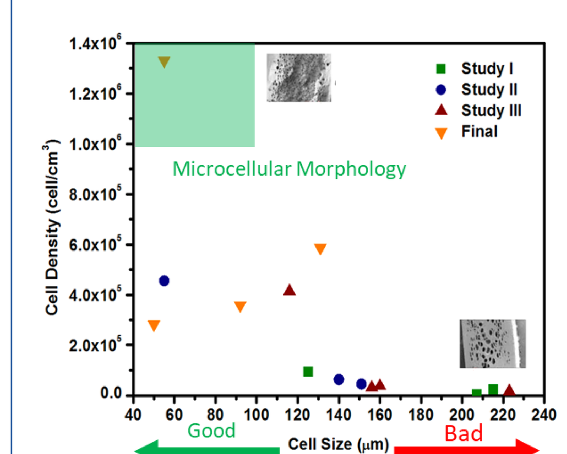
- The only work was by Xi and Kim et al [15] who used a modified cross model to describe the rheological properties of generic PP and nucleation models in Moldex 3D to predict foam morphology.
- There is a dearth of coupled process and mechanical modelling for TPO foams

Digital Life Cycle (Simulation Driven) MP2	Traditional MP2 (Experiment Driven)



- Digital life cycle leverages multiple simulation and validation steps provide OEMs the confidence to adopt new materials at shorter time scales.
- Traditionally, new material deployment takes years in order to experimentally gather the required data required to understand the interdependence of processing, structure, property and performance.
- This is time consuming and expensive primarily due to shear number of experimental inputs (e.g. tensile, flexural, impact, appearance).

Traditional (Experimental) Material-Process-Microstructure-Performance



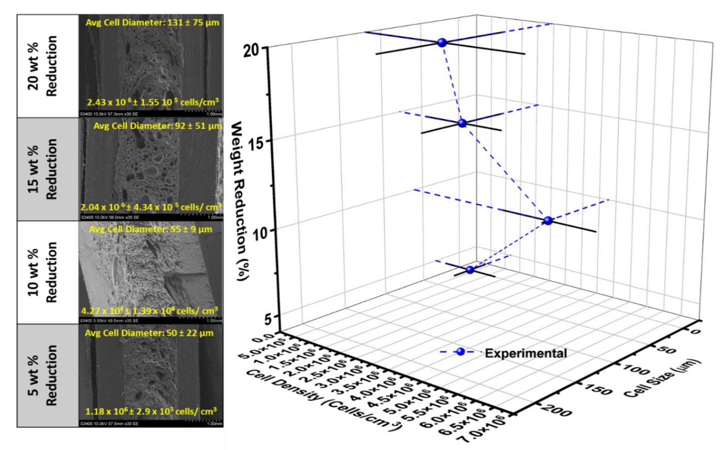
Study 1 :- To observe effect of lightweighting on foam morphology via reduced material usage and to study material foaming behavior.

Study 2 :- To observe effects of low gas dosage, processing temperature in order to improve foam morphology

Study 3 :- To observe effects of high gas dosage, processing temperature, and injection parameters in order to improve foam morphology

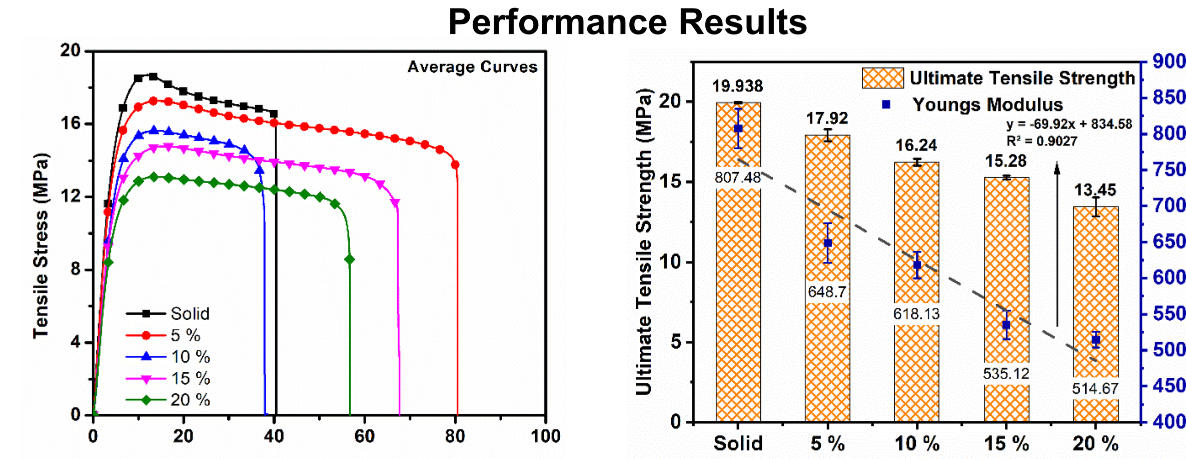
- Higher melt temperatures & ScF dosage with lower injection speed played a crucial role in improving ScF N2 solubility and obtaining microcellular morphology [17]

Microstructural Results

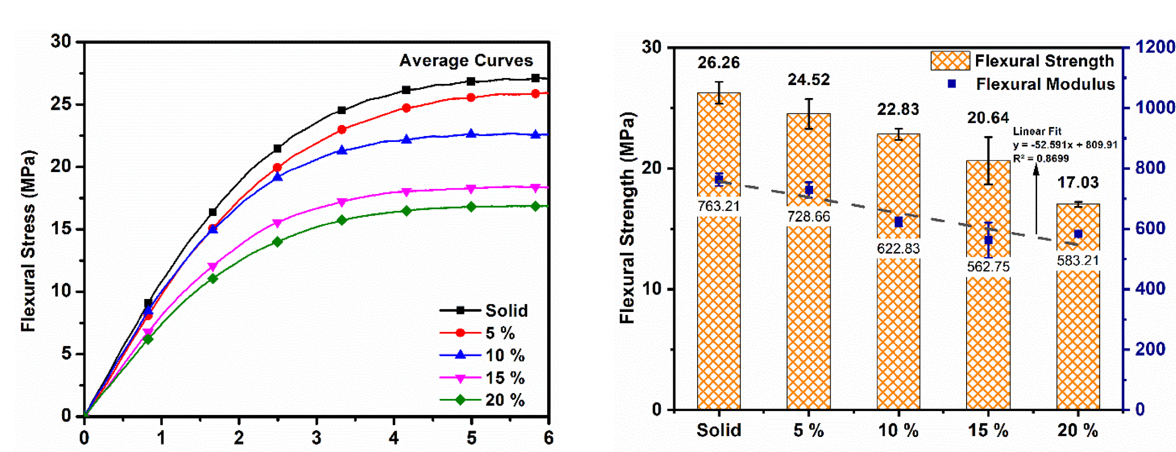


- Cell size increased with higher lightweighting compositions.
- Highest cell density was observed for 10 % lightweighting samples (ScF D2).

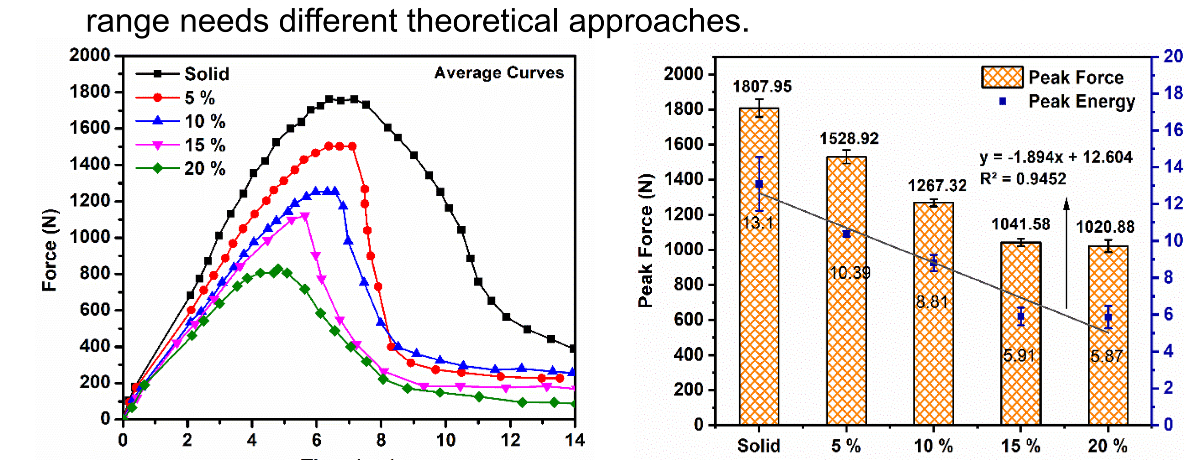
Performance Results



- The modulus and ultimate tensile strength show a linear or stepwise decline that is statistically significant.
- Interestingly the ultimate tensile strength only reduced by ~ 10 % for 5% weight reduction and 18 %, 23 % and 32 % for 10 wt %, 15 wt % and 20 wt % reductions, respectively.

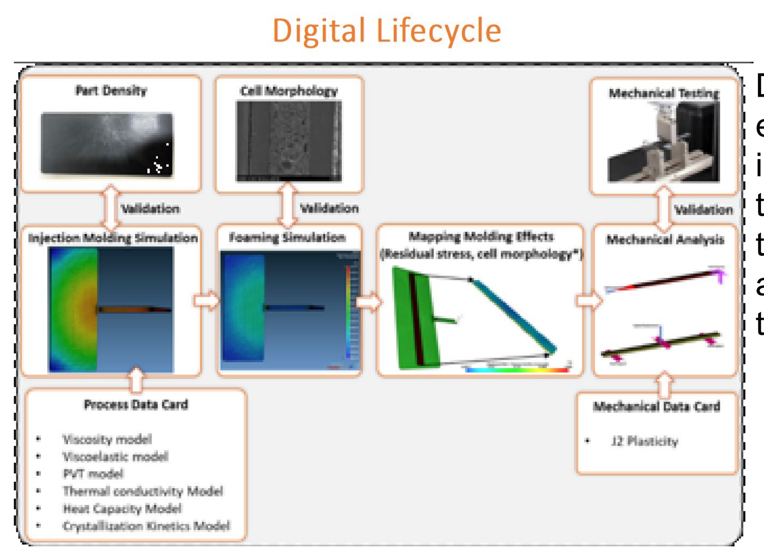


- The flexural strength showed a linear decline with increase in weight reduction.
- Theoretically predicting flexural modulus in 0 to 20 % density reduction range needs different theoretical approaches.

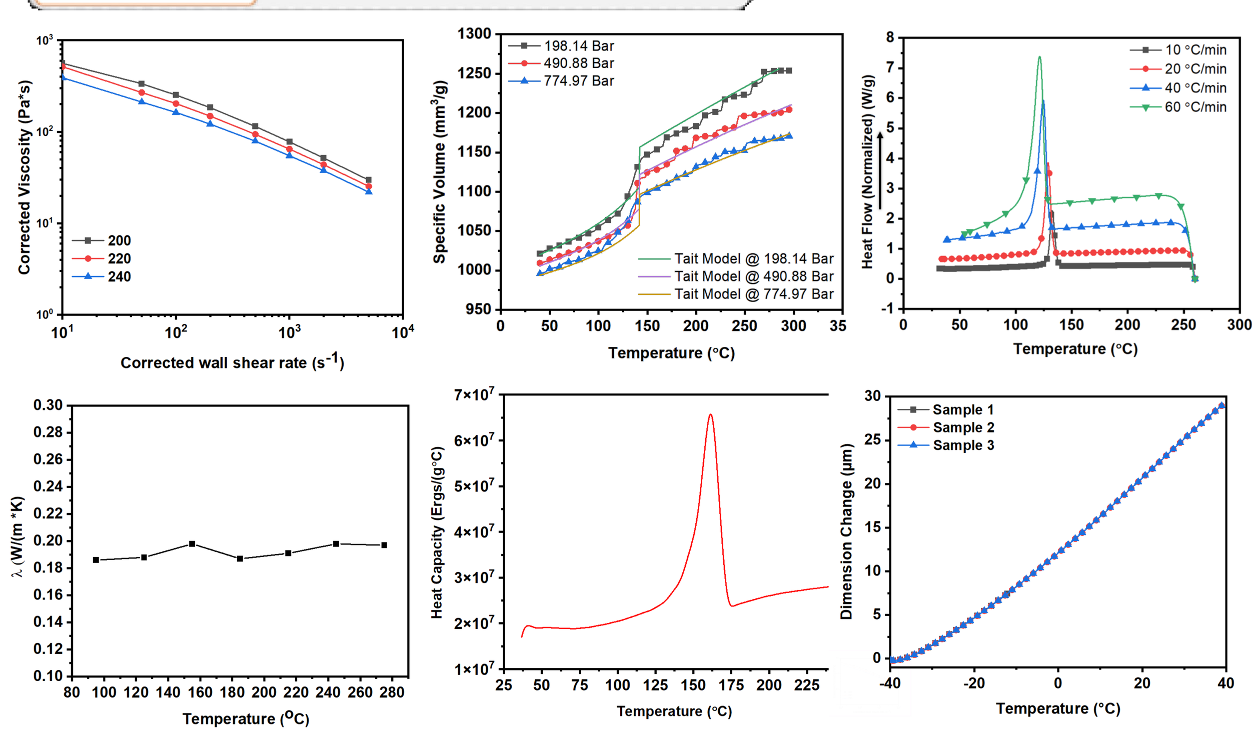


- The peak force and peak energy show a linear decline till 15 % weight reduction and plateau at 15 and 20 % weight reduction with no statistically difference in properties between 15 and 20 % wt reduction.

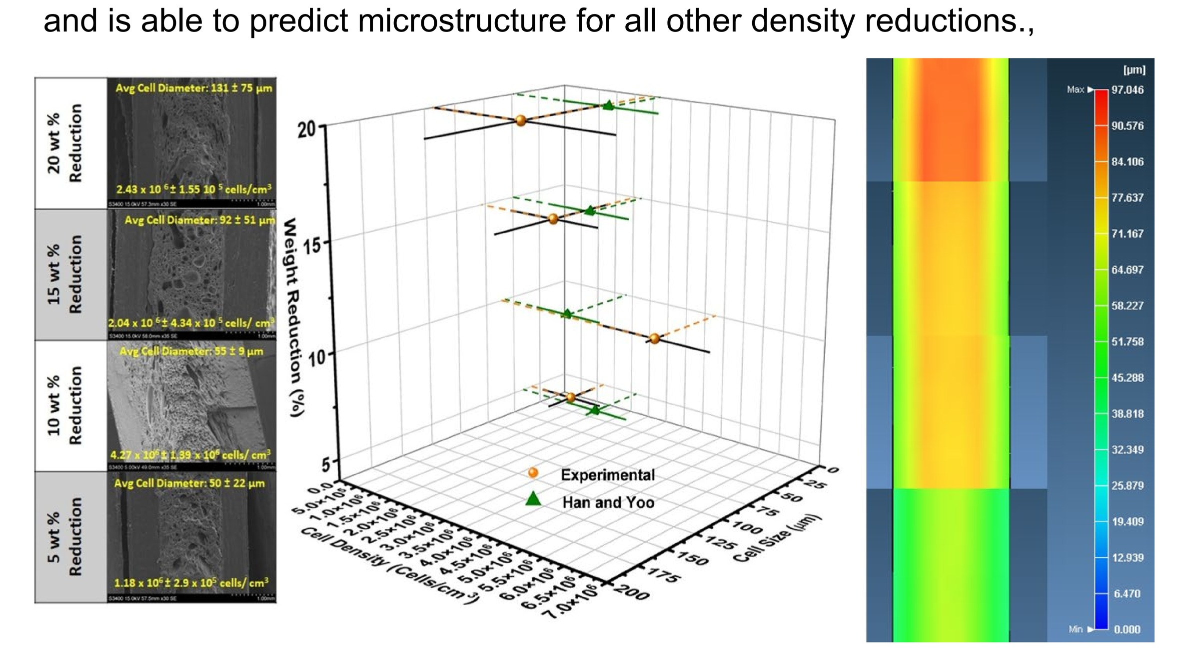
Digital Lifecycle (DLC) Pathway



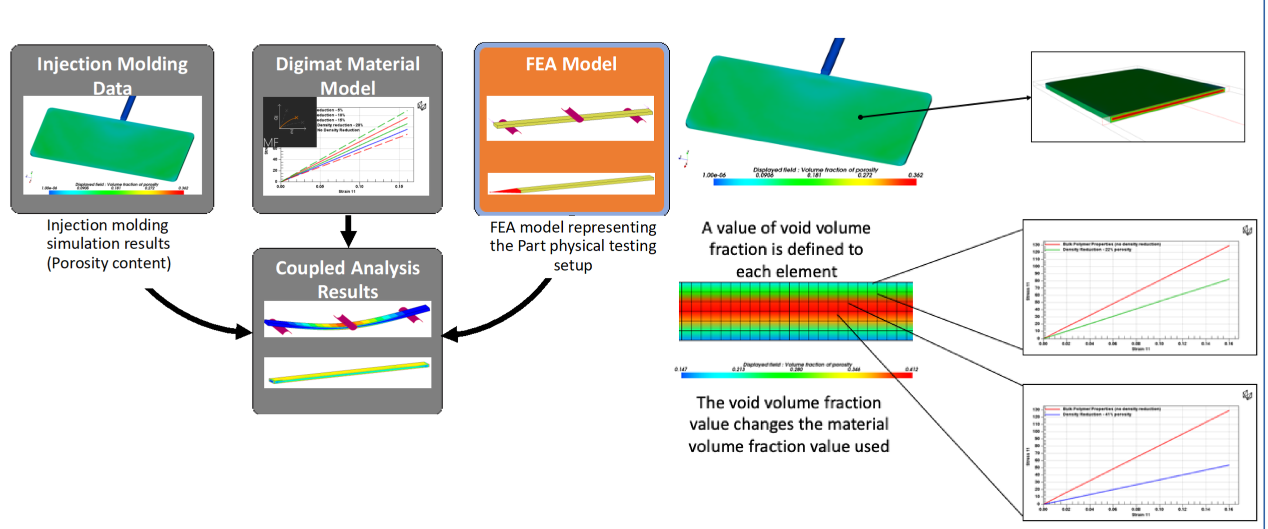
DLC circumvents the need for experimental inputs from SEM images, such as measured core thickness and skin thickness of the injection molded foam, that are necessary with most theoretical or analytical models.



- The DLC requires several experimental inputs in the form of shear viscosity, PVT, thermal conductivity, heat capacity, crystallization kinetics and mechanical data.
- DLC leverages different foaming models, calibrates to 15 wt % density reduction and is able to predict microstructure for all other density reductions.,

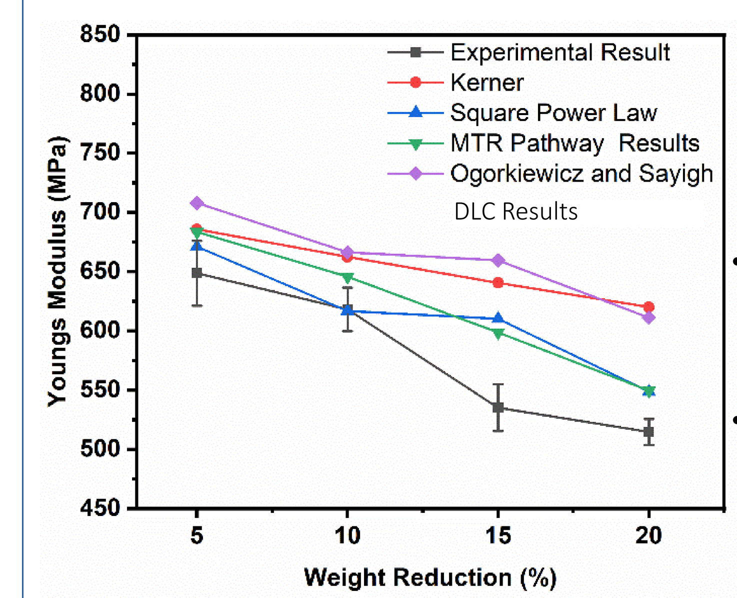


- Cell size and density were optimized using a correction factor when fitting for 15 % wt reduction and the Han and Yoo bubble growth model provided the closest correlation when compared to experimental results.
- The simulations were able to provide an accurate prediction of density and porosity when compared with experimentally characterized samples.



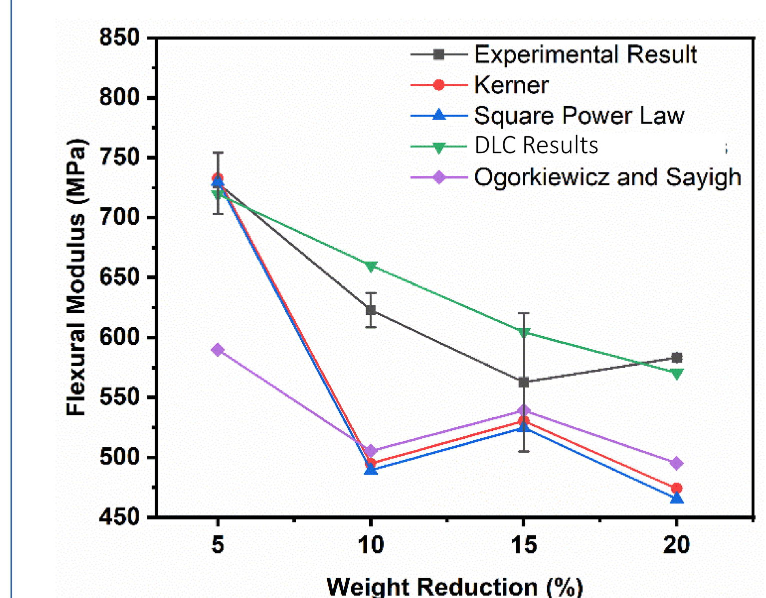
- Our current simulation approach takes advantage of mean-field homogenization for the material properties evaluation where the material model is built using the bulk material properties and using a void phase definition.
- This allows us to connect the material model to the void volume fraction at every element integration points – the local void volume fraction.

DLC Results



- The analytical models assume a uniform density distribution within the core, which is not the case/ with process parameters significantly affecting the cell size, cell distribution, and density distribution at a microstructure level.
- This approximation can result in overprediction or underprediction of mechanical properties.
- The workflow also mitigates the need for experiments and relies only on simulation results for the through-the-thickness porosity content definition.

Lightweight %	Flex Modulus [MPa] Experimental	Kerner [MPa]	Ogorkiewicz and Sayigh [MPa]	Square Power Law [MPa]	DLC Pathway - Simulation Results [MPa]
5%	728.66	732.75	589.86	730.09	719.54
10%	622.83	494.97	505.51	489.35	660.24
15%	562.75	530.45	539.06	524.76	604.64
20%	583.21	474.05	495.19	465.29	570.70
Avg Absolute Error		11.39 %	14.30 %	12.15 %	4.21 %



- These comparison, confirms the DLC pathway predicting the least error across different lightweighting and analytical models.
- Although the Square power law did show comparable results for Young's modulus, it failed to capture the correct trend in terms of property retention and, more importantly, performed worse in terms of predicting the flexural modulus.

Lightweight %	Youngs Modulus [MPa] Experimental	Kerner [MPa]	Ogorkiewicz and Sayigh [MPa]	Square Power Law [MPa]	DLC Pathway - Simulation Results [MPa]
5%	648.7	685.81	707.93	671.17	683.63
10%	618.13	662.43	666.33	616.87	645.86
15%	535.12	640.60	653.45	602.03	598.6
20%	514.67	620.16	616.38	555.46	549.49
Avg Absolute Error		13.27 %	14.70%	6.02%	7.12%

Future Work

Integration of Physics based Neural Networks to predict Material-Process-Microstructure-Performance

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References

Pradeep, Sai Aditya, et al. "A novel digital lifecycle for Material‑Process‑Microstructure‑Performance relationships of thermoplastic olefins foams manufactured via supercritical fluid assisted foam injection molding." Polymer Engineering & Science (2024). DOI: 10.1002/ pen.26700