

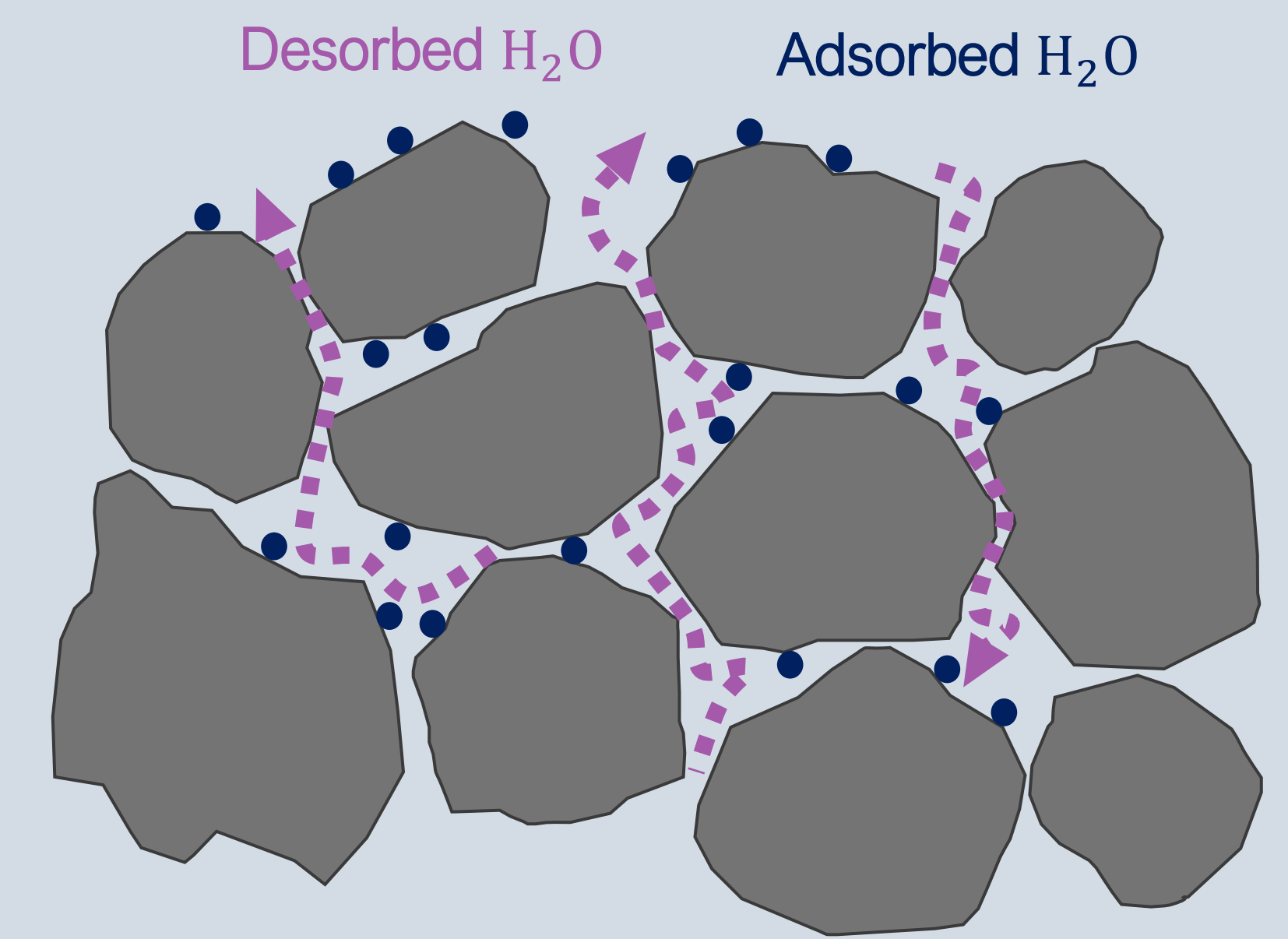
Methodology

The water adsorption profile is driven by temperature and concentration gradients. To investigate it, we solve the one-dimensional heat and mass transport equations with sorption as a sink/source (Eq. 1), using the Finite Volume Method. We distinguish between the adsorbed (c_a) and desorbed (c_d) water concentrations. The adsorbed concentration at equilibrium can be calculated using the Langmuir isotherm and the monolayer concentration (c_m) as shown in (Eq. 2). All our simulations have a spatial resolution of 200 cells and a domain length of 0.5 m.

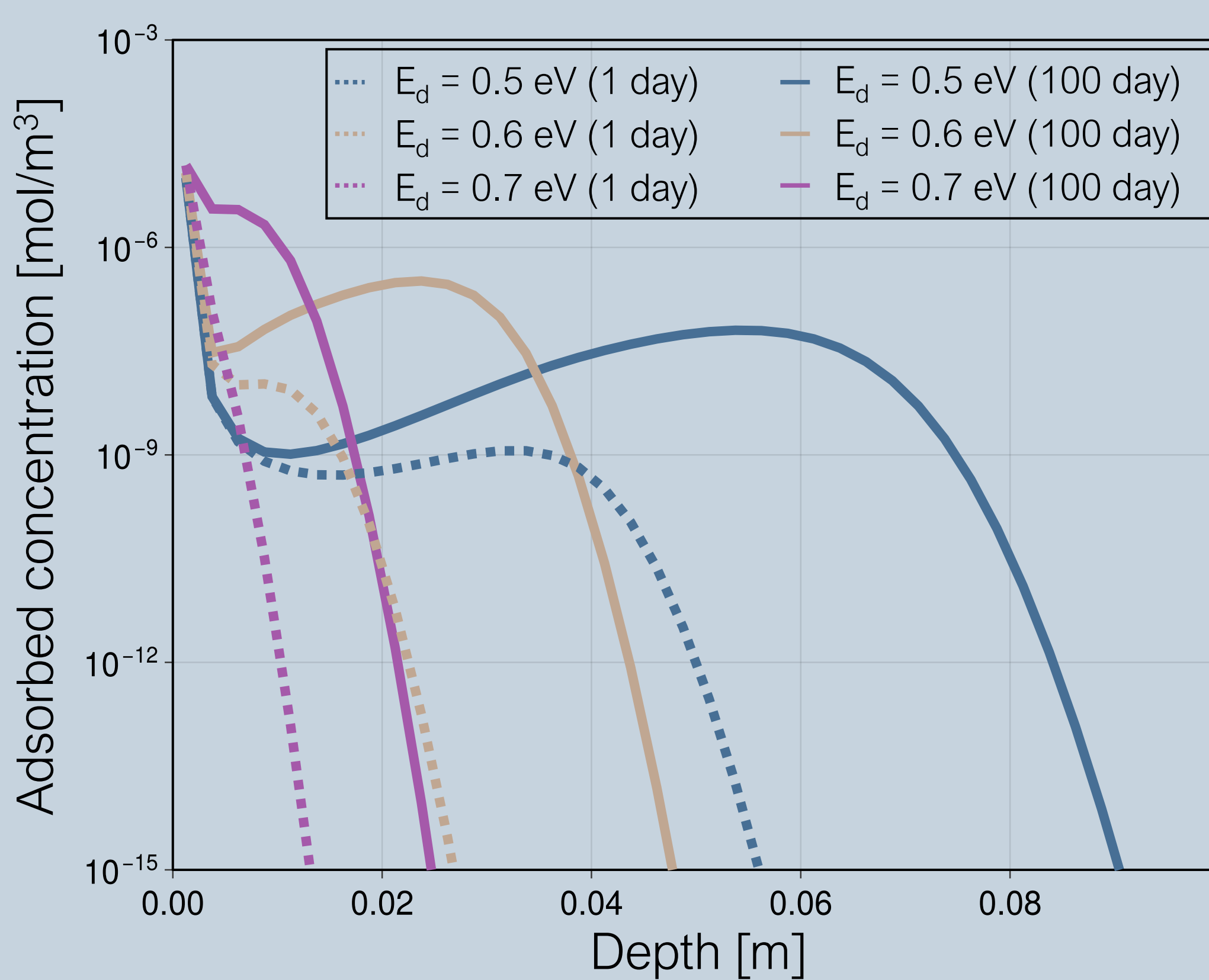
We define the surface temperature to follow the model of [1] at 80° latitude and a constant surface water supply as in [2]. Then, we simulate multiple lunar days to investigate the adsorption profile obtained.

$$\frac{\partial c_d}{\partial t} = \nabla \cdot (D \nabla c_d) - \frac{\partial c_a}{\partial t} \quad (\text{Eq. 1})$$

$$c_a = c_m \frac{bP}{1 + bP} \quad (\text{Eq. 2})$$



Adsorption profile



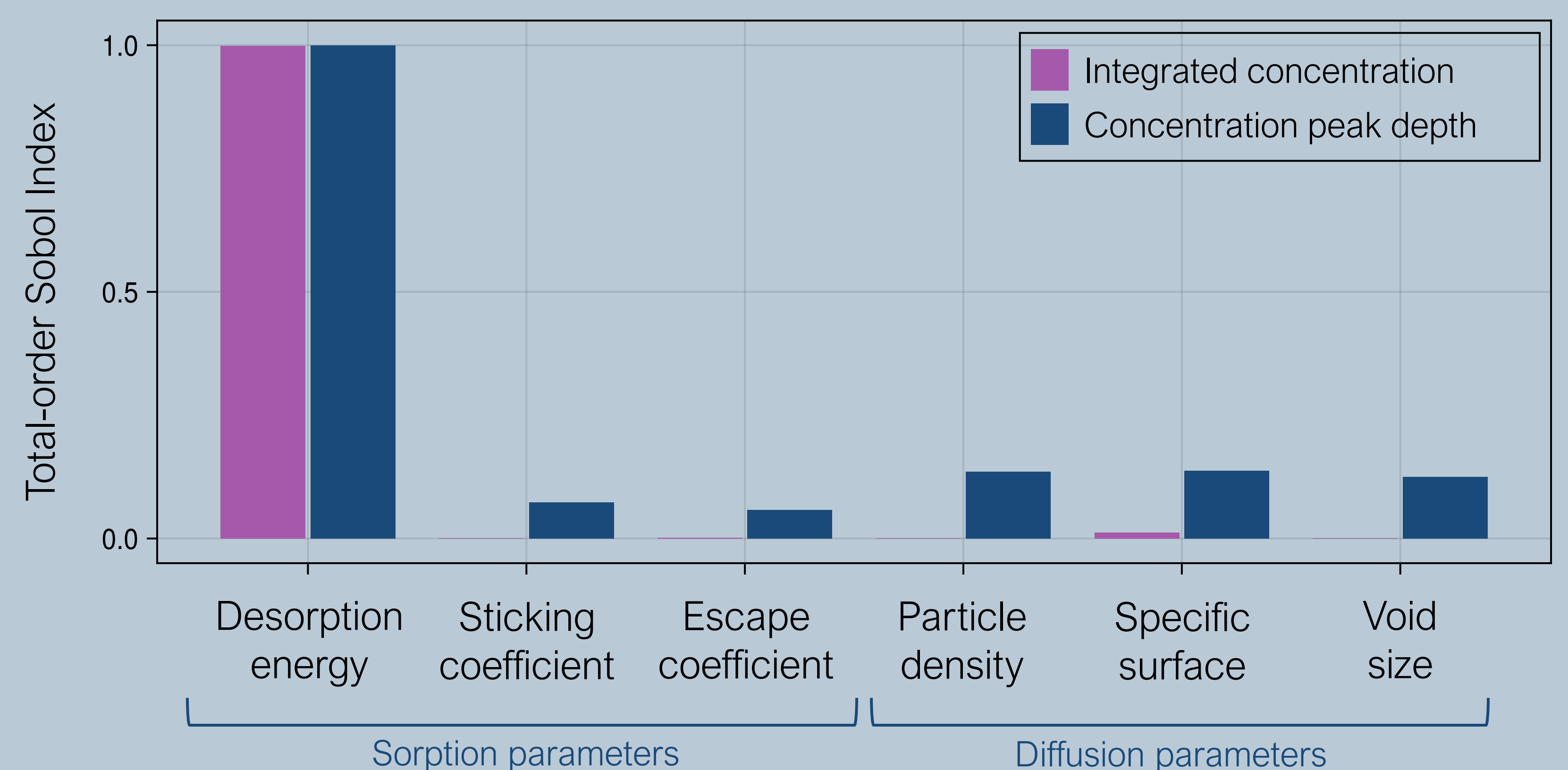
Similar to previous studies [2, 3], we observed a thermal pumping effect that accumulates water at a specific depth. After one lunar day, this effect can already be observed. Beyond that, the peak slowly drifts to lower depths.

The desorption energy (E_d) is needed to calculate the b parameter of (Eq. 2). We can see in the upper figure how its value greatly affects the resulting adsorption profile. This profile can be described by the **integrated concentration** and the **concentration peak depth**, the two target variables that we chose for our sensitivity analysis.

Sensitivity analysis

Parameter	Value range	Ref
Desorption energy	[0.45, 1.2] eV	[5]
Sticking error coefficient	[0.85, 1.15]	[6]
Escape coefficient	[0.5, 1.0]	-
Particle density	[2300, 3200] kg/m³	[4]
Specific surface	[20, 780] m²/kg	[4]
Mean void size	[5, 70] μm	[2]

To compare the effects of the different parameter uncertainties on the adsorbed profile, we computed the parameters' Sobol indices, with larger values indicating greater influence on the output's variance. To do so, we ran 10,000 simulations of one lunar day, starting from a dry sample. We assumed parameters to be uniformly distributed over the uncertainty ranges shown in the left table. The obtained Sobol indices are shown in the bottom bar plot.



Desorption energy is the most impactful parameter for water migration in lunar regolith

At 80° latitude, the thermal pumping effect can be observed after one lunar day of simulation. The parameters associated with the sorption process have a stronger influence on the water concentration profile than those associated with gas diffusivity, with the most impactful being the desorption energy. This highlights the need for a better understanding of this parameter and its variation with coverage.

[1] Hurlley, D. M. et al. (2015). An analytic function of lunar surface temperature for exospheric modeling. *Icarus*, 255, 159-163.
 [2] Reiss, P. et al. (2021). Dynamics of subsurface migration of water on the Moon. *Journal of Geophysical Research: Planets*, 126(5), e2020JE006742.
 [3] Schorghofer, N., & Aharonson, O. (2014). *The lunar thermal ice pump*. *The Astrophysical Journal*, 788(2), 169.
 [4] Carrier, W. D. et al. (1991). *Physical properties of the lunar surface*. In *Lunar Sourcebook* (Heiken, G. H. et al.), pp. 475-594, Cambridge University Press.
 [5] Poston, M. J. et al. (2013). *Water interactions with micronized lunar surrogates JSC-1A and albite under ultra-high vacuum with application to lunar observations*. *Journal of Geophysical Research: Planets*, 118(1), 105-115.
 [6] Haynes, D. R. et al. (1992). *Condensation and evaporation of water on ice surfaces*. *The Journal of Physical Chemistry*, 96(21), 8502-8509.