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Checking the post-processing of adsorption simulations: Henry coefficients, isosteric heats, IAST and stationarity tests validated against RASPA3

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Abstract

Grand canonical Monte Carlo (GCMC) isotherms are condensed into a few reported quantities: a Henry coefficient, an isosteric heat, fitted isotherm parameters, predicted mixture selectivities and a statement that each run was equilibrated. The post-processing code behind them is rarely tested. AdsorpQC is an open-source Python package that reads RASPA3 output and performs these steps; we validated each against known answers, using methane and carbon dioxide, pure and mixed, in silicalite-1 at 300 K. Henry coefficients extrapolated from the isotherms agreed with Widom insertion within 0.2%. The previous release, which fitted a line through the origin, was 4.5% low for methane and 22% low for carbon dioxide. The ideal adsorbed solution theory (IAST) solver agreed with pyIAST to $\mathbf{3 \times 10^{-12}}$ in relative terms, and it predicted the mixture GCMC loadings within 1.5% up to 100 kPa and within 4% at 1 MPa. The previous release reported a Henry-limit ratio under the name IAST: it missed the rise of the $\mathbf{CO_2/CH_4}$ selectivity from 5.9 to 6.9 at 1 MPa, and it was up to 7.7 times too high for model isotherms with unequal capacities. A stationarity test that compares the drift with its autocorrelation-corrected noise raised false alarms for 0.5% of stationary low-loading series, against 79% for the previous test. A small-sample information criterion selected the true isotherm model more reliably than AIC for two-parameter models but needed about ten points for four-parameter ones.

Keywords: grand canonical Monte Carlo, Henry coefficient, isosteric heat, ideal adsorbed solution theory, reproducibility, zeolite

1 Introduction

A grand canonical Monte Carlo (GCMC) study of adsorption usually ends with a handful of numbers. They include the Henry coefficient, the isosteric heat of adsorption, fitted isotherm parameters, selectivities for gas mixtures predicted by

the ideal adsorbed solution theory (IAST) (Myers and Prausnitz 1965; Walton and Sholl 2015), and a statement that each run was equilibrated. These numbers are what readers compare between materials, force fields and codes, and they are produced by post-processing scripts that are rarely published or tested. Experimental adsorption data show how much isotherms of nominally identical materials can scatter (Park et al. 2017). The simulation side carries its own sources of error, which are easier to control but also easier to overlook (Sturluson et al. 2019).

Each step has a known correct answer. A Henry coefficient extrapolated from an isotherm must agree with the Widom insertion estimate from the same force field (Widom 1963). An isosteric heat computed from particle–energy fluctuations must agree with the value that the simulation code accumulates over all cycles (Vlugt et al. 2008). IAST solutions can be checked against an established implementation (Simon et al. 2016) and, for the question of whether IAST applies at all, against mixture simulations (Walton and Sholl 2015; Gharagheizi and Sholl 2021). A stationarity test can be checked on series whose drift is known. Isotherm model selection can be checked on data generated by a known model (Akaike 1974; Hurvich and Tsai 1989).

AdsorpQC is an open-source Python package that reads RASPA3 output (Ran et al. 2024) and performs these steps. This article documents what it computes and tests every step against a known answer: real RASPA3 simulations of CH_4 and CO_2, pure and in binary mixtures, in silicalite-1, and simulated data where the truth is set by construction. The validation also changed the software. It exposed defects in version 1.0.0 that unit tests had not revealed, including a function that returned the Henry-limit selectivity under the name IAST. These defects are reported below and corrected in version 1.1.0.

2 Methods

An AI coding assistant (Claude, Anthropic) was used to write and test the code, to run the simulations and analyses and to draft the text; all numbers come from the deposited scripts, and the authors reviewed the code, the results and the text (see Statements and Declarations).

2.1 What AdsorpQC computes

Parsing. AdsorpQC reads the RASPA3 text output. It extracts the metadata, the block-averaged absolute and excess loadings of every component with their block errors, the enthalpy of adsorption, the Widom Henry coefficient, and the snapshot series of loading, number of molecules and potential energy written every `PrintEvery` cycles. A folder of runs at different pressures is assembled into an isotherm.

Henry coefficient. Writing the isotherm as $q/P = K_H - b\,q + \ldots$ (a first-order virial or Langmuir expansion), K_H is the intercept of a linear regression of q/P on q. The regression uses the lowest-pressure points with a loading below 15% of the largest one, and at least three points.

Isosteric heat. From the fluctuations of the number of molecules N and the total adsorbate energy U in the grand canonical ensemble (Vlugt et al. 2008),

$$q_{\mathrm{st}} = RT - \frac{\langle UN\rangle - \langle U\rangle\langle N\rangle}{\langle N^2\rangle - \langle N\rangle^2}, \tag{1}$$

with U in explicit units (RASPA writes U/k_B in K). When the code reports its own block-averaged enthalpy, AdsorpQC reports $q_{\mathrm{st}} = -\Delta H$ from it.

Isotherm models. Langmuir, dual-site Langmuir, Sips and Toth models (Foo and Hameed 2010) are fitted by non-linear least squares. The model with the lowest small-sample corrected Akaike criterion (Hurvich and Tsai 1989), $\mathrm{AIC_c} = n\ln(\mathrm{RSS}/n) + 2k + 2k(k+1)/(n-k-1)$ for n points and k parameters, is selected.

IAST. For a binary gas with mole fractions y_i at total pressure P, IAST (Myers and Prausnitz 1965) finds adsorbed-phase mole fractions x_i and pure-component pressures P_i^0 such that $Py_i = P_i^0 x_i$ and the reduced spreading pressures are equal,

$$\pi_1(P_1^0) = \pi_2(P_2^0), \qquad \pi_i(P^0) = \int_0^{P^0} \frac{q_i(p)}{p}\,\mathrm{d}p. \tag{2}$$

The total loading follows from $1/q_T = \sum_i x_i/q_i(P_i^0)$. AdsorpQC evaluates the integral in $\ln p$ with the fitted isotherm of each component and solves for x_1 by bracketing. The 95% interval of the selectivity $S_{12} = (x_1/x_2)/(y_1/y_2)$ comes from resampling the isotherm points of

each component and repeating the fits and the IAST solution (pairs bootstrap, 300 replicates). It therefore reflects the uncertainty of the fits, not the validity of IAST.

Stationarity. The production series is split into its first and last 20%. The difference of the two segment means is compared with its standard error, computed from the scatter and the statistical inefficiency g of the linearly detrended series; g uses the self-consistent window with $c = 6$ (Madras and Sokal 1988), as in automated equilibration detection for molecular simulation (Chodera 2016). A run is flagged `WARNING` when $z > 2$ and the difference exceeds 3% of the mean. It is flagged `FAIL` when $z > 3$ and the difference exceeds 8%. Version 1.0.0 used the percentage alone.

2.2 Simulations

All simulations used RASPA3 3.0.29 (Ran et al. 2024), the successor of RASPA (Dubbeldam et al. 2015), with a $2 \times 2 \times 2$ supercell of silicalite-1 (MFI) at 300 K. The force field is that of the RASPA3 examples for CO_2 and CH_4 in MFI. CO_2 and the framework follow García-Sánchez et al. (2009), with framework charges O $-1.025\,e$ and Si $+2.05\,e$ and Ewald summation, and CH_4 is the united-atom TraPPE model (Martin and Siepmann 1998). Lorentz–Berthelot mixing and a 12 Å cutoff were used. Pure-component isotherms were computed at seven pressures from 1 kPa to 1 MPa. The CH_4 runs had 5000 initialisation and 40 000 production cycles, and the CO_2 runs 5000 and 30 000. The Henry coefficient of each gas was computed by Widom insertion (Widom 1963). Binary CO_2/CH_4 mixtures were simulated at $y_{CO_2} = 0.5$ and 10 kPa, 100 kPa and 1 MPa, and at $y_{CO_2} = 0.1$ and 100 kPa. Uncertainties are the block errors reported by RASPA3 (Flyvbjerg and Petersen 1989).

2.3 Known-answer studies

The IAST solver was compared with pyIAST 1.4 (Simon et al. 2016) for three pairs of model isotherms, at three compositions and four pressures, using the exact model parameters in both codes. The pairs were Langmuir components with equal capacity, for which IAST reduces to extended Langmuir; Langmuir components with capacities 2 and 6 mol kg^{-1}; and dual-site Langmuir components.

The stationarity test was applied to 1000 synthetic series per case in two regimes:

- high loading, with an autoregressive process of coefficient 0.5 and a 5% coefficient of variation;
- low loading, with Poisson counts of mean 2, as at the lowest pressures of an isotherm.

The series had 40 or 400 samples. Stationary series were compared with series carrying a linear drift of 5%, 20% or 50% of the mean over the run.

Model selection was tested on isotherms with 7 or 12 pressures and 1% Gaussian noise, generated by a Langmuir model (capacity 3 mol kg^{-1}, $K = 1$ bar^{-1}) or a dual-site Langmuir model. There were 500 replicates per case.

3 Results and discussion

3.1 Henry coefficients

Widom insertion gave $K_H = 3.525 \times 10^{-5}$ (CO_2) and 6.108×10^{-6} mol kg^{-1} Pa^{-1} (CH_4), with statistical errors of 0.7%. The coefficients extrapolated by AdsorpQC from the isotherms agreed within 0.16% and 0.11% (Fig. 1b). Version 1.0.0 fitted a straight line through the origin to the four lowest pressures, whatever their curvature. It was 4.5% low for CH_4 (6 standard errors of the Widom value) and 22% low for CO_2 (33 standard errors). CO_2 is the more strongly adsorbed gas, and its isotherm already bends at 30 kPa (Fig. 1a). The size of this error therefore depends on the pressures chosen, which a reader cannot know.

3.2 Isosteric heats

The block-averaged enthalpies reported by RASPA3 gave q_{st} rising from 19.0 to 20.2 kJ mol^{-1} for CH_4 and from 26.9 to 30.3 kJ mol^{-1} for CO_2 between 1 kPa and 1 MPa (Table S1). Eq. (1) applied to only the 40 snapshots written during production reproduced these values within 2.4 kJ mol^{-1}, and within 0.3 kJ mol^{-1} at the pressures with the largest fluctuations. Version 1.0.0 applied the same formula to the loading in mol kg^{-1} instead of the number of molecules, which scales the covariance term. It also combined energies in K with RT in kJ mol^{-1}, and took the absolute value of the result, which hides sign errors. The snapshot estimate is noisy, so

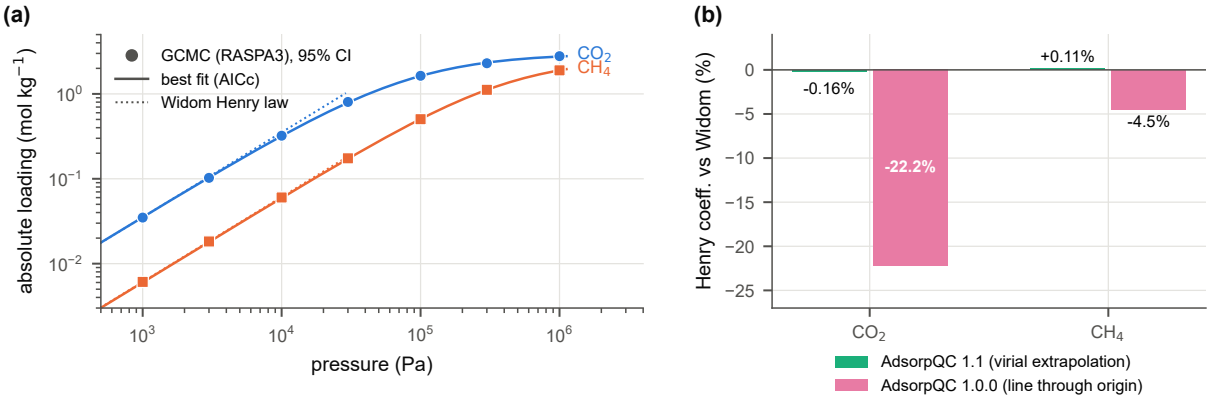


Fig. 1 Single-component isotherms of CO_2 and CH_4 in silicalite-1 at 300 K from RASPA3. (a) Absolute loadings with 95% intervals (smaller than the symbols), the model selected by AIC_c (Langmuir for CO_2, Toth for CH_4) and the Henry law from Widom insertion. (b) Henry coefficient obtained from the isotherm, relative to the Widom value, by AdsorpQC 1.1 and by the line through the origin of version 1.0.0.

the engine's value, accumulated over every cycle, should be reported when it is available.

3.3 IAST

For all 36 comparisons with pyIAST, the mixture loadings computed by AdsorpQC agreed to within 3×10^{-12} in relative terms. For equal capacities they reproduced the extended-Langmuir selectivity $K_1/K_2 = 10$ exactly. The function that version 1.0.0 called IAST returned $(q_{\mathrm{sat},1}K_1)/(q_{\mathrm{sat},2}K_2)$, the Henry-limit selectivity, whatever the pressure and composition. For Langmuir components with capacities of 2 and 6 mol kg^{-1}, the IAST selectivity falls from 8.8 at 0.01 bar to 1.15 at 10 bar, whereas version 1.0.0 returned 8.9 at every pressure, 7.7 times the IAST value at 10 bar.

Against the mixture simulations, IAST predicted the CO_2 loading within 0.9% in all four mixtures (Fig. 2a, Table 1). It predicted the CH_4 loading within 1.5% up to 100 kPa and within 3.8% at 1 MPa, where the GCMC error of the CH_4 loading is itself 4%. IAST is expected to hold well for this pair in silicalite-1, where the two gases compete for the same channels (Walton and Sholl 2015; Gharagheizi and Sholl 2021). The selectivity is the quantity most often reported. IAST reproduced its value within the GCMC uncertainty at every condition, including its rise from 5.9 to 6.9 at 1 MPa (Fig. 2b). The constant 5.70 of version 1.0.0 was 2.6–4.4% low at the lower pressures, 1.2–3.3 standard errors from the GCMC values, and 17% low at 1 MPa. For this nearly ideal pair with similar capacities, the Henry-limit shortcut is therefore only moderately wrong at low pressure. It is qualitatively wrong at high pressure and for components with different capacities. The bootstrap interval of the IAST selectivity widens from about ±7% at the lower pressures to 5.8–11.5 at 1 MPa, because the pure-component pressure of CH_4 then exceeds the highest simulated pressure and the prediction rests on the extrapolated isotherm. AdsorpQC reports this interval so that such extrapolations are visible.

3.4 Stationarity test

For stationary series, the 1.0.0 test failed 79% of the low-loading series of 40 samples and 50% of those of 400 samples (Fig. 3a). At low loading, Poisson fluctuations alone move the first and last 20% of a run apart by more than 8% of the mean. On the fourteen single-component RASPA3 runs of this work, the 1.0.0 test failed eleven: five of the seven CH_4 runs and six of the seven CO_2 runs. The 1.1 test failed 0–0.9% of stationary series in every regime and none of the RASPA3 runs. It flagged all fourteen with a `WARNING`, because their 45 snapshots give fewer than 50 effective samples, not because of drift. It detected a 20% drift at high loading in 90% of runs of 40 samples and in all runs of 400 samples. At low loading a drift of that size was hardly detectable (0.4% and 5% of runs failed for 40 and 400 samples) because it is small compared with the Poisson noise. The 1.0.0 test failed such runs more often, but it failed stationary runs almost as often, so its alarms did not distinguish drift from noise.

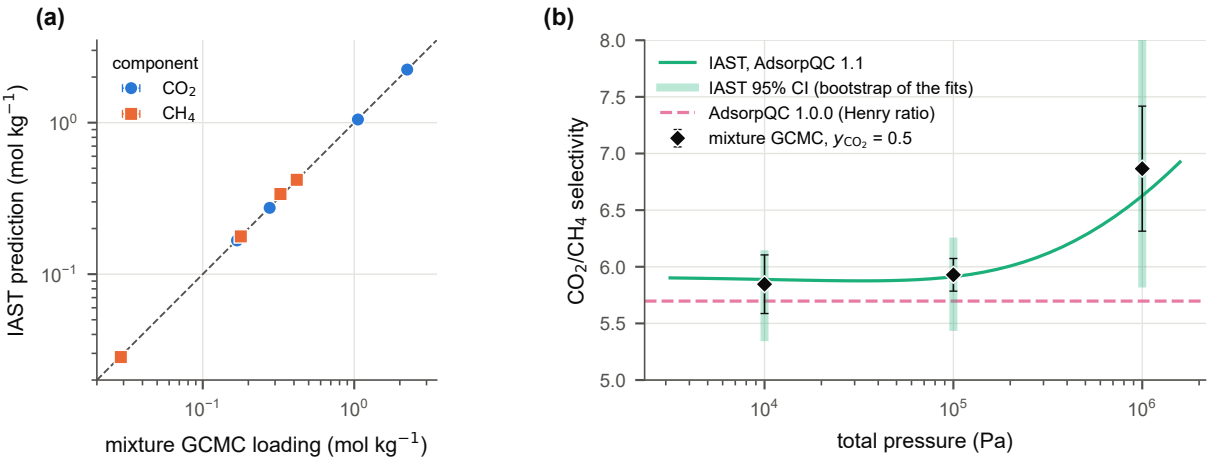


Fig. 2 IAST against binary-mixture GCMC for CO_2/CH_4 in silicalite-1 at 300 K. (a) Component loadings predicted by IAST from the single-component isotherms against the mixture simulations (four mixtures; error bars are 95% intervals of the GCMC loadings). (b) CO_2/CH_4 selectivity at $y_{CO_2} = 0.5$: mixture GCMC, IAST with its bootstrap interval (shaded bars; the interval at 1 MPa extends to 11.5), and the constant value of version 1.0.0.

Table 1 Binary CO_2/CH_4 mixtures in silicalite-1 at 300 K: loadings from mixture GCMC (block error in the last digits in parentheses) and from IAST, and CO_2/CH_4 selectivity from GCMC, IAST (with its 95% bootstrap interval) and AdsorpQC 1.0.0.

y_{CO_2}	P (kPa)	q_{CO_2} (mol kg^{-1})		q_{CH_4} (mol kg^{-1})		selectivity CO_2/CH_4		
		GCMC	IAST	GCMC	IAST	GCMC	IAST [95% CI]	1.0.0
0.1	100	0.276(3)	0.274	0.4175(46)	0.4196	5.96(9)	5.88 [5.37, 6.14]	5.70
0.5	10	0.168(3)	0.167	0.0288(4)	0.0284	5.85(13)	5.89 [5.34, 6.15]	5.70
0.5	100	1.058(8)	1.050	0.1784(18)	0.1775	5.93(7)	5.91 [5.43, 6.26]	5.70
0.5	1000	2.237(22)	2.241	0.3257(130)	0.3382	6.87(28)	6.63 [5.82, 11.48]	5.70

3.5 Model selection

With seven points, AIC_c selected the true model for 91% of Langmuir-generated isotherms, against 59% for AIC, which often preferred three- or four-parameter models (Fig. 3b). For dual-site Langmuir data the ranking reversed. AIC_c selected the true four-parameter model in only 31% of cases and preferred the three-parameter Toth model, whereas AIC selected it in 91%. With twelve points both criteria selected the dual-site model in about 90% of cases. AdsorpQC uses AIC_c because an over-fitted isotherm extrapolates badly, which matters for IAST. Four-parameter models, however, need about ten or more points to be identified.

3.6 Defects of the previous release

Validation against real output exposed several defects of version 1.0.0 that its unit tests, written on hand-made inputs, had not revealed:

1. The parser returned no loading, no cycle counts and a default pressure for RASPA3 files.
2. The command line discarded the loading, the Henry coefficient and the isosteric heat.
3. The Henry coefficient was biased low.
4. The isosteric heat used the wrong variable and mixed units.
5. The function named IAST did not solve IAST.
6. The stationarity test ignored noise.

All are corrected in version 1.1.0 and covered by tests on the RASPA3 outputs used here.

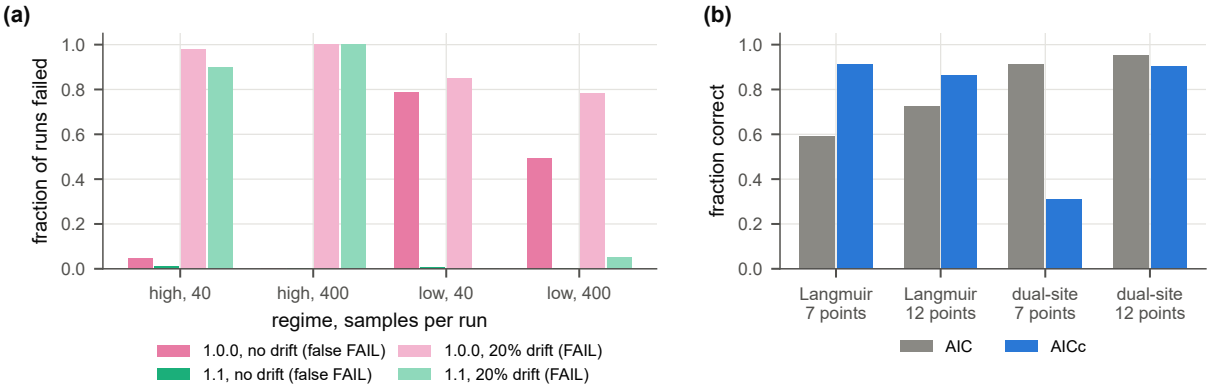


Fig. 3 Known-answer studies. (a) Fraction of synthetic GCMC loading series failed by the stationarity test of versions 1.0.0 and 1.1, for stationary series and for series with a 20% drift, at high loading (autoregressive, 5% coefficient of variation) and low loading (Poisson counts, mean 2), with 40 or 400 samples (1000 series per bar). (b) Fraction of simulated isotherms for which AIC and AIC_c selected the generating model (500 isotherms per bar).

4 Limitations and recommendations

The validation uses one framework, two small non-polar or weakly polar gases and one temperature. More strongly interacting systems, such as water or CO_2 in frameworks with open metal sites, will stress the isotherm fits and IAST more, and IAST may fail there for physical reasons (Walton and Sholl 2015; Gharagheizi and Sholl 2021). The comparison with mixture GCMC tests the IAST implementation together with the ideal-solution assumption; the comparison with pyIAST tests the implementation alone. The stationarity test compares only the first and last parts of a run and will miss slow oscillations. The isosteric heat from snapshots depends on the print frequency. The model-selection study uses independent Gaussian noise, whereas GCMC errors grow with loading.

From these results we recommend the following:

1. Report Henry coefficients from Widom insertion, or check isotherm extrapolations against it.
2. Take isosteric heats from the engine's block averages over all cycles.
3. Report IAST selectivities together with the pressure range of the pure-component isotherms, and check them against at least one mixture simulation.
4. Judge stationarity against the statistical noise of the run, not against a fixed percentage.
5. Fit four-parameter isotherm models only to ten or more points.

5 Conclusions

AdsorpQC 1.1 reads RASPA3 output and computes Henry coefficients, isosteric heats, isotherm fits, IAST predictions and stationarity tests that agree with independent answers: Widom insertion, the engine's own averages, pyIAST and mixture GCMC. The validation exposed errors in the previous release of up to 22% in Henry coefficients and 17% in selectivities for a benign system, and larger ones for model isotherms. It also exposed false stationarity alarms for most low-loading runs. Post-processing code deserves the same testing against known answers as the simulations themselves, and the scripts and outputs deposited with AdsorpQC allow each of these checks to be repeated for other systems.

Supplementary information. The Supplementary Information contains the single-component loadings and isosteric heats (Table S1), the comparison with pyIAST (Table S2) and the full results of the known-answer studies (Tables S3 and S4).

Statements and Declarations

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Competing interests. The authors declare no competing interests.

Ethics approval and consent to participate. Not applicable: the study uses no human or animal subjects and no personal data.

Consent for publication. Not applicable.

Data availability. The RASPA3 input and output files, the analysis scripts and all results are available at https://github.com/sircalch/adsorpqc (directories `validation/` and, for the pure-methane RASPA3 runs, `tests/data/raspa3_mfi_ch4/`) and archived on Zenodo (version 1.1.0, 10.5281/zenodo.23072031).

Materials availability. Not applicable.

Code availability. AdsorpQC is open source (MIT licence) at https://github.com/sircalch/adsorpqc.

Author contributions. A. Monreal-Hernández: conceptualization, methodology, software, validation, formal analysis, investigation, data curation, visualization, writing – original draft, writing – review and editing. S. L. Franco Amaya: validation, writing – review and editing. C. I. Martínez Osorio: supervision, writing – review and editing.

Use of AI tools. An AI coding assistant (Claude, Anthropic) was used to write and test code, run the simulations and analyses, and draft the text. All numbers were produced by the deposited scripts. The authors reviewed the code, the results and the text, and take full responsibility for the content.

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