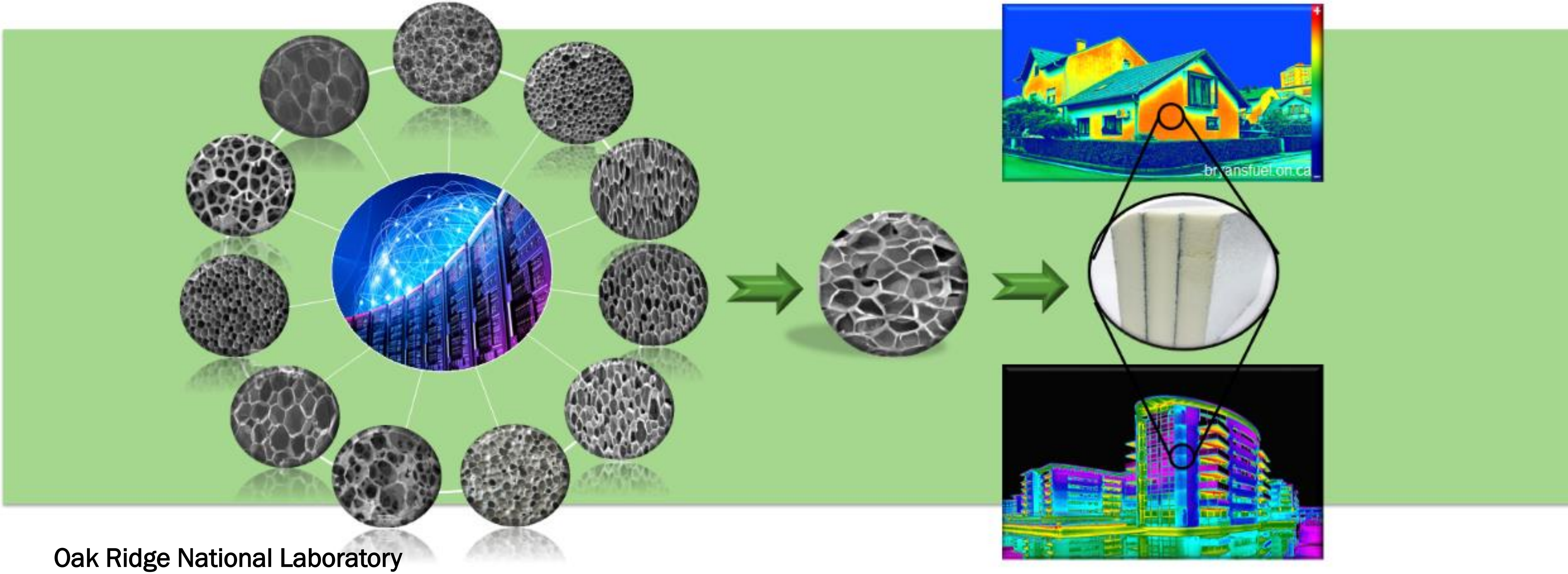
Multi-Scale Simulations and Machine Learning-Guided Design and Synthesis of High-Performance Thermal Insulation Materials



Oak Ridge National Laboratory
Som S Shrestha, Senior R&D Staff | Building Envelope Materials Research Group
865-241-8772. shresthass@ornl.gov
Bokyung Park, Postdoctoral Research Associate | Building Envelope Materials Research Group
BTO-03.01.03.124, BENEFIT FOA 2196

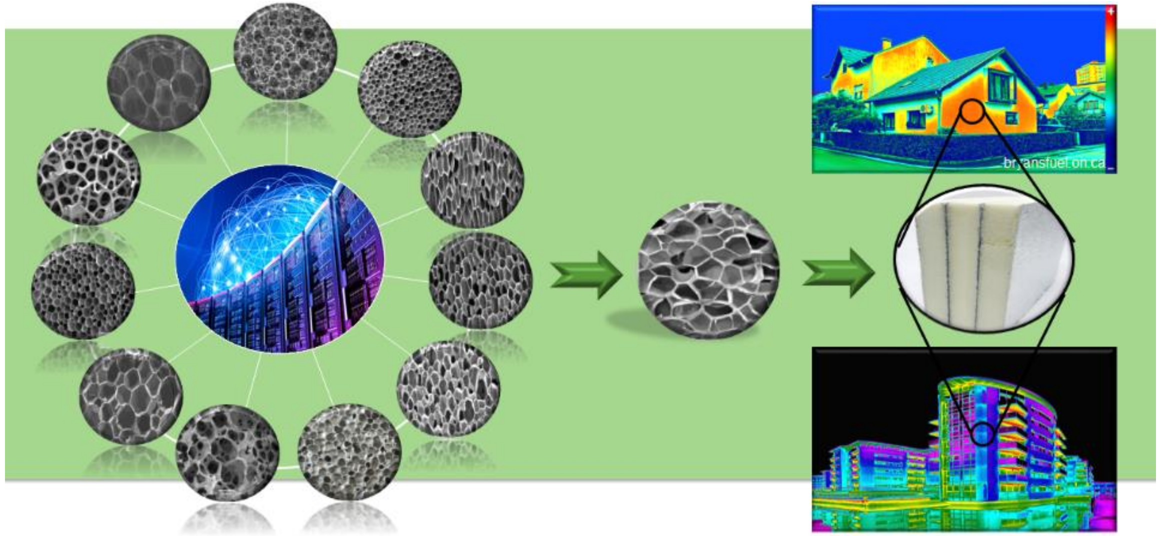
Project Summary

Objectives

- Develop novel foam insulation with higher thermal performance and comparable cost compared to the state-of-the-art.
- Enable building envelopes with tight spaces to meet thermal building code requirements.

Outcome

R10/in foam that does not require vacuum and can be produced with minimal adjustments to current manufacturing practices.



Team and Partners

OAK RIDGE National Laboratory

THE UNIVERSITY OF UTAH

GAF

Stats

Performance Period: 10/1/21 to 9/30 24
DOE budget: $1,600k, Cost Share: $400k
Milestone 1: Develop foam design concepts for ≥R10/in.

Milestone 2: Produce ≥R10/in foams and cost of goods sold (COGS) analysis.

Milestone 3: Identify large-scale manufacturing process to produce new insulation with minimum modification to current process.

Problem

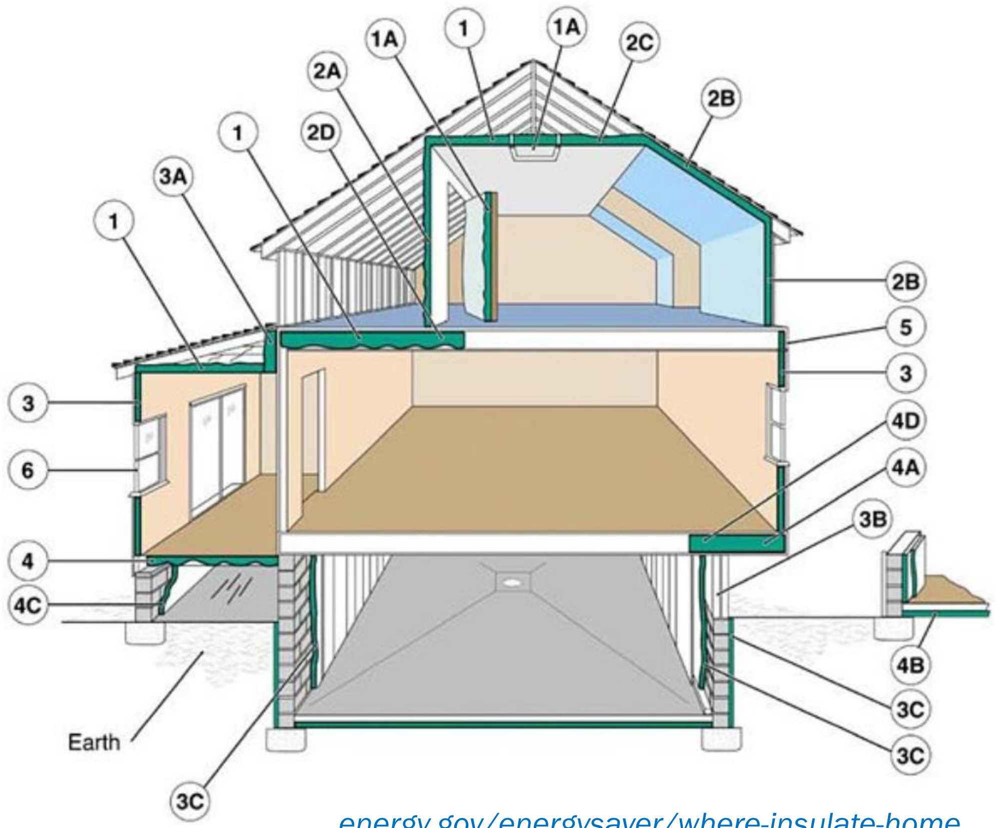
- Around 44 % of US households spend > 8.6 % of their income on energy bills*.

- High-performance insulation can improve building energy efficiency but currently used insulation limits ~R6/in.

Solution:

- Multi-scale simulations and machine learning can guide the design and development of R10/in. foam that does not require evacuation or nanopores.

Envelope areas that require higher thermal performance



energy.gov/energysaver/where-insulate-home

* DOE LEAD Tool https://www.energy.gov/scep/slsc/lead-tool

Alignment & Impact

- Insulation is a key contributor heating and cooling costs.
- Higher R-value of insulation

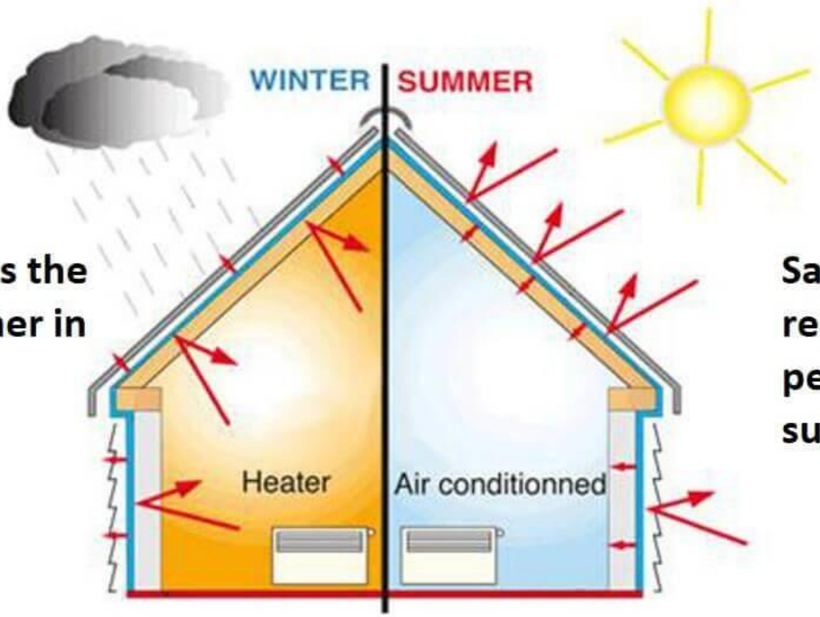
  - Can save >1 quad energy/year** (~$10 billion in energy cost).

Increase building energy efficiency

Reduce onsite energy use intensity in buildings 30% by 2035 and 45% by 2050, compared to 2005

- Successful R10 foam
  – Minimal modifications are required to the current manufacturing process.
  – Cost competitive with available insulation materials

Save energy as the home is warmer in winter



Save energy by reducing heat penetration in summer.

** DOE, Research and Development Opportunities Report for Opaque Building Envelopes

Image: roofinsulations.co.za/summer-insulation-benefits/

State-of-the-art Insulation Materials

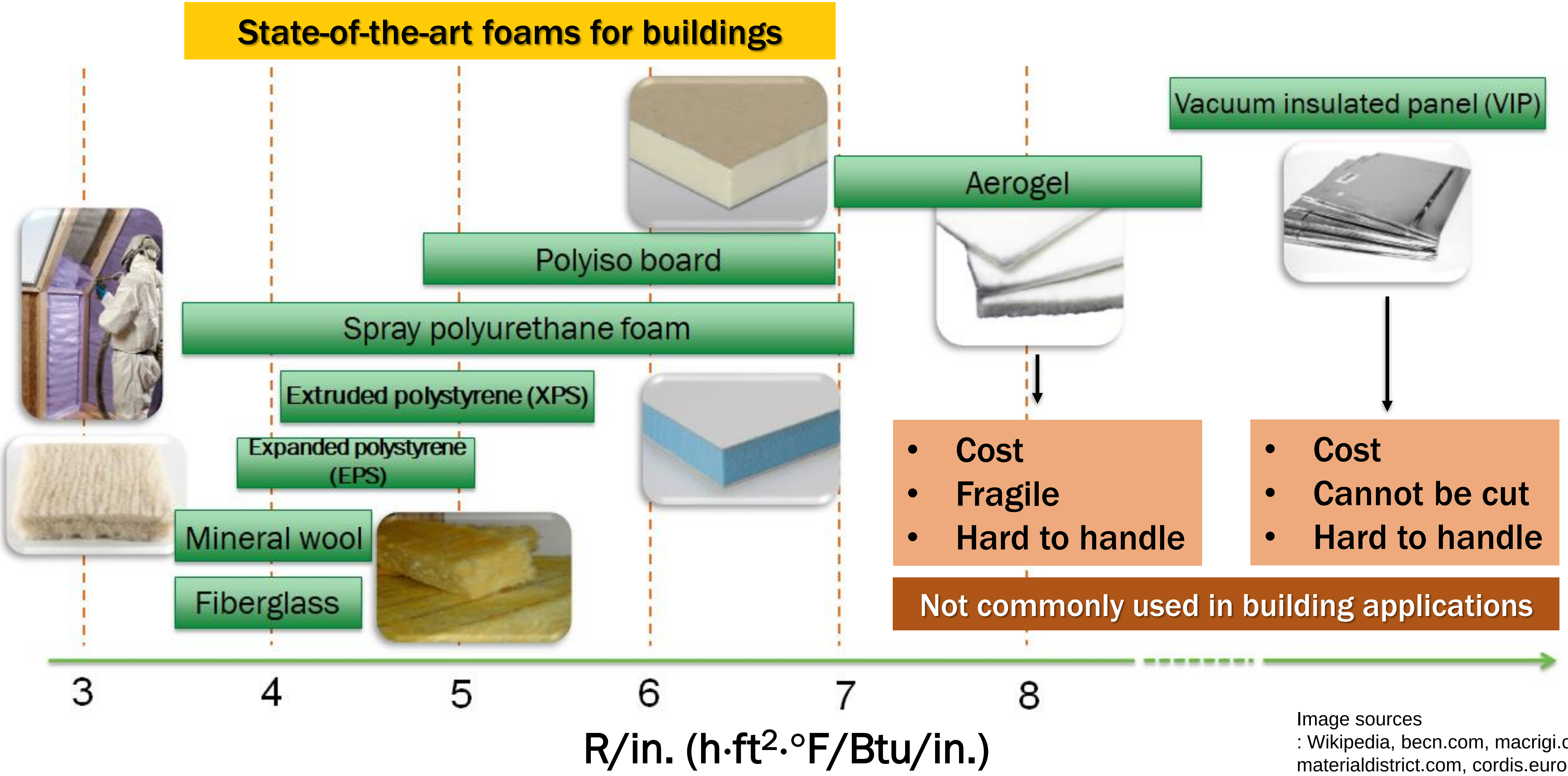


Image sources
: Wikipedia, becn.com, macrigi.com, materialdistrict.com, cordis.europa.eu

Challenges, Risks, Validation, and Commercialization

Technical challenges

Translate simulation results into actual foam designs

Risks and mitigation strategies

Numerous parameters affect thermal performance of foam insulation

- Use experimental results from the literature and this project to train ML algorithms that will identify and guide most relevant parameters

Validation

Reproducibility of foam prototypes and thermal performance

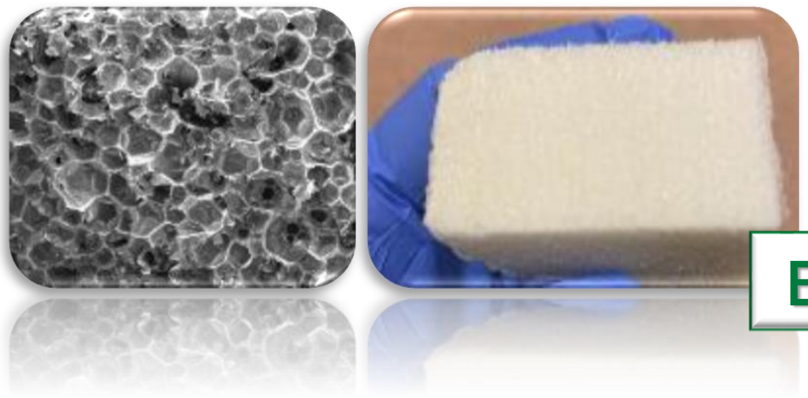
- Work with GAF to translate lab-scale to large-scale production

Commercialization

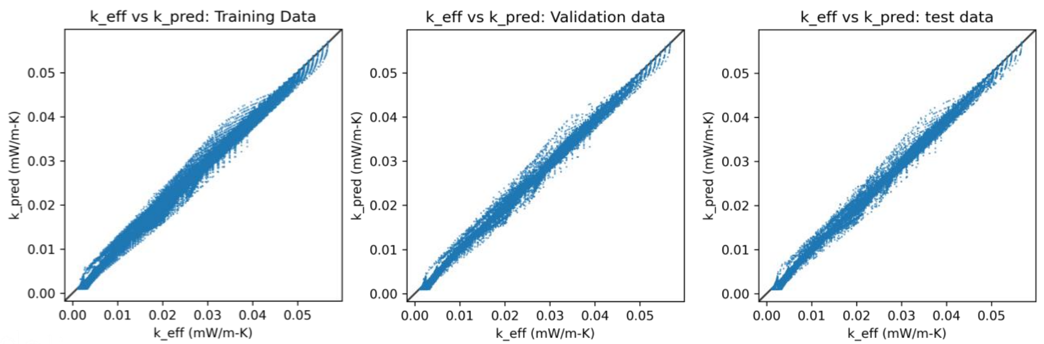
Feasible designs that consider scalability, cost, and durability

- Identify the design that requires minimum modifications in the current manufacturing process
- Cost comparable with current foam insulation on $\$/ft^2/R$ basis

Approach and Novelty



Experiment

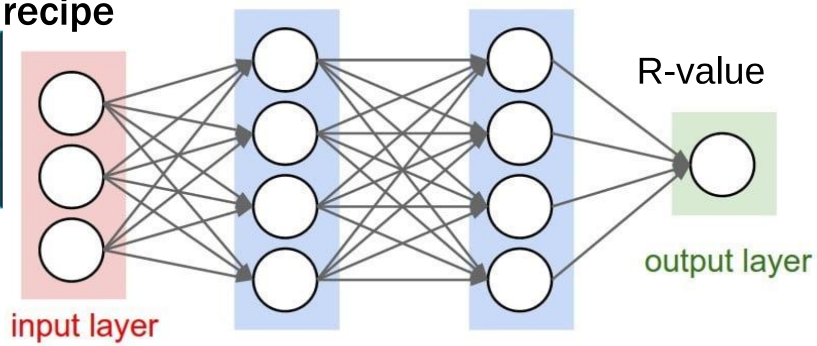


Validation

Input geometry or recipe

Using experimental results to develop/train ML

Machine learning

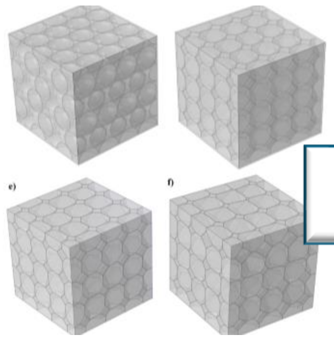


Machine learning

Simulation

ThermoPI

+



Multi-scale model for $\lambda_{gas}, \lambda_{solid}, \lambda_{rad}$

High-throughput finite-element

Simulation guides the design of foam insulation → Reduce trial and error

Current Solutions and Challenges

Thermal conductivity of foams → **three coupled** heat transfer mechanisms

$$\boldsymbol{\lambda_{foam}} = \lambda_{gas} + \lambda_{solid} + \lambda_{rad}$$

λ_{gas}:
- **Porosity**
- Cell size
- Gas species

λ_{solid}:
- **Porosity**
- Cell structure
- Material

λ_{rad}:
- **Porosity**
- Cell size
- Cell-wall thickness
- Opacifier

- Tradeoff between heat transfer mechanisms.
- Current commercial PIR foam is already at the optimal point (for pentane) → limitation of current solutions
- ~97% porosity is optimum.

Current optimum

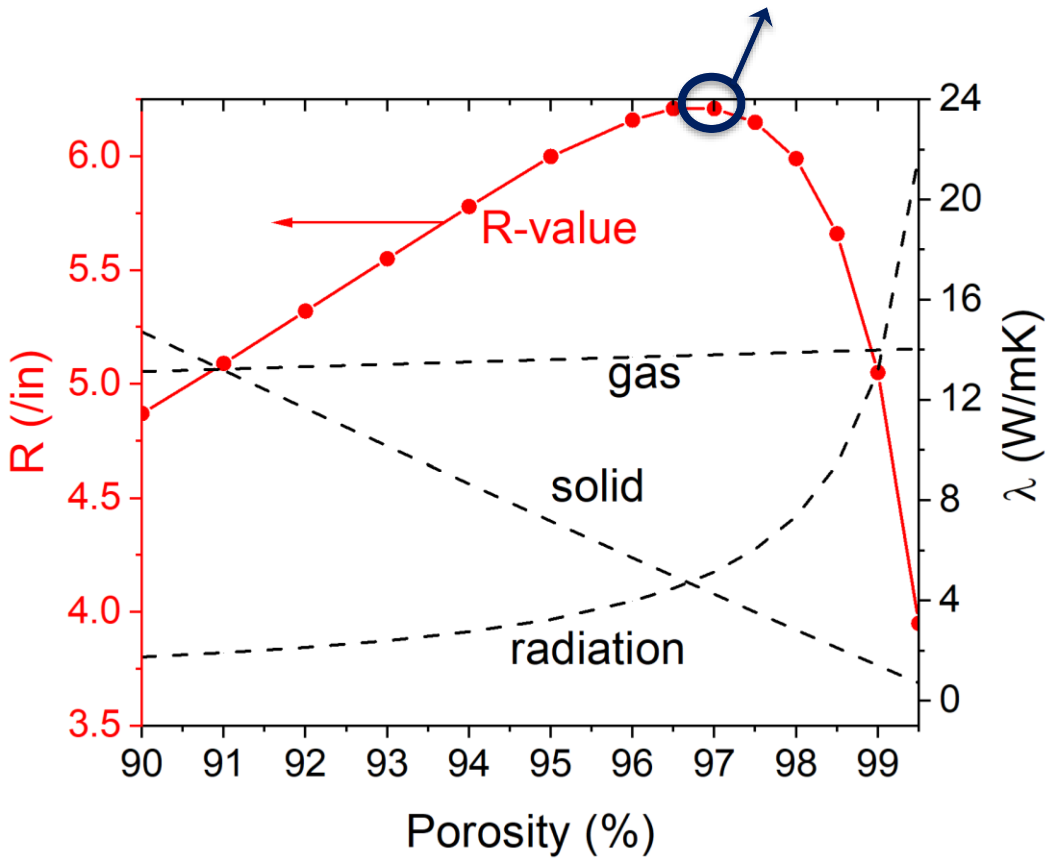
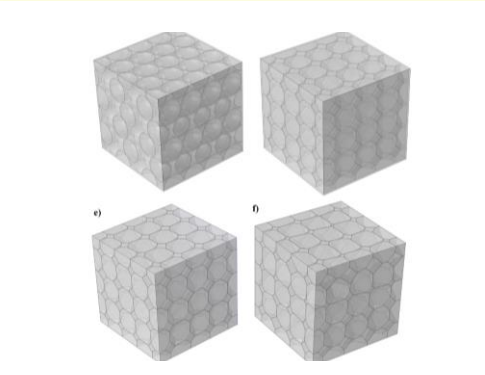


Figure generated using *ThermoPI (ORNL)*
thermopi.ornl.gov/calculate

Approach and Novelty: Simulation Guidance to Foam Designs

Simulation



Pore geometry
(FE simulation)

+

$$\lambda_{foam} = \lambda_{gas} + \lambda_{solid} + \lambda_{rad}$$

ThermoPI

λ_{gas}:
- Porosity
- Cell size
- Gas species

λ_{solid}:
- Porosity
- Cell structure
- Material

λ_{rad}:
- Porosity
- Cell size
- Cell-wall thickness
- Opacifier

Consider different approaches to overcome current limits
(multi-scale simulation)

✓ : Picks for our work

- Open-cell foam

or

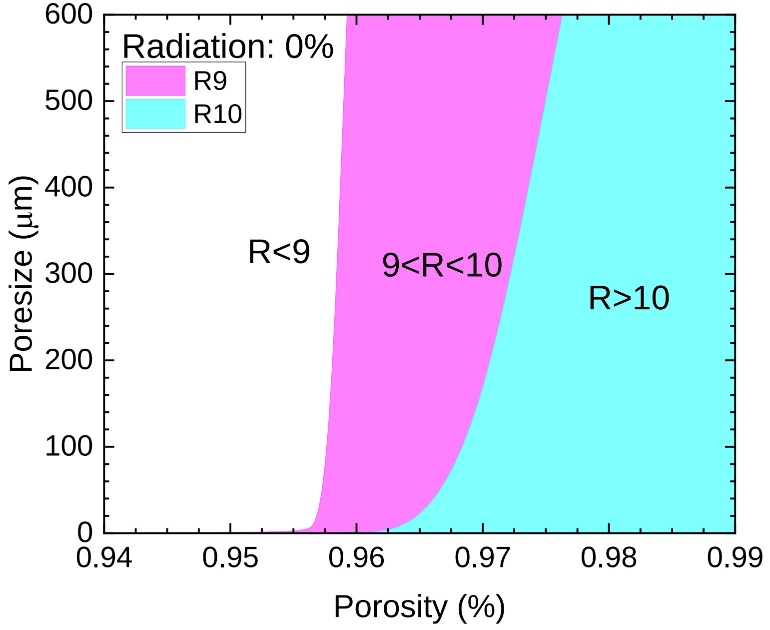
- Closed-cell foam ✓

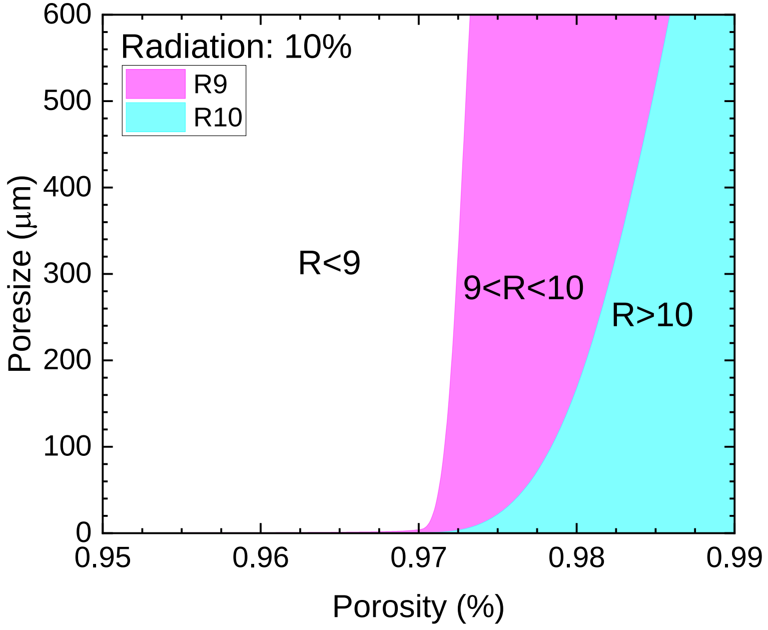
- Reduce cell size to nanometers
- Control cell morphology ✓
- Remove radiation (add opacifier) ✓

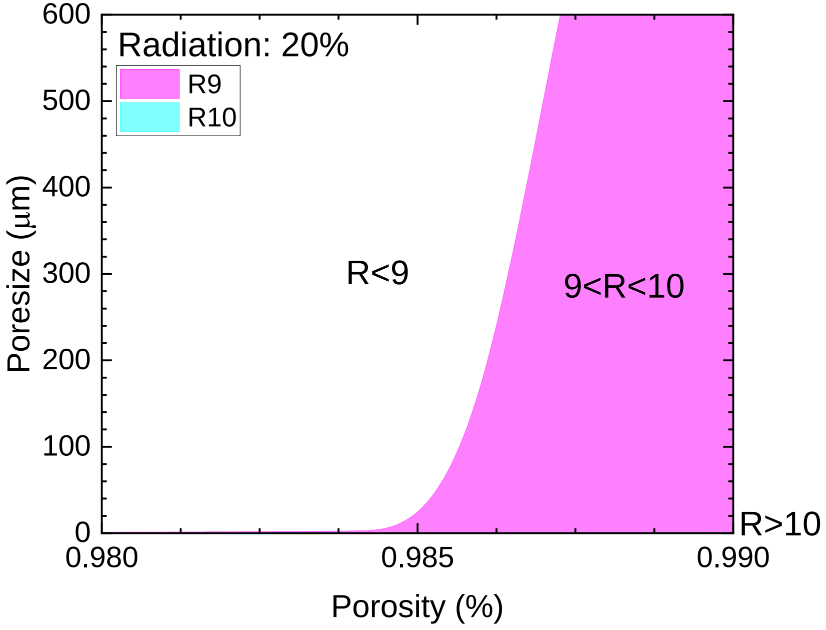
- Optimize formulation ✓
- Optimize co-blowing agents ✓

Approach/Progress: R-10/in. Design Concepts for Closed-cell Foam

Closed-cell (Polyiso) design space with HFO as blowing agent:







If radiation = 0

- R10 is feasible

If radiation = 10%

- R10 is feasible

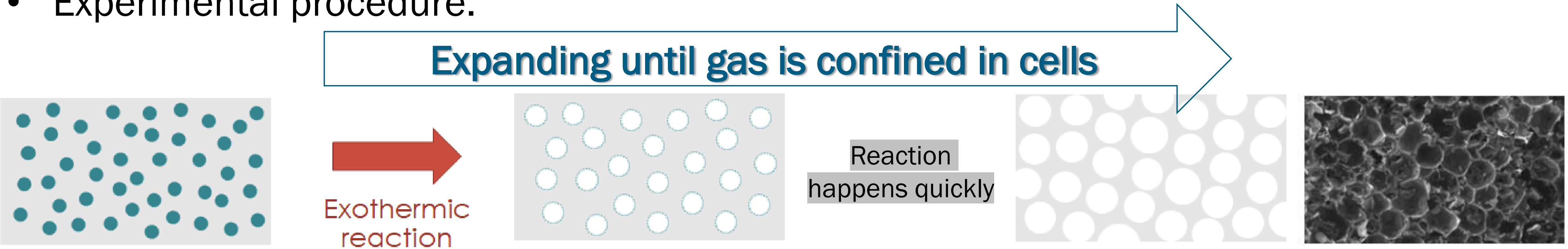
If radiation = 20%

- R10 is challenging
- R9 is possible

With reduced radiation, R10/in. can be achieved without nm-scale cell structure

Approach/Progress: Polyiso Foam Formation

- Experimental procedure:

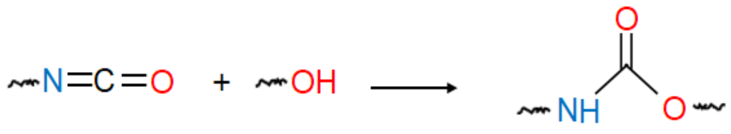


Dispersed physical blowing agent (liquid status)

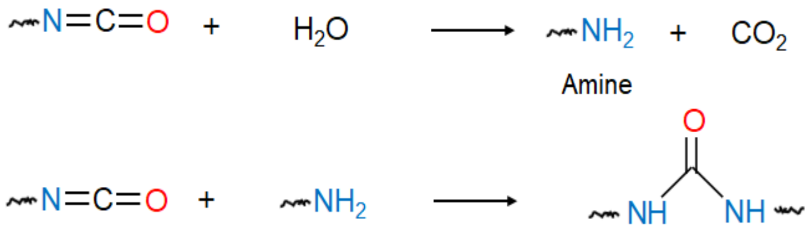
Expansion of blowing agent (Gaseous status)

Packing of cells (cell-foam formation)

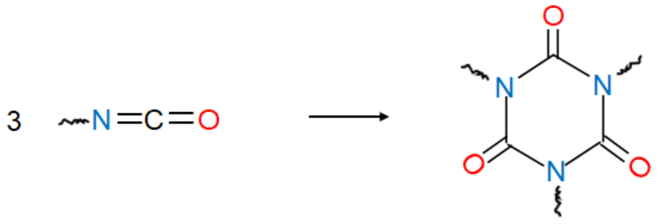
Exothermic reactions : Isocyanate reacts with polyol, water, isocyanate



Isocyanate Polyol Urethane



Isocyanate water Urea + CO_2 ↑



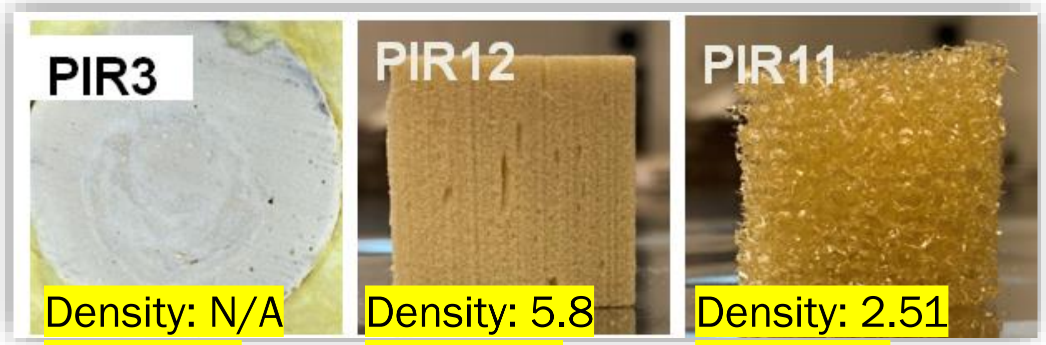
Isocyanate Polyisocyanurate

Simulation results indicate polyiso foam's R-value can be increased to R10/in.

Progress: Experimental Challenges

Density: lb/ft^3
R/in: h.ft^2.F/Btu/in.

- Too much blowing agent → too brittle, large pores



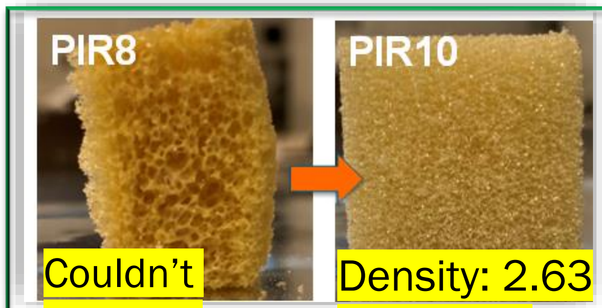
PIR3	PIR12	PIR11
Density: N/A	Density: 5.8	Density: 2.51
R/in. 4.33	R/in. 4.84	R/in. 3.19

Poor structure & thermal performance

- Excessive Isocyanate → poor thermal performance

	NPIR7	NPIR14
pMDI	Iso Index ~380 →	Iso Index ~270
Density	2.94	3.0
R/in.	6.28	6.69

- Same additive behaves opposite on different formulation



PIR8	PIR10
Couldn't measure	Density: 2.63
	R/in. 4.07

More additives → improved structure & thermal performance

PIR9	PIR11
Density: 2.62	Density: 2.51
R/in. 4.56	R/in. 3.19

More additives → poor structure & thermal performance

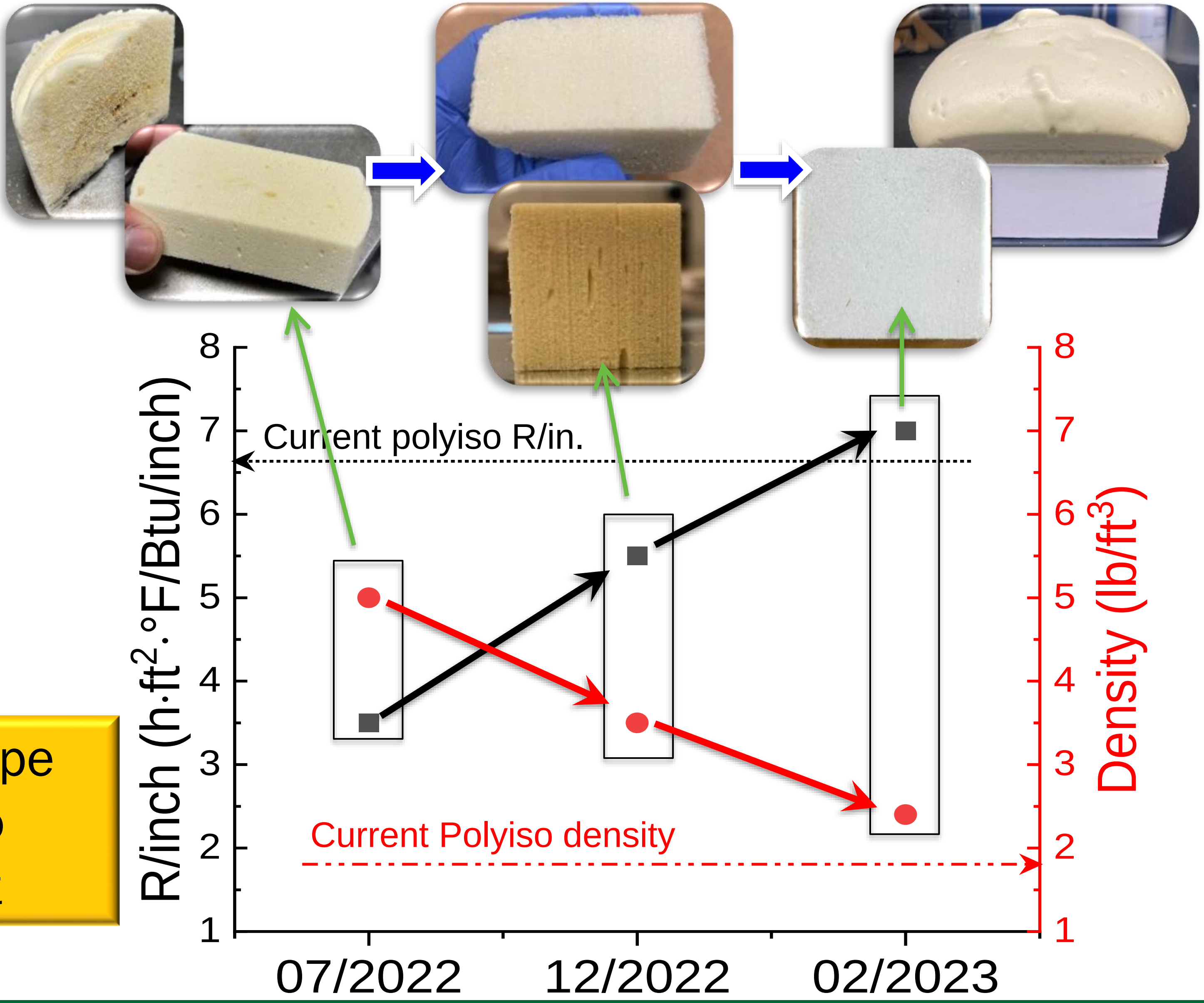
Formulation → control cellular structure → use the results for ML

Progress: Experimental Obstacles and Significant Progress

Formulation

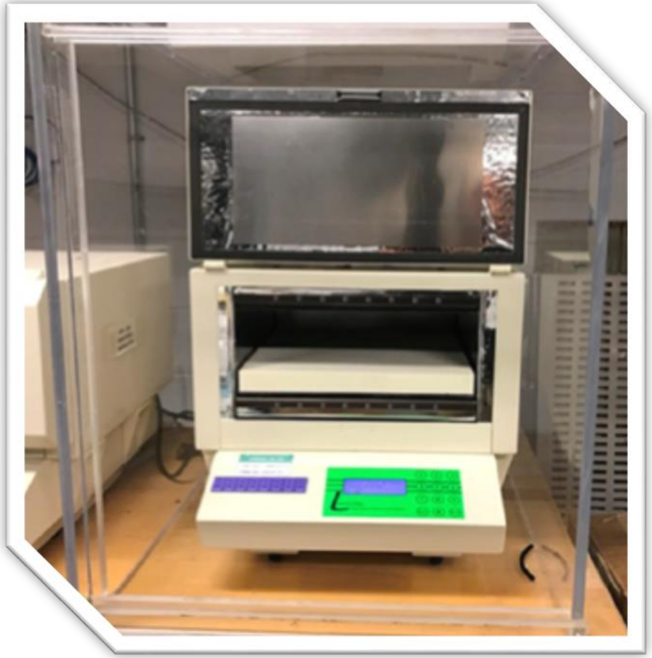
Material	
A-side	
Iso Index	270
B-side	Parts per weight (PBW)
Polyol	100
Catalysts, water, and other additives	varies

- Significant improvement in our recipe
- Wide range of experimental data to feed for ML algorithm development



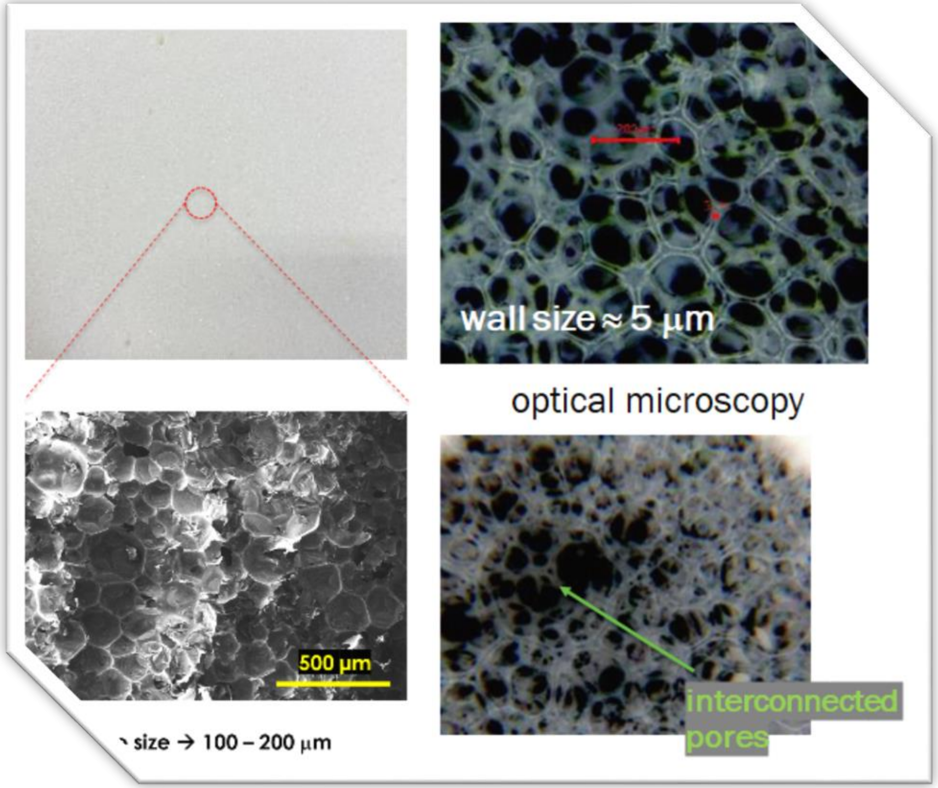
Progress: Thermal Performance and Morphology Analysis for ML

- Heat flow meter
(thermal conductivity)
ASTM C518



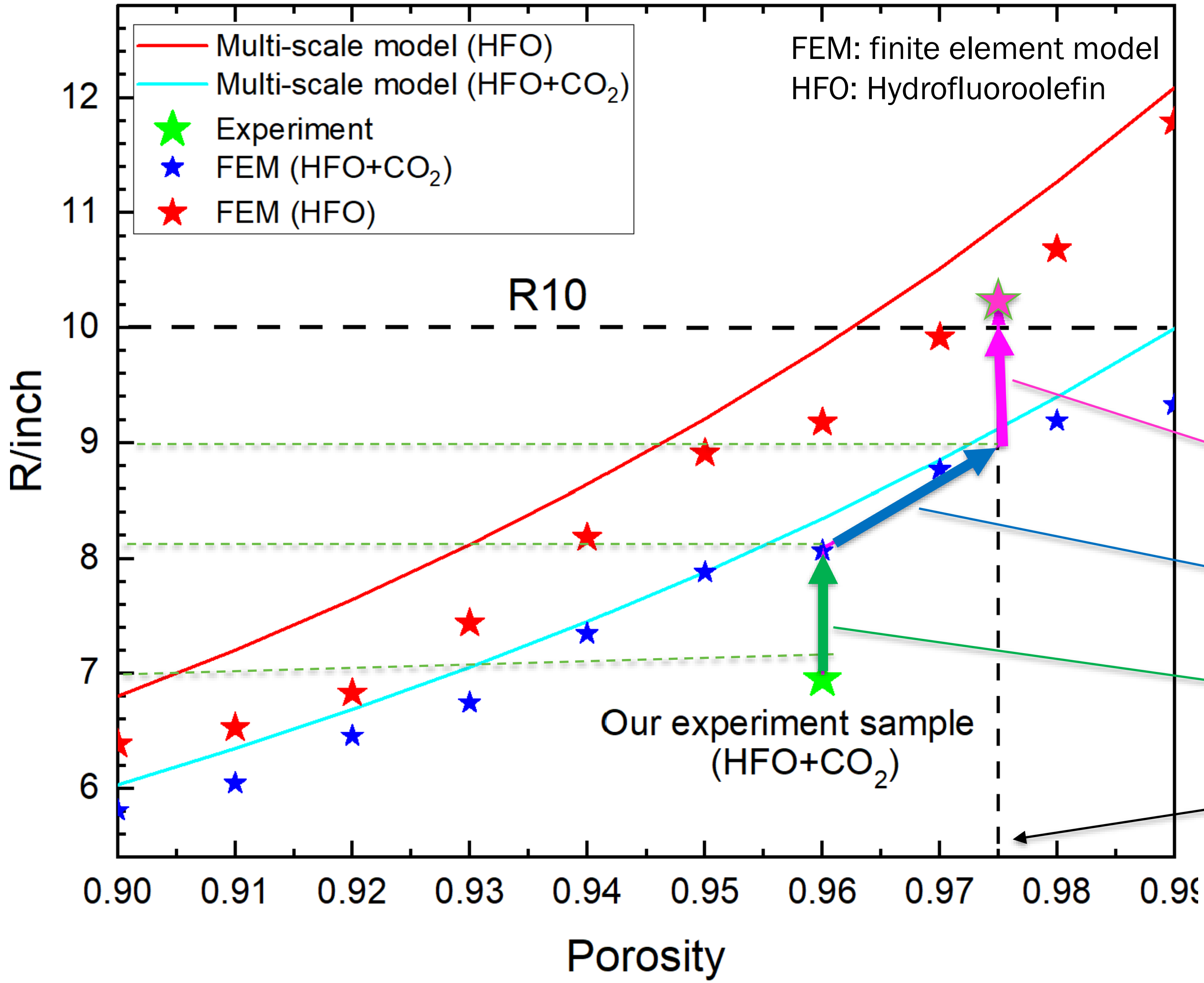
- Pycnometer
(closed-cell contents)
ASTM D 6226

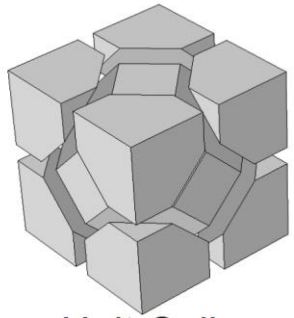
- Microscopy
(morphology investigation)

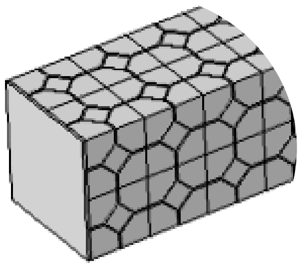


Collecting important performance parameters to feed to ML algorithm

Next Experimental Steps Guided by Simulations to Reach R-10/in.







Eliminate CO_2 generation → Control water in formulation

Increase porosity → Explore different additives & control processing condition

Eliminate radiation & open cells → Optimize opacifier (material, shape, size)

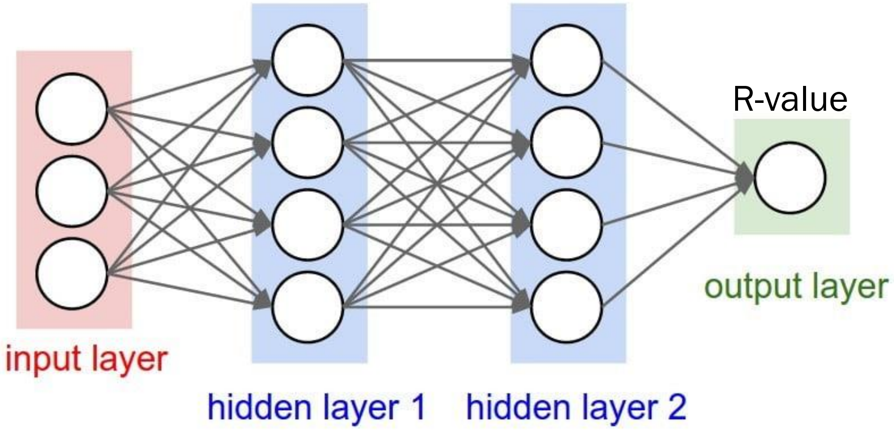
Commercial foam porosity (97.5%)

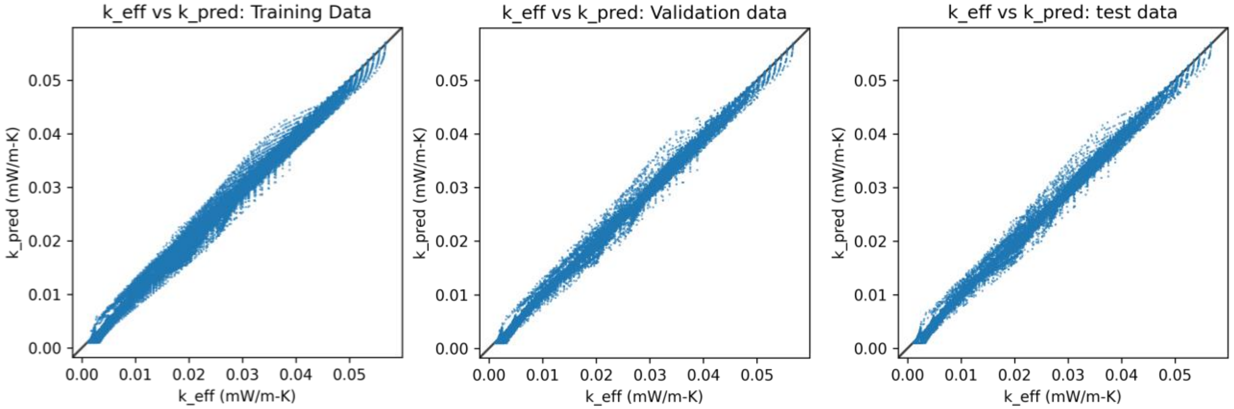
Assumption: no radiation, large pore (No Knudsen effect)

Next modelling effort: Machine learning

R-value prediction by foam structures

Porosity
Pore size
Gas composition
Solid
Anisotropic ratio
……

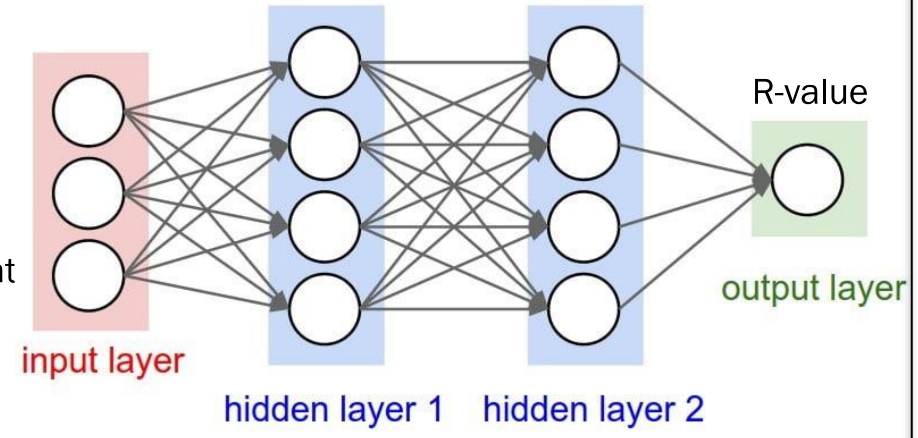




Our ML model predicts very well thermal conductivity

R-value prediction by recipe

Materials
Temperature
Mixing time
Catalyst
Polyol
Flame retardant
Surfactant
Opacifier
……



- ML model is built and ready
- As soon as we have more experimental data, we will be able to train the model and optimize the recipe

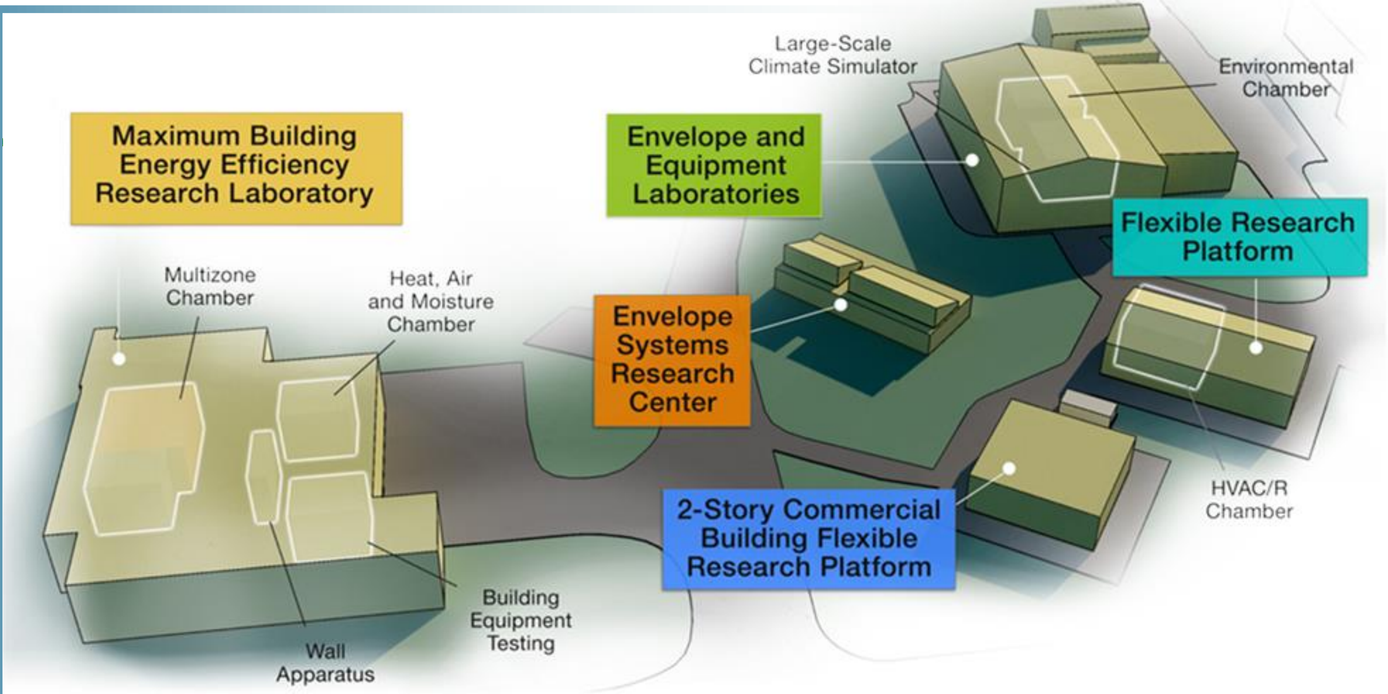
Future Work

- Optimize the manufacturing conditions for a minimum foam thermal conductivity by using the trained ML model
- Optimize the porous structures to achieve ≥R10/in. by multiscale simulations, FE analysis, and ML
- Fabricate the ML-optimized foam prototypes and characterize the thermal conductivity with a target of >R10/in.
- Identify a method for mass production of the new foam and minimize the cost

Thank you

Oak Ridge National Laboratory
Som Shrestha, Senior R&D Staff
(865)-241-8772 | shresthass@ornl.gov
Bokyung Park, Postdoctoral Research Associate

WBS # BTO-03.01.03.124, BENEFIT FOA Project # 2196-1726



ORNL's Building Technologies Research and Integration Center (BTRIC) has supported DOE BTO since 1993. BTRIC is comprised of 60,000+ ft^2 of lab facilities conducting RD&D to support the DOE mission to equitably transition America to a carbon pollution-free electricity sector by 2035 and carbon free economy by 2050.

Scientific and Economic Results
236 publications in FY22
125 industry partners
54 university partners
13 R&D 100 awards
52 active CRADAs

BTRIC is a DOE-Designated National User Facility

REFERENCE SLIDES

Project Execution

	FY2022	FY2023	FY2024
Planned budget	500,000	600,000	500,000
Spent budget	316,000	417,000	NA

No	Deliverable/Milestones	Year 1				Year 2				Year 3			
		Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4
Task 1. Finalize Overall Project Management and Planning													
1.1	Finalized Overall PMP	Milestone											
Task 2. Collect and analyze the experimental data													
2.1	Collect the experimental details and TC for at least 20 foam designs				Milestone								
2.2	Process and analyze at least 20 foam design data.				Milestone								
Task 3. Optimize the Manufacturing Conditions for a Minimum Foam Thermal Conductivity													
3.1	Optimize the manufacturing conditions to minimize the foam thermal conductivity by using the existing manufacturing methods				Milestone								
Task 4. Optimize the Porous Structures to Achieve ≥R10/in. by Multiscale Simulations													
4.1	Obtain foam morphologies to achieve ≥R10/in.				Go/No-Go								
Task 5. Obtain the Foam's Cell Morphology Details Needed for Performing Machine Learning Optimization													
5.1	Obtain the foam's cell morphology details for the at least 20 foam designs					Milestone							
Task 6. Optimize the Porous Structures to Achieve ≥R10/in. by Multiscale Simulations, FE Analysis, and ML													
6.1	Train ML algorithm and predict the TC and foam structure with 90% accuracy							Milestone					
6.2	Obtain the TC of porous structures by using multiscale models and FE simulations.								Milestone				
6.3	Obtain at least three optimized porous structures with ≥R10/in. by ML								Go/No-Go				
Task 7. Conduct a cost of goods sold (COGS) analysis to understand the cost distribution of foam manufacturing													
7.1	Collect cost details to conduct cost of gods sold (COGS) analysis							Milestone					
7.2	Complete the COGS analysis and rank-order cost objects. Identify cost reduction opportunities to attain the cost of polyiso foam.								Milestone				
Task 8. Identify new gas blends with a lower TC than currently industry used ones													
8.1	Obtain the pressure-dependent TC of CO_2 + HCFO blends						Milestone						
8.2	Identify new gas blends with lower TC and condensation point of <-40 °C							Milestone					
Task 9. Develop a method to fabricate foams with small pore size and high porosity													
9.1	Produce at least two types of foams with pore size ≤0.5 µm and porosity ≥ 0.9.								Milestone				
Task 10. Fabricate the ML optimized foam prototypes and characterize the TC with a target of >R10/in.													
10.1	Produce at least two prototype foams that achieve ≥R10/in.									Milestone			
10.2	Produce closed-cell foams with facers to achieve ≥R10/in.										Milestone		
10.3	Fabricate at least one 6×6×1 in. foam that achieves ≥R10/in.											Milestone	
Task 11. Identify a method for mass production of the new foam and minimize the cost													
11.1	Identify options to modify the current commercial foam manufacturing processes that will be needed to produce new insulation that will potentially achieve ≥R10/in.										Milestone		
11.2	Identify and trail a large-scale manufacturing process that will enable producing new insulation with ≥R10/in. with a minimum modification in the current manufacturing												Milestone

Milestone | Go/No-Go

Team member

Thermal Analysis

Som Shrestha, Diana Hun, Andre Desjarlais
Buildings Envelope Materials Research, ORNL

Design / Synthesis of Foam

Tomonori Saito, Sungjin Kim
Chemical Sciences Division, ORNL

Bokyung Park
Buildings Envelope Materials Research, ORNL

Physical Characterization

Catalin Gainaru
Chemical Sciences Division, ORNL

Industry Partner

Kevin McGrath, Kenneth Willoughby, Kevin Pollack
GAF Materials Corporation

Simulation / Computational Analysis

Tianli Feng, Janak Tiwari
University of Utah

Daniel Howard
Buildings Envelope Materials Research, ORNL