Supporting Information

Adsorption-based atmospheric water harvesting: impact of material and component properties on system-level performance

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Table S1. Variables used in the sorption kinetics and heat transfer model.

Variable	**Definition**
C	Vapor concentration
C_μ	Vapor concentration in the adsorbent crystal
T	Temperature
t	Time
D_v	Intercrystalline diffusivity
D_k	Knudsen diffusivity
d_p	Characteristic void size
P	Pressure

Table S2. Material properties used in the sorption kinetics and heat transfer model.

Material property	**Description**	**Input value (MOF-801)[1]**
r_c	Crystal radius	0.5 μm
D_μ	Intracrystalline diffusivity	1.2E-16
ε	Packing porosity	variable
D_{vap}	Vapor molecular diffusivity in air	~3E-5 m^2/s
ρ	Average density	~910 kg/m^3 (dependent on uptake)
c_p	Average specific heat capacity	~800 J/kg/K (dependent on uptake)
k	Average thermal conductivity	4 W/m/K
h_{ad}	Adsorption enthalpy	3055 kJ/L
C_{eq}	Equilibrium concentration	From material isotherm

Table S3. Boundary conditions used in the sorption kinetics and heat transfer model.

Boundary condition	**Term**	**Value**
Heat loss	h	10 W/m^2/K
	$T_{external}$	25 °C
Ambient relative humidity	RH	30%
Condenser temperature	$T_{external}$	25 °C

References

(1) Kim, H.; Rao, S. R.; Kapustin, E. A.; Zhao, L.; Yang, S.; Yaghi, O. M.; Wang, E. N. Adsorption-based atmospheric water harvesting device for arid climates. *Nature Communications* **2018**, *9*, 1191-1191.