

Atmospheric Water Extraction Enabled by Smart Moisture Absorbing Foams (SMAFs)

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Cascade Designs Inc.

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Physical Sciences Inc.

Our Team

VG-2021-197-1



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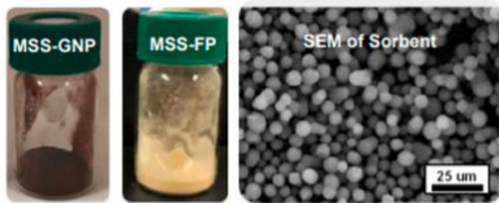
Physical
Sciences Inc.

UMass Amherst

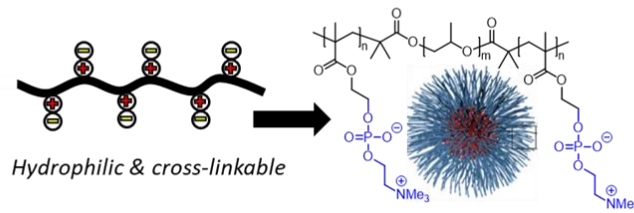
CASCADE DESIGNS®

Team Members and Roles

- **Physical Sciences Inc., PSI (Program Lead)**
 - **Program Role:** Sorbent development, evaluation and optimization (TA1). AWE system modelling, design, prototyping and evaluation (TA2). Management and reporting.
 - **Expertise:** Tech development for large government programs.
- **University of Massachusetts Amherst, UMass (TA1 Partner)**
 - **Program Role:** Sorbent material synthesis, characterization and scale-up.
 - **Expertise:** World class Polymer Science and Engineering program.
- **Cascade Designs, CDI (TA2 Partner)**
 - **Program Role:** Prototype system development, optimization and field testing. Commercialization partner, owner of Mountain Scientific Research (MSR) brand.
 - **Expertise:** Design and manufacture of individual sustainment gear.



PSI Smart Sorbent Platform



UMass Functional Materials



MSR/CDI Water Filtration Systems



Program Summary

- **Team:**

- Physical Sciences Inc. (PSI), Andover, MA (PI: Gamliel, PM: Warren)
- University of Massachusetts Amherst, Amherst, MA (Co-I: Emrick)
- Cascade Designs Inc (CDI), Seattle, WA (Co-I: Norris)

- **Primary Objective** – Develop a man portable system capable of extracting potable drinking water from air, obviating the need for costly and dangerous transportation (Expeditionary Track).

- **TA1 Goal:** Create a new and revolutionary class of sorbents that have high capacity, rapid water uptake and release sorbed water by compression-enabled switching from hydrophilic to hydrophobic state.
- **TA2 Goal:** Design, construct and optimize a system capable of meeting the DARPA SWaP and output requirements by leveraging the SMAF compressive release capability developed in TA1.



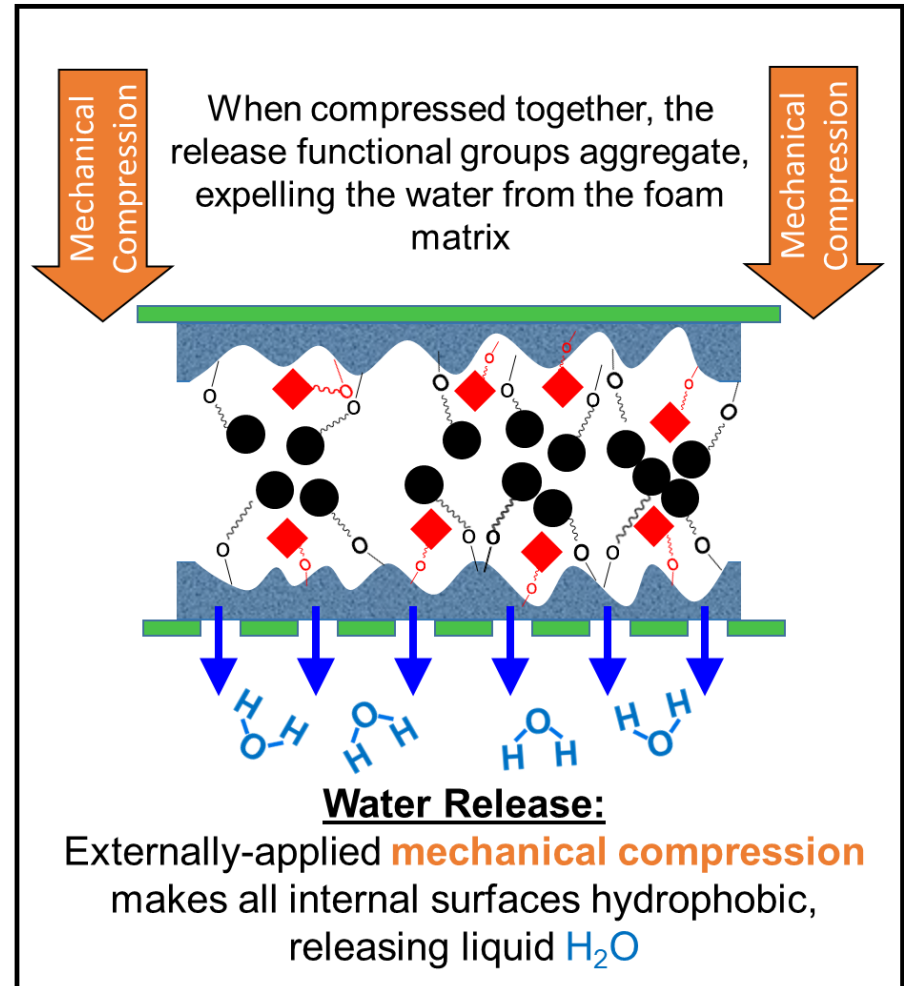
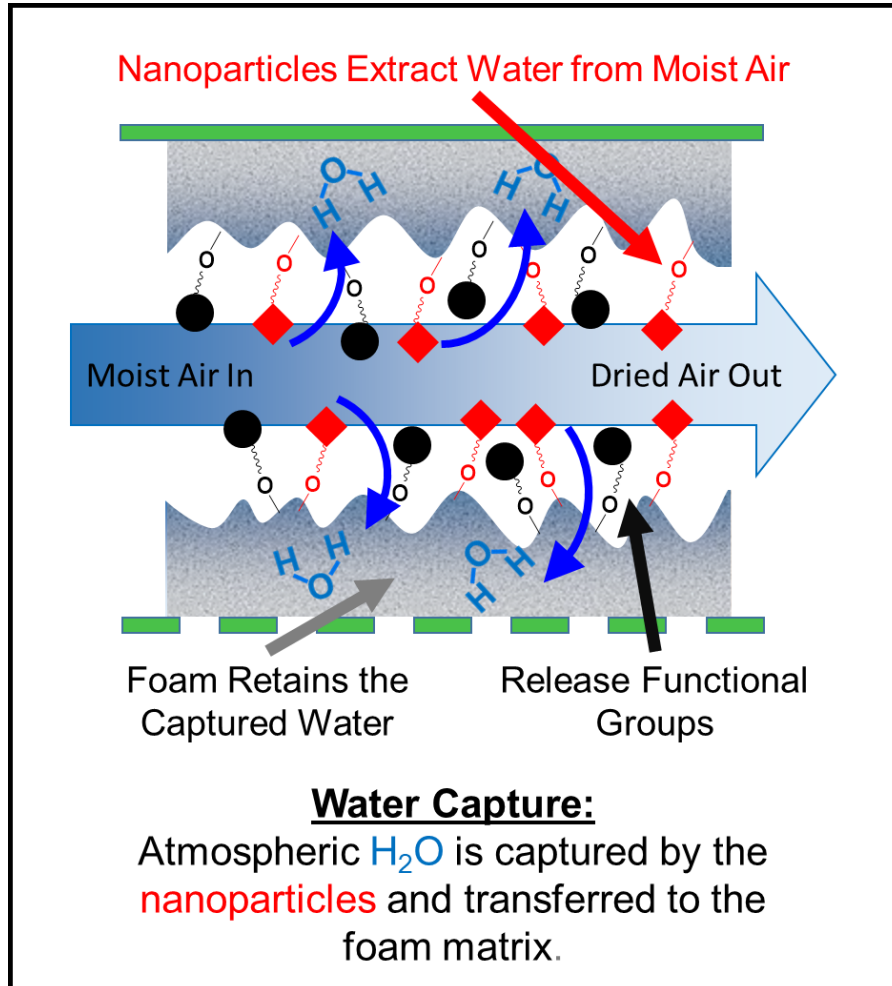
DARPA BAA Requirements

- **Topic** – DARPA BAA HR001120S0014 Atmospheric Water Extraction (AWE)
- **Broad Need** – Water transport to the warfighter is mission-critical but logistically challenging, requiring equipment, fuel, and personnel that limits tactical maneuver and decision space. Warfighter requires 3-7 L/day of drinking water.

Metrics	Phase I Objective	Phase II Objective
Water Production Rate	≥1 L/day @ ~4 °C, 50% RH ≥1 L/day @ ~27 °C, 10% RH ≥1 L/day @ ~43 °C, 60% RH	≥5.5 L/day @ ~4 °C, 50% RH ≥5.5 L/day @ ~27 °C, 10% RH ≥7.5 L/day @ ~43 °C, 60% RH
System Dry Weight	≤7 kg	≤2.5 kg
Power	Must be contained onboard	Must be contained onboard
Volume	6 L (0.21 ft ³)	1.5 L (0.05 ft ³)
Desired Properties	-	Water meets TB-Med-577 potability standards, Operational for >30 days at 24 hr runtime

- *“The world’s ultimate weapon runs on water; everything else runs on fuel”*

Key Innovation – Compressive Release



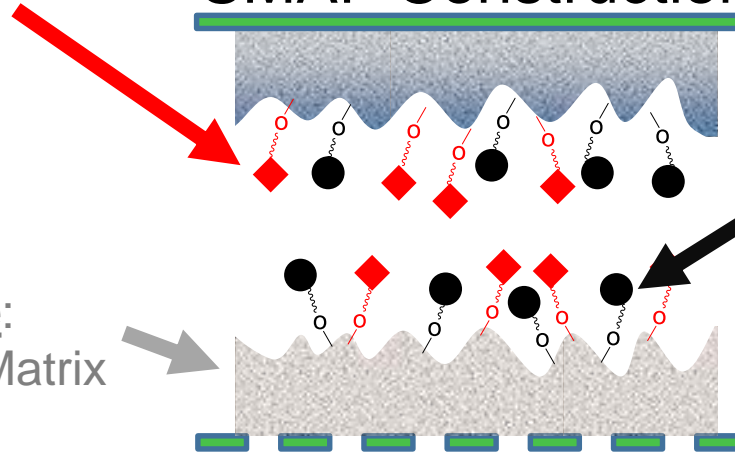
TA1 Smart Moisture Absorbing Foam (SMAF) designed to have **water capture, storage and **release** functionality (non-thermal release mechanism)**

TA1: Material Level Concept

Water Capture: Ionic grafting, polymers, and microporous materials

Water Storage: Biopolymer Foam Matrix

SMAF Construction

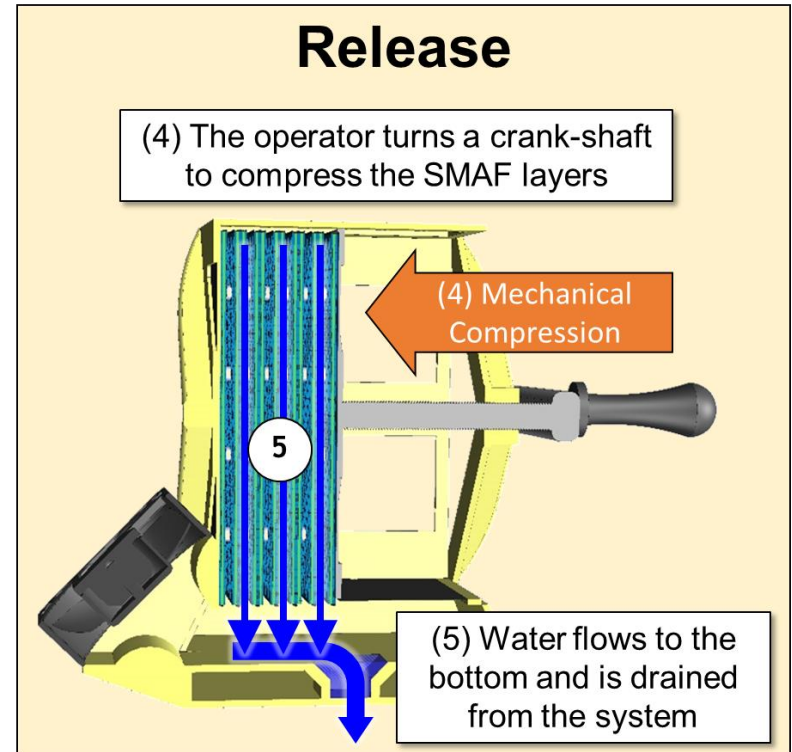
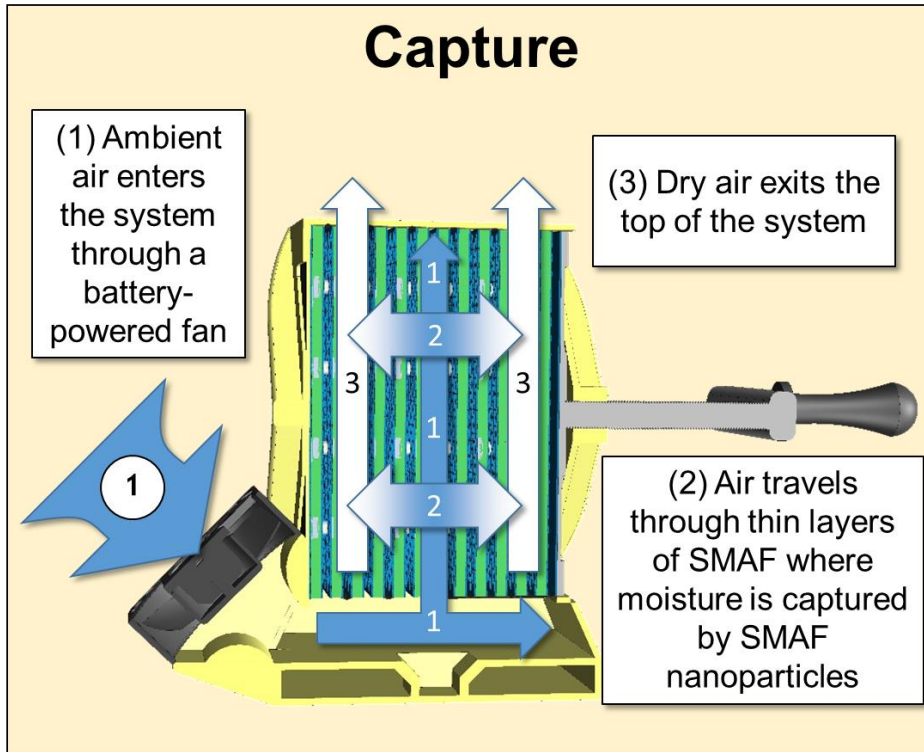


Water Release: Hydrophilic/Hydrophobic Organo-Silicate

Exp. Results	Milestone 1.1 Metric	Matrix 1	Matrix 2
Water Uptake at 100% RH (g_{H_2O}/g_{foam})	> 10	12.5	11

Functional groups selected based on experimental evaluation

TA2: System Level Concept



TA2 design leverages high SMAF capacity and mechanical release to drastically reduce system SWaP

TA1 - Screening Methods

Water Capture

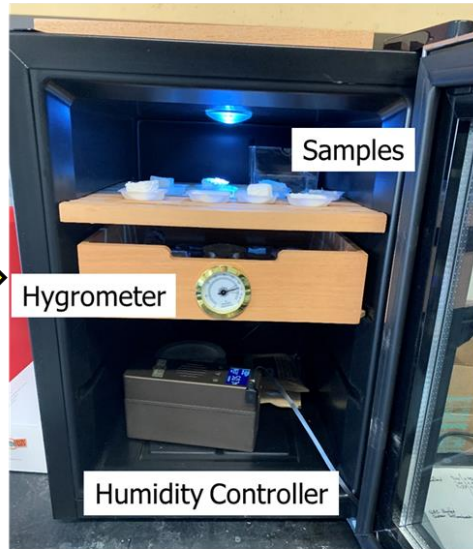
Water Release

Dynamic Vapor Sorption (DVS)



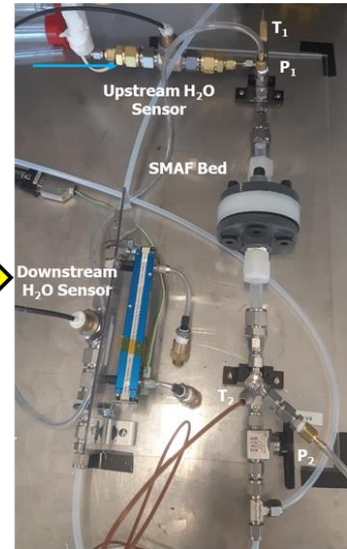
Measurement:
Water Uptake
Isotherm
(mg scale)

Humidity Chamber



Measurement:
Single-Point
Uptake
(100 mg scale)

Fixed-bed



Measurement:
Water Capture in
Flow Configuration
(g scale)

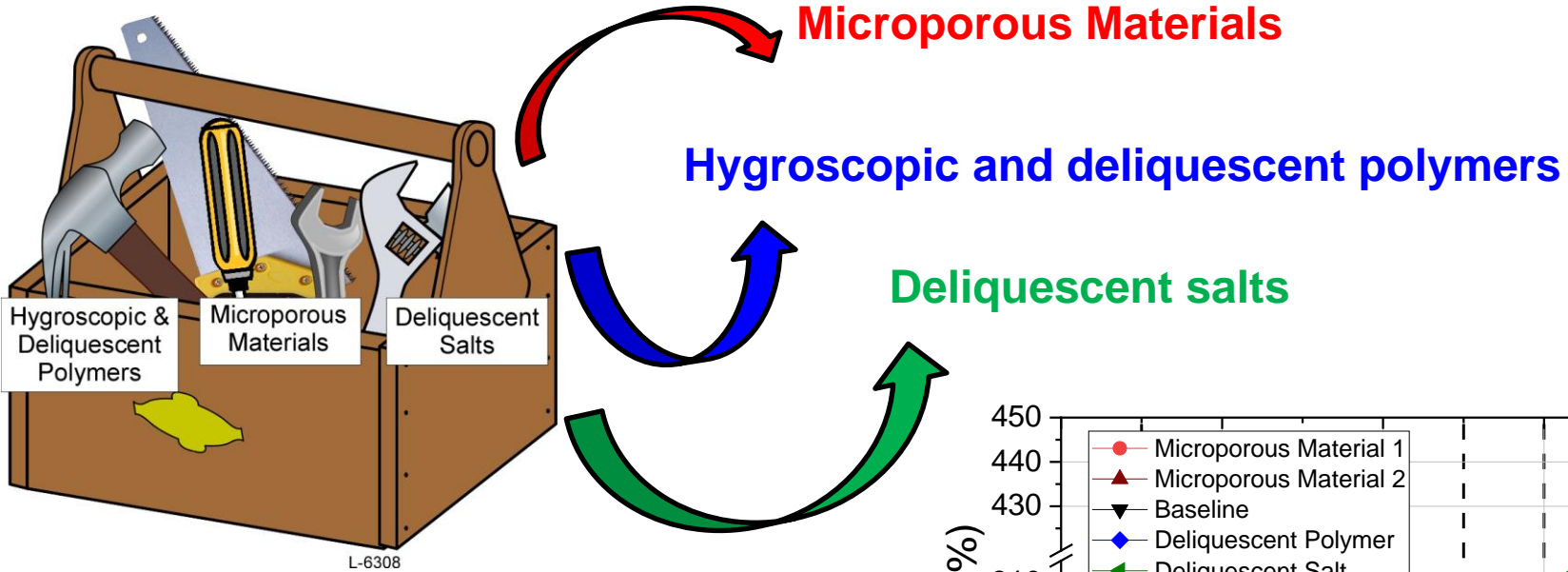
Compression Test



Measurement:
Force Required for
Water Release
(g scale)

We have assembled the equipment necessary to measure water capture and release under the relevant conditions

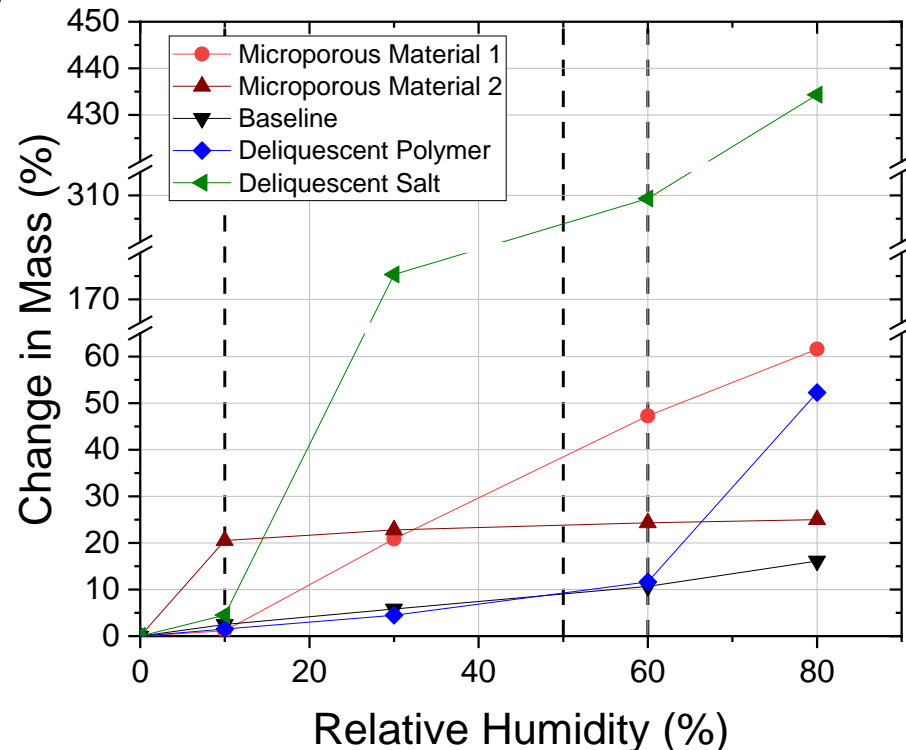
TA1 - Capture Materials Toolbox



Selection Criteria:

- Water capture capacity
- Rapid water uptake kinetics
- Material stability
- Scalable synthesis

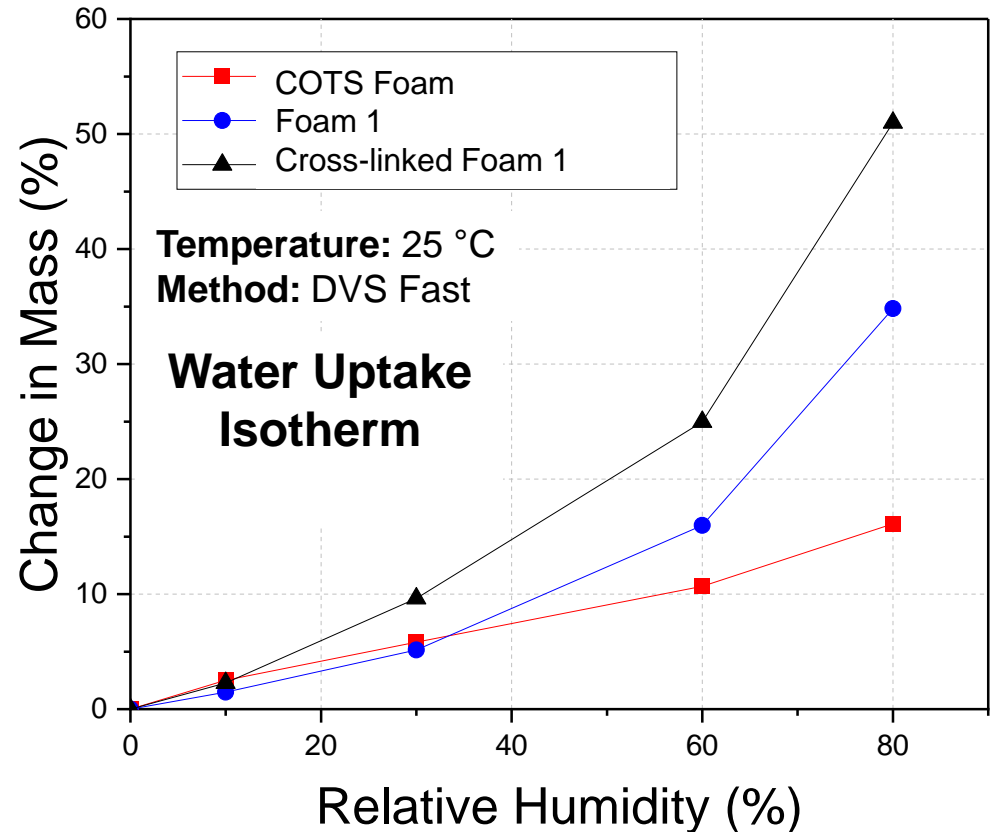
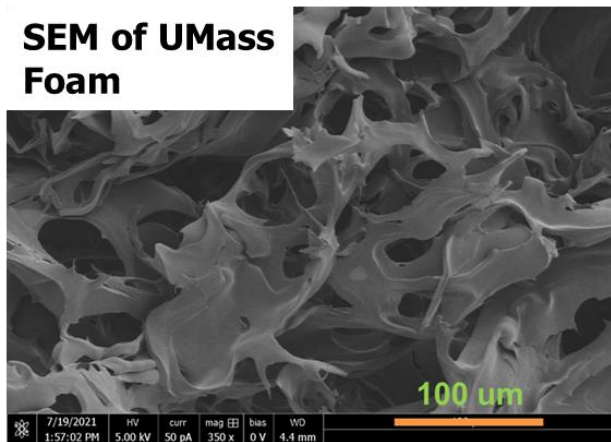
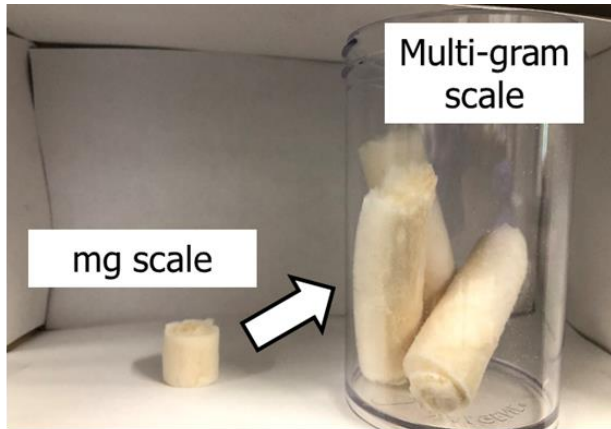
Combination of water capture functionalities provides desired water capture performance



TA1 - Water Storage Development

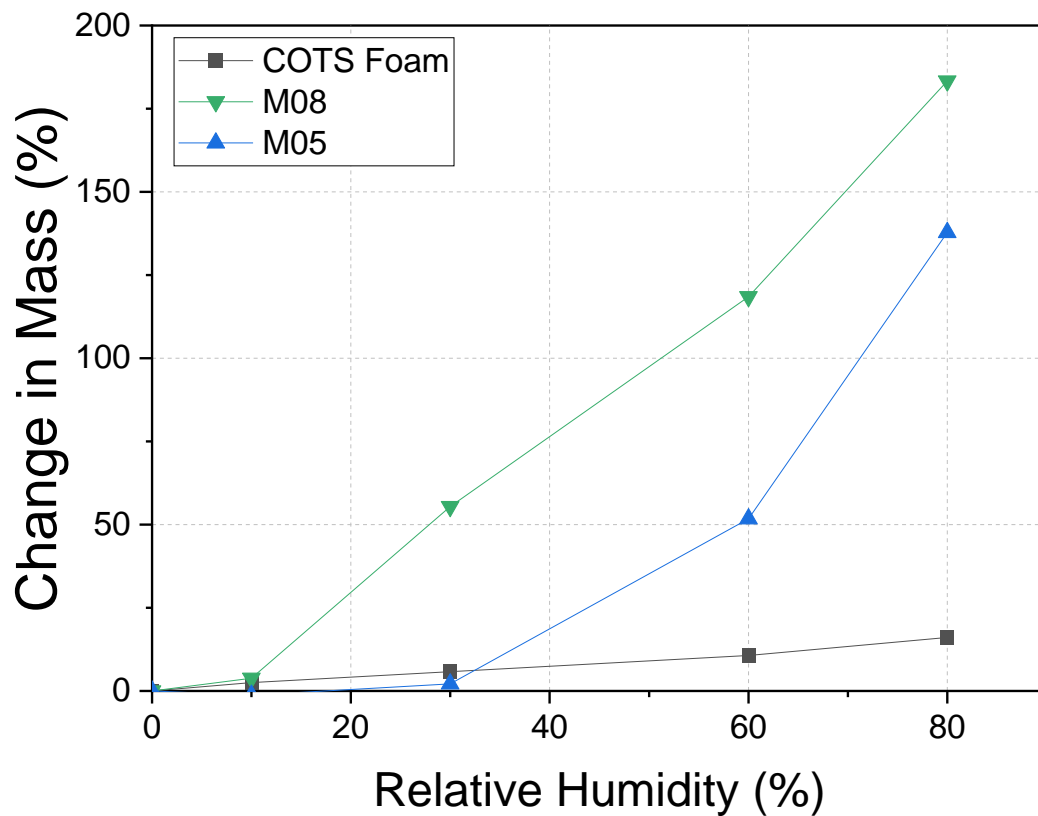
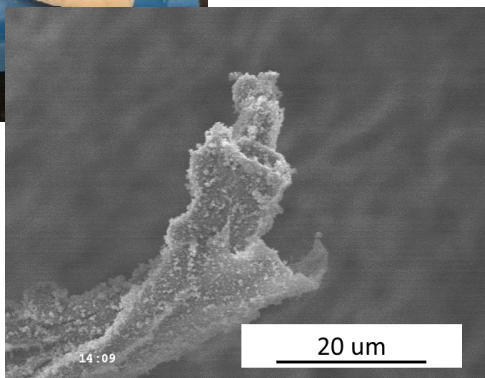
Goal: Exceed baseline water uptake of commercial off-the-shelf biopolymer foam

Methods: Examine biopolymer foaming (by lyophilization) with and without crosslinking



Engineered foams promote greater water uptake than baseline off-the-shelf foam

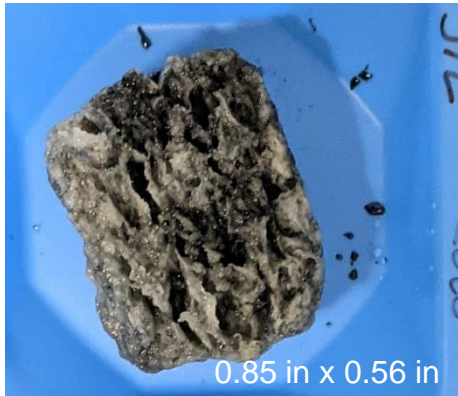
TA1 – Best Performing Materials To Date



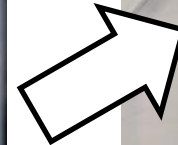
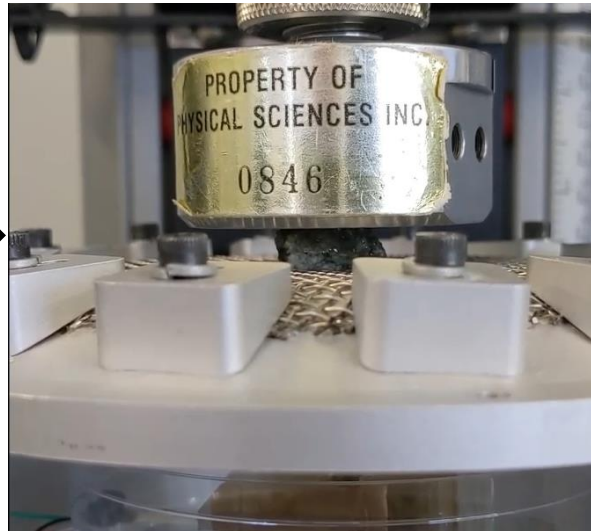
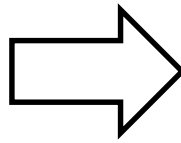
M05 and M08 SMAFs have been the best performing materials with both capture and release functionality incorporated

TA1 - M05 SMAF Demonstration

- **Objective:** Demonstrate water release from SMAF material loaded at 70% RH
- **Methods:** Perform water uptake in humidity chamber, followed by release using compression set-up
 - ^1H NMR spectrum indicated contamination of water with polymers



SMAF coupon loaded at 70% RH



Filtration
(0.45 μm)



Filtered Water

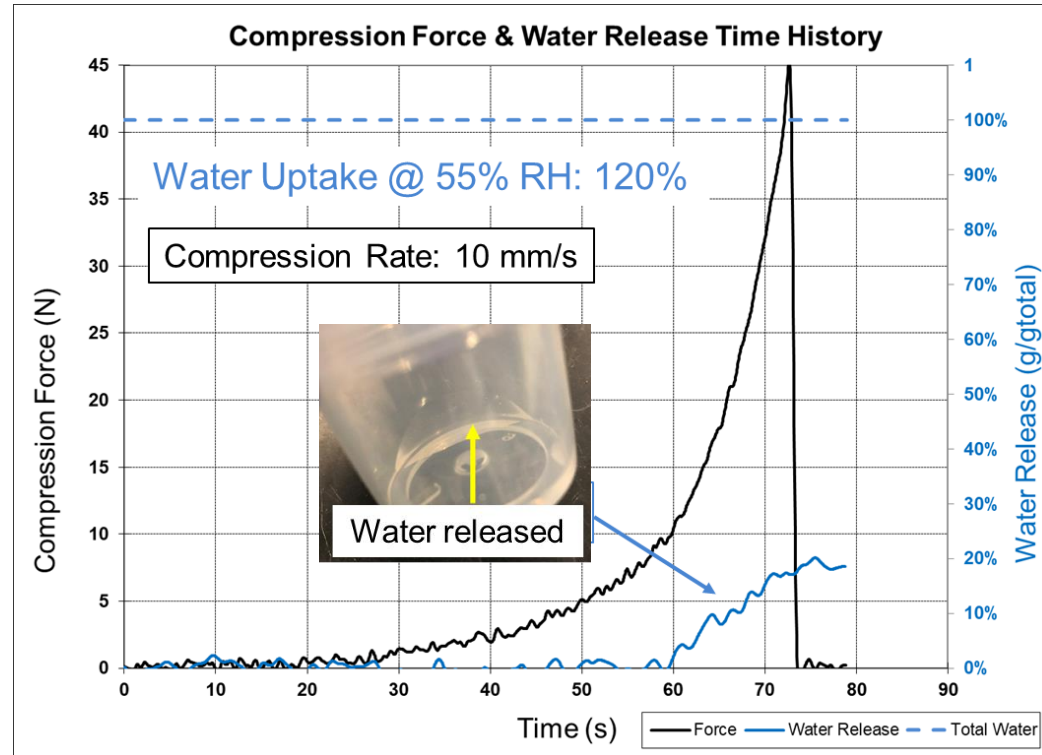
Video demonstrates water release upon SMAF compression

TA1 - M08 SMAF Demonstration

- **Objective:** Demonstrate water uptake and compressive release at 55% RH (M05 demonstrated at 70 % RH)
 - Fulfills one out of the three DARPA performance conditions (10%, 50%, 60%)



M08 SMAF coupon reached 120% water uptake after 16 hr at 55% RH



Achieved 20% water release with a 45 N force

SMAF water capture and compressive release demonstrated at 55% RH

TA2 – SMAF Model Key Equations

Governing Equations

Humid Air Flow Through SMAF

- Navier-Stokes (momentum equation)
- Assumptions: constant fluid and SMAF properties, laminar flow, no mass source/sink, gravity negligible
- Brinkman (B) Equations: continuity and momentum conservation for flow through porous media

$$\nabla \cdot \mathbf{U} = 0$$

$$\underbrace{\frac{\rho}{\varepsilon_p} \left(\frac{\partial \mathbf{U}}{\partial t} + \frac{1}{\varepsilon_p} (\mathbf{U} \cdot \nabla \mathbf{U}) \right)}_{\text{Inertia}} = \underbrace{-\nabla p}_{\text{Pressure Source}} + \underbrace{\frac{\mu}{\varepsilon_p} \nabla^2 \mathbf{U}}_{\text{Viscous Diffusion}} - \underbrace{\frac{\mu}{\kappa} \mathbf{U}}_{\text{Foam Permeability}}$$

Water Vapor (c_v) and Liquid Water (c_l) Mass Transport

- Assumptions: constant fluid and SMAF properties, liquid water advection negligible
- Advection-Diffusion (AD) equation with reaction rate defines mass transport:

$$\underbrace{\frac{\partial c_i}{\partial t}}_{\text{Transient}} = \underbrace{D_i \nabla^2 c_i}_{\text{Diffusion}} - \underbrace{\mathbf{U}_i \cdot \nabla c_i}_{\text{Advection}} + \underbrace{R_i}_{\text{Vapor to Liquid Source/Sink}}$$

Key Parameters

Water Capture

- Assumptions: sample size in DVS small enough for diffusion to be negligible, advection also negligible
- LDF model fit to DVS data at various RH:

$$R_l = -R_v = k(c_{l,eq} - c_l)$$

- k , and $c_{l,eq}$ both function of RH – calculated from local c_v

Key Dimensionless Numbers

- Non-dimensionalization of Advection-Diffusion equations yields three key dimensionless numbers:

- Diffusivity ratio:

$$\lambda = \frac{H_2O \text{ in SMAF}}{H_2O \text{ in air}} = \frac{D_l}{D_v}$$

- Peclet number:

$$Pe_v = \frac{\text{advection}}{\text{diffusion}} = \frac{u_v L}{D_v}$$

- Damkohler number, 2nd kind:

$$Da_v = \frac{\text{water capture rate}}{\text{diffusion}} = \frac{kL^2}{D_v}$$

Navier-Stokes and Advection/Diffusion Equations used to model water transport and capture by SMAF material

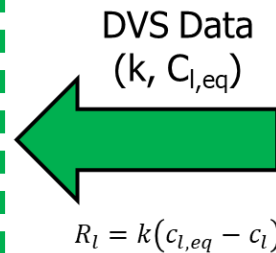
TA2 – SMAF Model Inputs and Outputs

Inputs

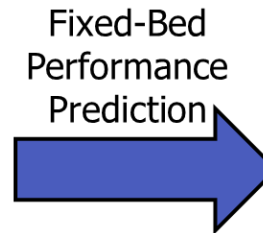
- SMAF Properties
 - Physical properties – form factor, density, porosity, permeability, stress-strain curve
 - Water capture/storage/release – isotherm define equilibrium capacity and rate constant, diffusivity, release vs. strain, unreleased capacity
- Environmental Conditions
 - Humid air temp, RH, and specific discharge
- System Properties
 - Common – turnovers per day, compression strain, battery power density, air handler efficiency
 - Specific – architecture specific parameters, e.g. material selection, air gap thickness, number of layers

Outputs

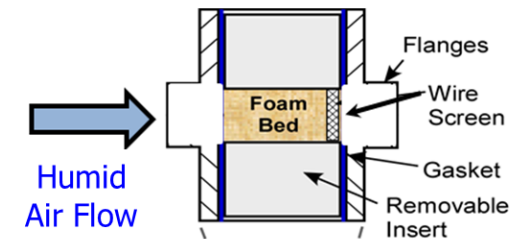
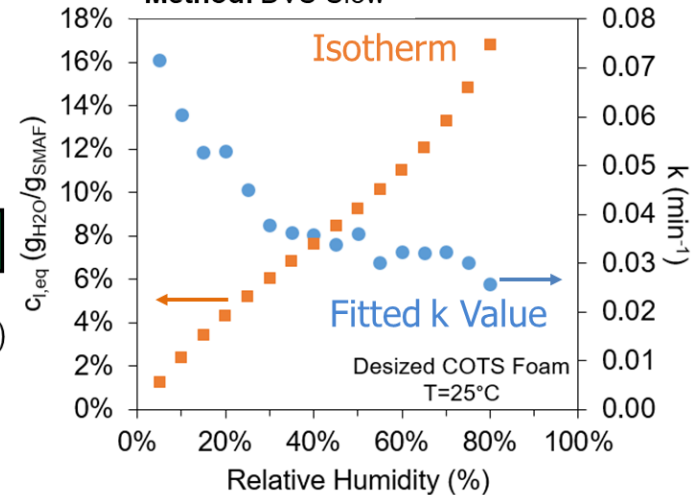
- Water Output
 - Water capture rate, total water capture per SMAF mass
 - Water released and required force from Instron testing
- System SWaP



$$R_l = k(c_{l,eq} - c_i)$$



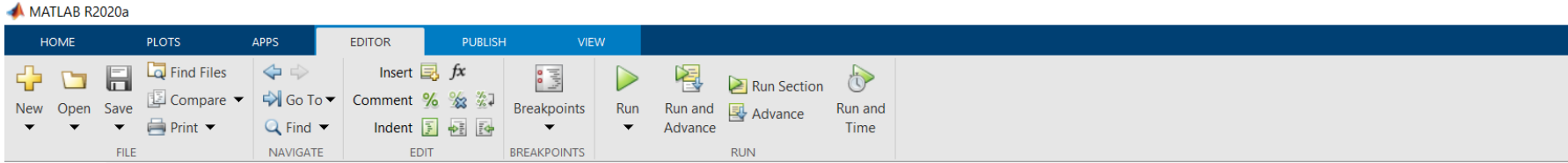
Temperature: 25 °C
Method: DVS Slow



The goal of this modeling effort is to correlate intrinsic foam properties (DVS data) to performance in a flow geometry (prototype system)



TA2 – SMAF Model Construction



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Editor - G:\Deployable Technologies\temery\8068 - AWE\Calculations\BAD_2DCyl_PDEPE.m

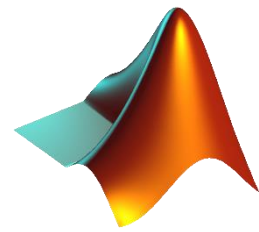
- Bubble Collision Model
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- ~\$Flow Calcs_TSE.xlsx
- ~\$ror Analysis Equations.docx
- ~\$Transient capture.xlsx
- 1D Brinkman.xlsx
- 1D Brinkman and AD.xlsx
- 89_4mm_270SCCM.csv
- 89A_isotherm.csv
- 89A_isotherm_avg.csv
- BAD_1D.m
- BAD_1D.pptx
- BAD_1D_Graphing.m
- BAD_1D_NonDim.xlsx
- BAD_1D_NonDim_Graphing.m
- BAD_1D_ODE.m
- BAD_1D_PDEPE.m
- BAD_1D_PDEPE_NonDim.m
- BAD_2D_Cylindrical.pptx
- BAD_2DCyl_Graphing.m
- BAD_2DCyl_PDEPE.m
- Brinkman.pptx
- Cellulose_isotherm.csv
- coeffteter.m
- COTS_20mm_270SCCM.csv
- COTS_isotherm.csv
- Error Analysis Equations.docx
- fdcoeff.m
- Flow Calcs_DPG4.xlsx
- Flow Calcs_TSE.xlsx
- foam_2D.m

```

29 % Get inlet conditions
30 P=101325; % assumed pressure for air props [Pa]
31 % Humid Air properties
32 % p_wv [Pa], p_wvs [Pa], x [g_wv/g_da], AH [g/m^3], rho [kg/m^3], y_wv [-], mu [Pa-s]
33 [~,p_wvs,x_in,AH_in,rho_in~,mu_in] = getHAprops(T,P,RH_in);
34 D_v=(8.125E-6*T^2+9.875E-4*T+0.219)*1E-4; % water vapor diffusivity in air [m^2/s]
35 cv_in=AH_in/M_wv; % water vapor concentration in humid air [mol/m^3]
36 cl_eqin=interp1(isotherm(:,1),isotherm(:,2),RH_in,'linear','extrap'); % inlet equilibrium liquid water concentration [mol/m^3]
37 mdot_da=mdot_daSCCM/298.15*M_da/(R/101325*100^3)/60; % dry air mass flow rate [g/s]
38 mdot_ha=mdot_da*(1+x_in); % humid air mass flow rate [g/s]
39 Vdot_ha=mdot_ha/1000/rho_in; % humid air volumetric flow rate [m^3/s]
40 u_avg=Vdot_ha/(pi*rm^2); % Specific discharge/superficial velocity [m/s]
41 % Reynolds number - check for laminar assumption
42 Re_open=rho_in*u_avg*2*rm/mu_in; % open tube
43 Re_foam=rho_in*u_avg*sqrt(kappa/eps_p)/mu_in; % through foam
44
45 % Max water capture
46 m_wcmax=vol_SMAF*cl_eqin*M_wv*1000; % max water capture [mg]
47 M_tmax=m_wcmax/m_SMAF; % max relative water capture [g_H2O/g_SMAF]
48
49 % Domain discretization
50 dz=0.0001; % z spatial resolution [m]
51 z=linspace(0,zm,zm/dz+1); % z domain [m]
52 dr=0.00005; % r spatial resolution [m]
53 r=linspace(0,rm,rm/dr+1).'; % r domain [m]
54 [zG,rG]=meshgrid(z*100,r*100); % gridded [z,r] domain [cm]
55 t=[0:0.001:1 10:10:100000].'; % time domain [s]
56

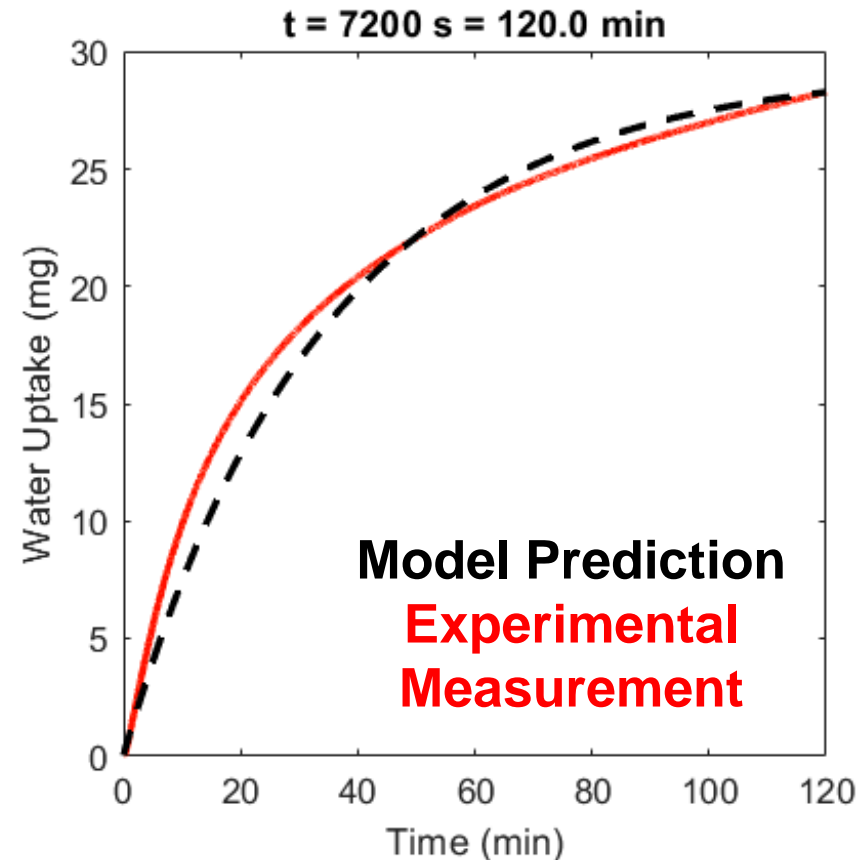
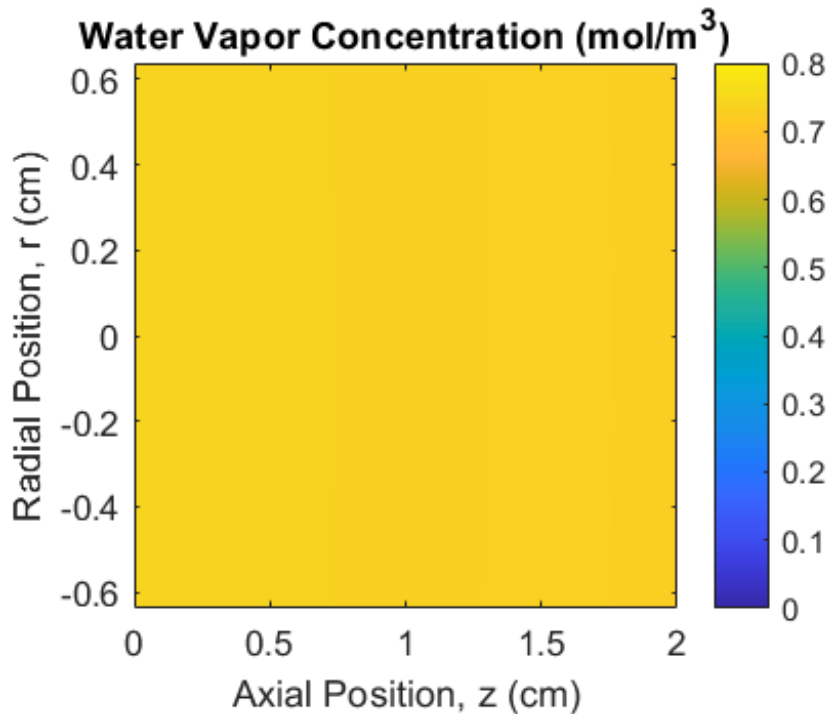
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SMAF model constructed in MATLAB



TA2 – Predicting SMAF Water Capture Performance

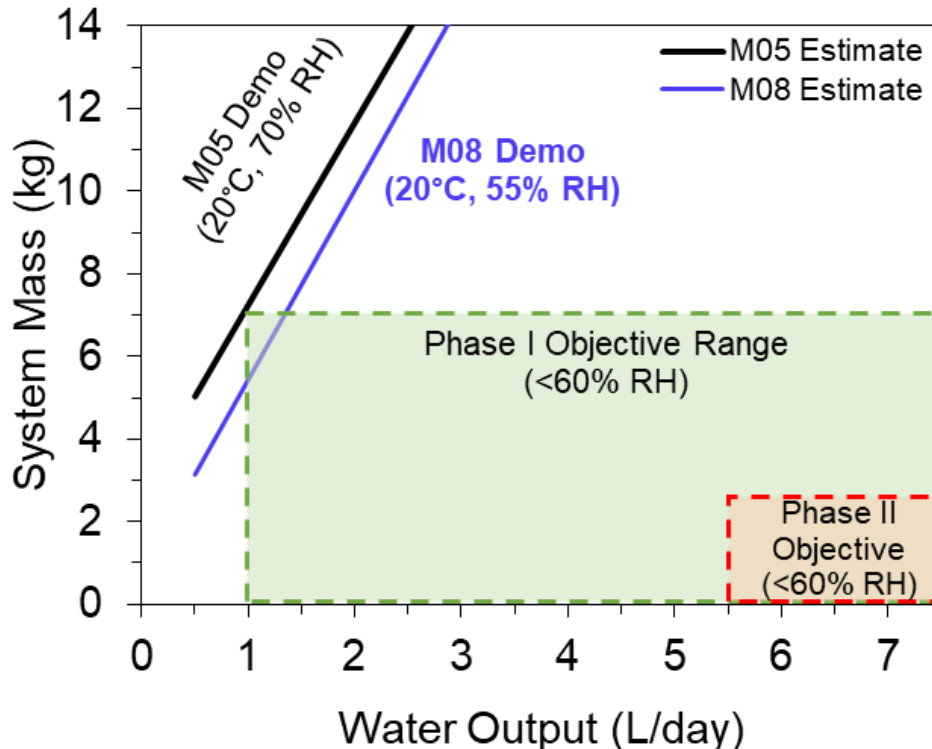
PSI SMAF Model was used to predict the performance of a SMAF material



Animation shows that the PSI model prediction has good correlation with the experimental measurement

TA2 – Tracking Progress Towards Implementation

- **Goal: Provide a predictive modeling to assist in the overall design and ensure the required performance metrics are being met.**
 - **Black line** represents M05 demonstration
 - **Blue line** represents M08 demonstration
 - Computed using PSI rubber model using several key assumptions



Key Assumptions:

- No SMAF material degradation over time
- Layered system model as initially proposed to estimate housing mass
- Minimal additional pressure drop as SMAF fills. Air flow requirements used to estimate fan and battery mass
- Two capture/release cycles per day
- Water is potable after filtration

Improvements in performance at lower relative humidity and system performance have been achieved

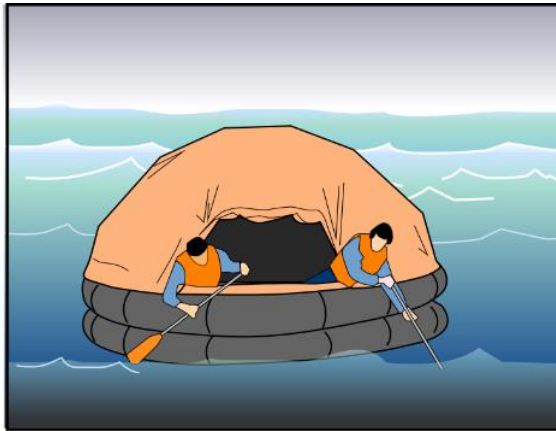
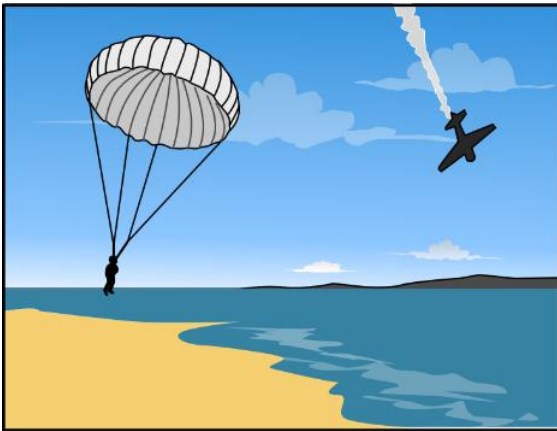
Potential Technology Use Cases

- **Goal:** Identify potential use cases to which our SMAF approach can be tailored to both defense and commercial applications:
 - 1. Downed Pilot Scenario**

Key Advantage: Low anticipated system noise generation
 - 2. Lifeboat Operation**

Key Advantage: Surrounding conditions maintained at high RH
 - 3. Initial Household Water Generation after Disaster Event**

Key Advantage: Ideal solution for use in tropical regions, where water production can be maximized.

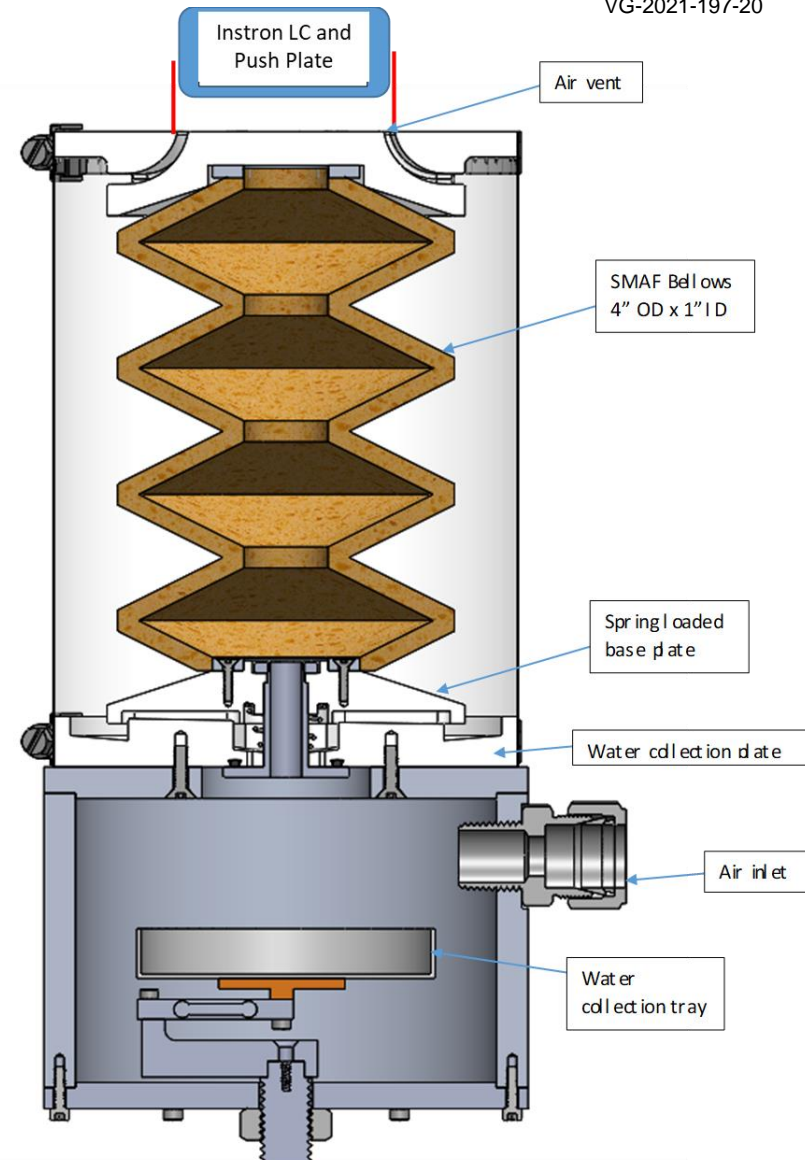


The team is taking into consideration potential applications to guide prototype development

Conclusions and Next Steps

VG-2021-197-20

- The PSI/UMass/CDI team is developing a new material called a Smart Moisture Adsorbing Foam (SMAF)
- SMAF material captures water from the atmosphere and releases water by compression
- Core concept has been demonstrated at 55% and 70% relative humidity
- SMAF model developed to describe transport and adsorption in foam media
- Next steps include further optimization of SMAF formulation and construction of an operable prototype (due to IV&V team in July)





Physical Sciences Inc.

Backups

VG-2021-197-21



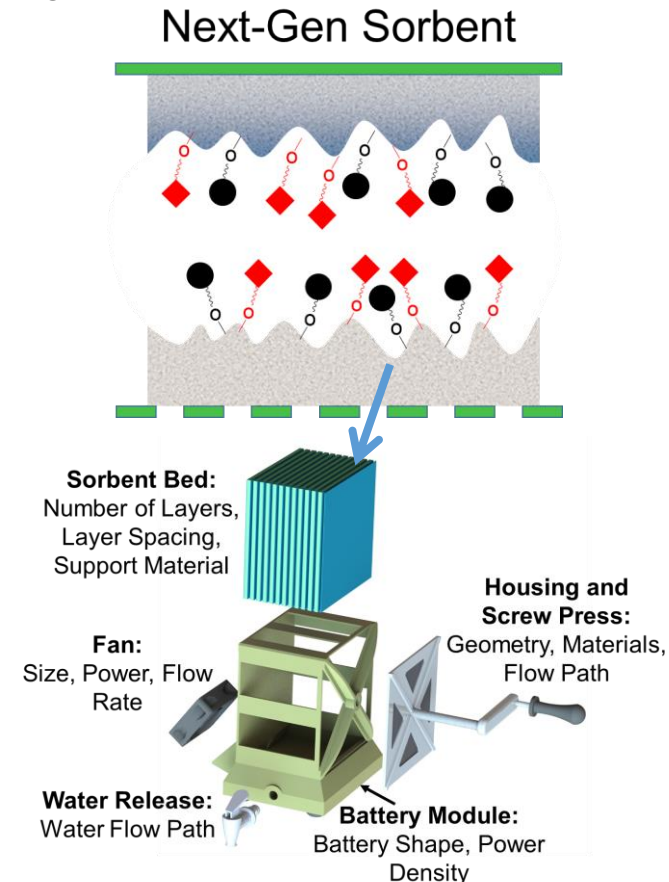
DARPA BAA Requirements

- **Topic – DARPA BAA HR001120S0014** Atmospheric Water Extraction (AWE)
- **Broad Need –** Water transport to the warfighter is mission-critical but logistically challenging, requiring equipment, fuel, and personnel that limits tactical maneuver and decision space. Warfighter requires 3/7 L/day.
- *The world’s ultimate weapon runs on water; everything else runs on fuel*

Metrics	Phase I Objective	Phase II Objective
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System Dry Weight	≤7 kg	≤2.5 kg
Power	Must be contained onboard	Must be contained onboard
Volume	6 L (0.21 ft ³)	1.5 L (0.05 ft ³)
Unit Cost	-	-
Desired Properties	-	Water meets TB-Med-577 potability standards, Operational for >30 days at 24 hr runtime

PSI Team Program Objectives

- **Program Goal:** Develop a system capable of extracting potable drinking water from air, obviating the need for costly and dangerous transportation (Expeditionary Track).
 - Program broken into 2 technical areas (TAs)
 - TA1: Transformational Sorbent Materials Development
 - TA2: Extractor Modelling, Engineering and Sorbent Integration
- **TA1 Goal:** Create a new and revolutionary class of sorbents that have high capacity, rapid water uptake and release sorbed water by compression-enabled switching from hydrophilic to hydrophobic state.
- **TA2 Goal:** Design, construct and optimize a system capable of meeting the DARPA SWaP and output requirements by leveraging the SMAF compressive release capability developed in TA1.





TRL Analysis*

- **Entering Phase I Program = TRL1/2**
 - Technology concept and/or application formulated.
 - Limited analytic studies
 - Process in place to produce and evaluate SMAF materials
 - System concept created

- **Exiting Base Program = TRL3/4**
 - Analytical and experimental critical function and/or characteristic proof of concept. Component and/or breadboard validation in laboratory environment
 - Material optimization performed
 - Breadboard system demonstration

- **Exiting Option Programs = TRL6**
 - Components and/or breadboard validation in relevant environment
 - Scalable sorbent production
 - Field demonstration in relevant environment (IV&V)