

HPC4

ENERGY INNOVATION

HPC4
MATERIALS

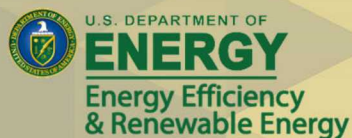
HPC4
MANUFACTURING

HPC4
MOBILITY

Polyurethane Foam Process Models Using a Population Balance Method

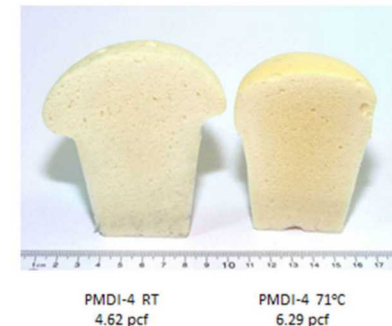
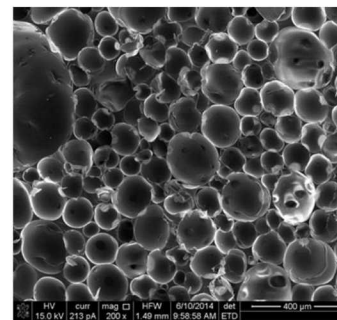
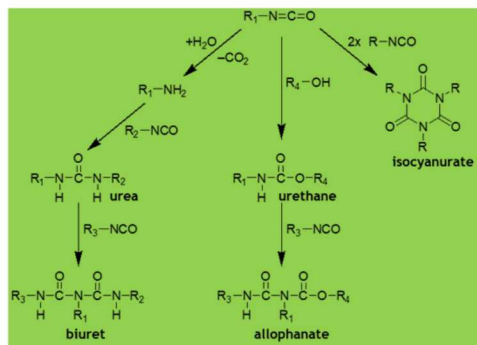
Rekha Rao & Christine Roberts (SNL)

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Industry need

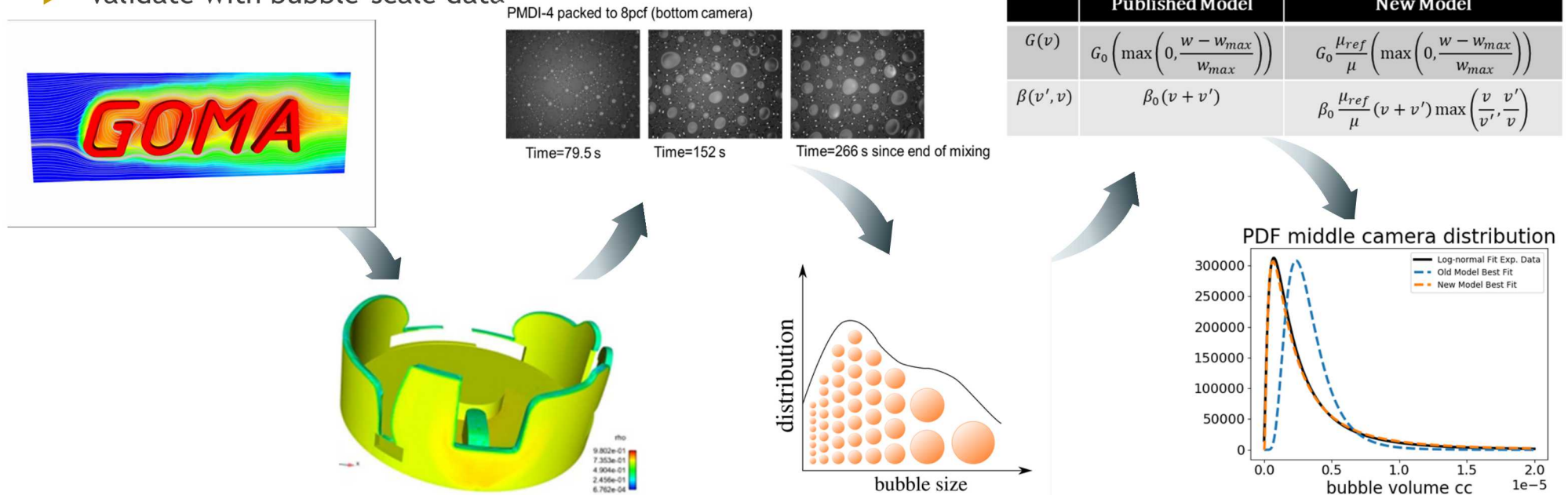
- ▶ Polyurethane foams are widely used as insulators
- ▶ Insulation efficiency is a complex function of gas fraction, solid/gas thermal conductivity, and foam cell size distribution
- ▶ A HPC-based polyurethane (PU) foaming model to predict the impact of formulation changes on bubble-scale thermal properties is needed
- ▶ A PU model would expedite the timeline for more energy efficient foams and appliances



Computational models can help produce more insulating foam with less waste

Approach

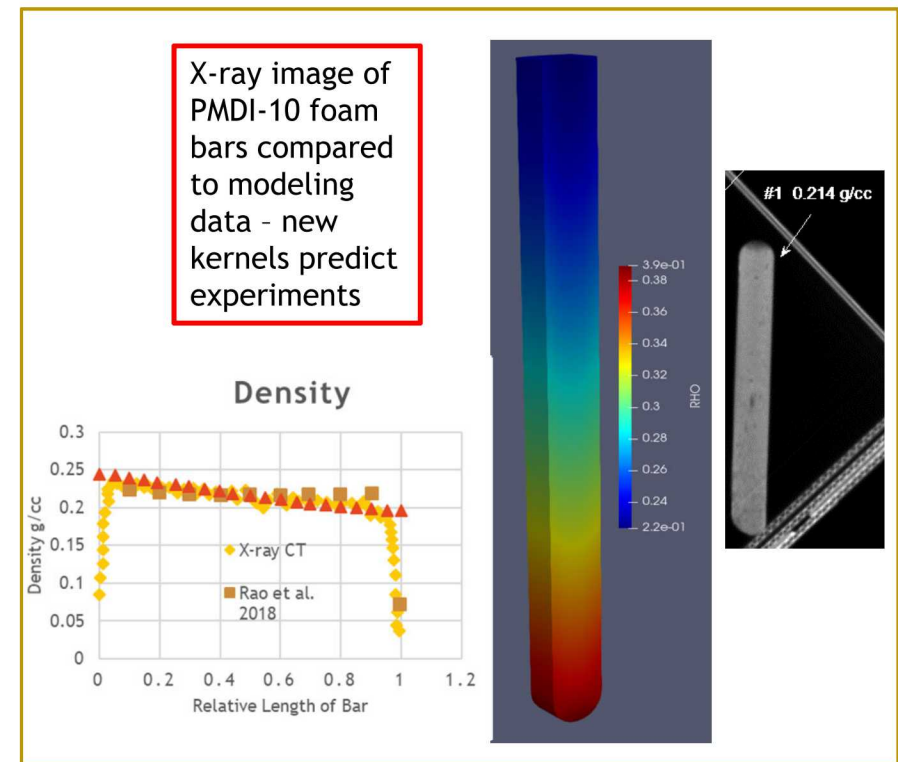
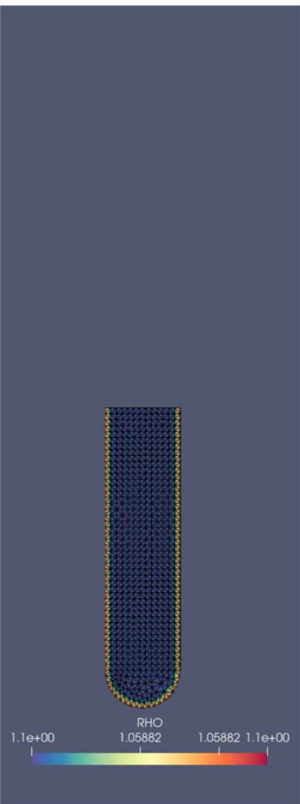
- Implement Sandia foam kinetics into an open source code
- Add population balance equations for bubble size evolution => improve model
- Validate with bubble-scale data



Coupled CFD-PBE for polyurethane process model and property predictions

Results

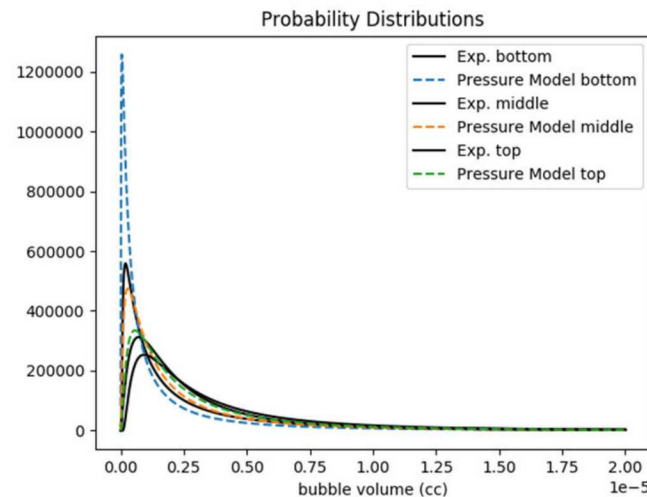
- ▶ New model can predict density gradients seen in X-ray CT experiments for the first time
- ▶ Predicts density and thermal conductivity based on bubble size
- ▶ Python version of model released to Dow for simple “numerical” foam rise experiments
- ▶ PBE equations poorly behaved with level set
- ▶ Numerical improvements underway for PBE in complex molds including adaptivity, tetrahedral elements, and upwinding



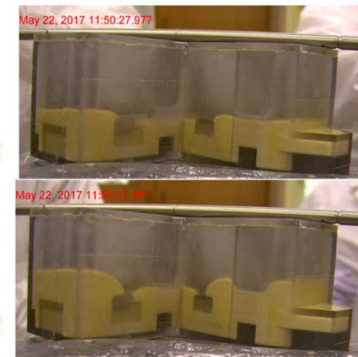
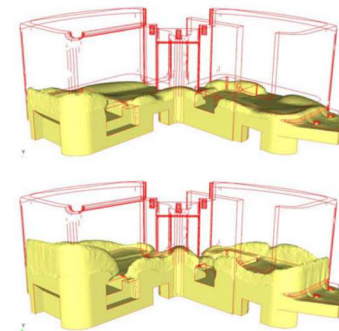
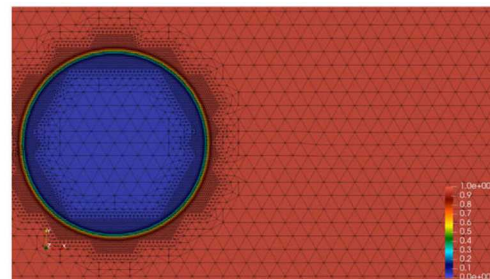
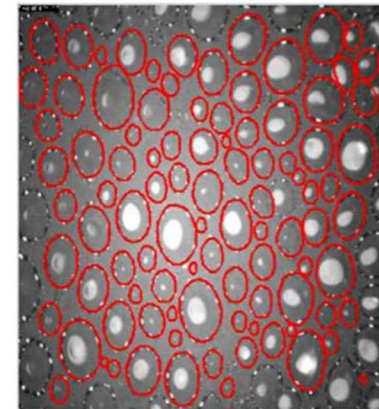
Model can now predict foam filling, curing, and bubble-size distribution for thermal conductivity

Benefits

- ▶ New bubble-scale model can help improve insulation efficiency while reducing precursor waste
- ▶ Energy savings expected once Dow starts using the code to help customers with mold and process design
- ▶ Dow currently using Python model
- ▶ Working on a paper: CFD-PBE model compared to Sandia experimental results



MATLAB script
counts
bubble-size
evolution over
time creating
bubble
volume data



Goma 7.0 release with full model expected October 2020



<https://www.buildinggreen.com/blog/epa-raises-health-concerns-spray-foam-insulation>

[US Korea Hotlink](#)

[PU Vacuum Foaming Molds | Refrigerator Door, Cabinet](#)

<https://github.com/goma/goma>

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