Next Generation Adsorbent Composites: Material Discovery by way of Artificial Neural Networks informed by Finite Element Analysis

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Material Discovery by way of Artificial Neural Networks informed by Finite Element Analysis

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Abstract

We present our efforts to computationally investigate methodologies and material designs capable of leveraging breakthroughs in material synthesis. Micro-porous adsorbents have found incorporation into a wide range of industrial processes. Our area of investigation is atmospheric water extraction (AWE). A key design hurdle in AWE is optimizing sorbent/substrate networks for increased vapor uptake while mitigating rate limiting enthalpies. The developed optimization framework utilizes dolfin-adjoint to solve a coupled adsorption FEM script by iteratively evaluating a function of interest and its gradient at different points. The function of interest is the distribution of a phase change material homogenously imbedded in the sorbent/substrate optimized to limit the swings in temperature exhibited by the composite thereby increasing uptake/release cycling.

Adsorption based Atmospheric Water Harvesting Incorporating Phase Change Materials

Much of our world is built with the expectation that water will return to us through natural systems and in abundance. Population growth, untreated industrial wastewater, and climate change have resulted in daunting cleanup challenges, rivers with reduced flow, and reservoirs with depleting supplies. Passive adsorption based Atmospheric Water Harvesting (AWH) is a potential breakthrough technology.

Adsorption is an exothermic process wherein the process of capturing vapor generates heat which inhibits vapor capture. A focus of our research has been a search for; designer adsorbents with idealized isotherms, composite designs which sink heat away through substrate structures or metal inclusions, and now the inclusion of phase change materials in the adsorbent bed.

This work is part of a broader effort described in Figure 2 for the development of a Multi-scale schema for high throughput topologically optimized studies to determine and design water collecting structure and materials.

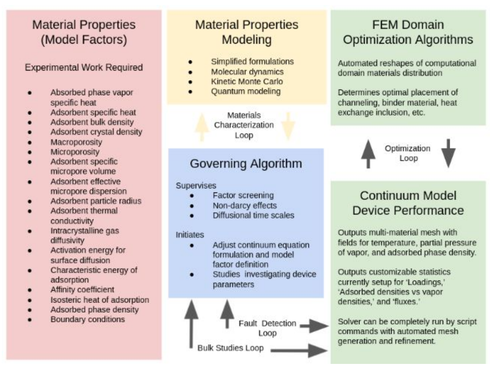


Figure 2: Multi-scale schema for high throughput topologically optimized studies

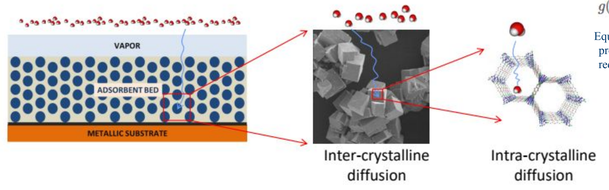


Figure 1: (left) Vapor capture by adsorbent bed with heat sink substrate. (center) Macroporosities characterize vapor diffusion and are temperature dependent. (right) Microporosities characterizes saturation limitations with rate limited temperature dependence.

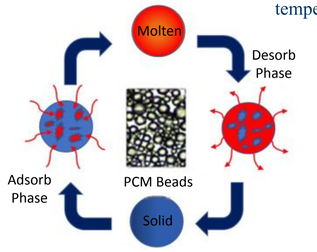


Figure 3: Phase Change Material Cycle, During the Adsorb phase the PCM captures heat and during the Desorb phase the PCM releases heat.

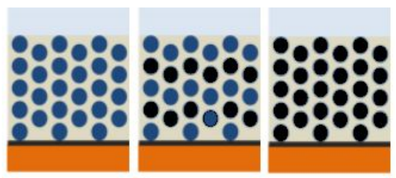


Figure 4: Each iteration of the ANN optimization increases the distribution of the Phase Change Material beads (black) replacing Adsorbent beads (blue) . The results of such iterations are displayed to the right.

Optimizing Phase Change Distribution with L-BFGS

$$\min_{u,m} J(u,m) \quad \text{subject to} \quad F(u,m)=0,\ l_u \le m \le l_b,\ g(m) \le 0$$

$$\min_{m} J(u(m),m) \quad \text{subject to} \quad l_u \le m \le l_b,\ g(m) \le 0$$

Equations 1, 2, and 3: PDE-Constrained optimization problems, general form (left), reduced form (right), reduced form can be seen as function depending on the optimization variable *m* (below).
m, is a vector of PCM

$$\hat{J}(m) := J(u(m),m)$$

The physics model is a set of time-dependent coupled partial differential equations expressed as the vector expression F, with all terms on the LHS. The PDE solution *u* can be considered an implicit function u(m) of the parameters *m* related through the PDE F(u,m) ≡ 0. J represents the quantity to be optimized by minimizing the misfit between PDE observations and OPT computations. Derivatives of the functional direct where to step next in parameter space and allow gradient-based optimization algorithms to converge onto a local minimum with reduced computational effort.

This PDE-constrained optimization problem involves; 1) starting with an initial guess for the parameters, *m*, 2) Computing Jˆ (m) using the forward PDE and its gradient using the adjoint method (Hermitian transpose), 3) passing values to the L-BFGS optimization algorithm which returns a new point in the parameter space with a better functional value, 4) if gradient is 0 or max iterations reached, terminate, else return to 2.

The L-BFGS (Limited-memory Broyden Fletcher Goldfarb Shanno) method intends to minimize the performance function, J, subject to the bound constraints 0_u and l_b. L-BFGS uses the approximated second order gradient information to converge towards a minimum. It does not scale well with multiple parameters but for this implementation that is not a problem and these equations were solved on a 4-year old laptop over the course of 30 min.

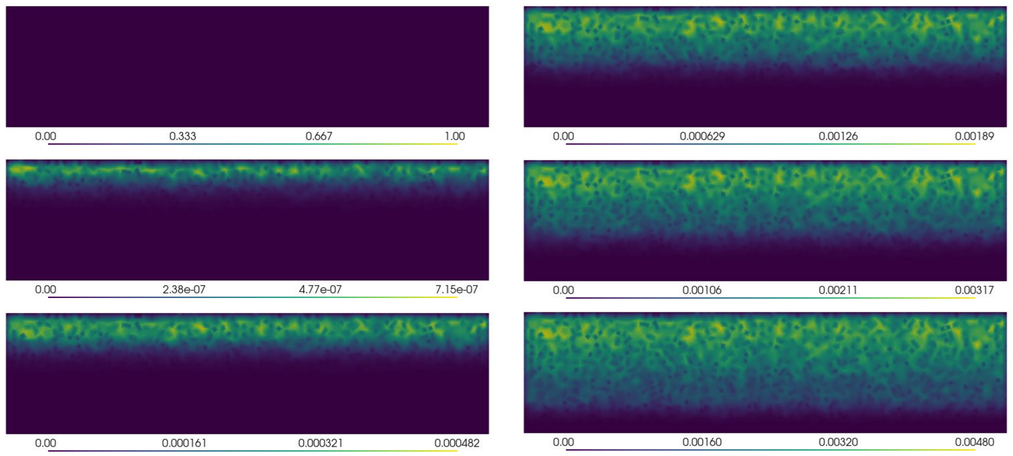
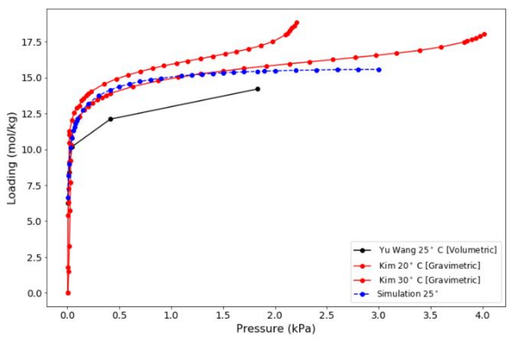


Figure 7: Increasing PCM distribution homogeneously starting with 0 to 1. PCM distribution is visualized above.

Finite Element Model



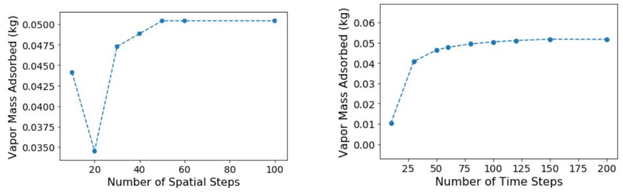


Figure 6: Convergence Studies (left) Spatial Convergence: the mesh adequately resolved at nx = 50. nx = 60 was used for subsequent investigation. (right) Temporal Convergence: the time stepping adequately resolved at nt = 125. nt = 150 was used for subsequent investigation.

Figure 5: Validation Study Results: Isotherm Loading The volumetrically determined Adsorption Equilibrium are plotted in black with simulation results in blue. The model was specified with the Dubinin-Astakhov for adsorption density equilibrium, Vant Hoff fitting for the enthalpy of adsorption, Vasiliev method for the mass transfer coefficient, Kozeny-Carman approximation with no constants for permeability, Modified Zehnder-Schlunder for effective thermal conductivity, and Antoine fitting for the local adsorbed gas density.

The difference in vapor collected between the lowest bounded PCM distribution and the highest iterated PCM distribution was **2.5e-6 [kg] vapor mass adsorbed**. The incorporation of PCM resulted in more vapor collected despite replacing adsorbent with PCM.

References

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