Supplementary material for: An Open-Source IDAES Framework for Simulating Inductively Heated Adsorption Processes

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Abstract:

Isotherm data for CO2 and N2 adsorption for Fe3O4@HKUST1 (MOF) and Mass and Energy balance equations for Magnetic Inductive Swing Adsorption system.

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Supplementary material for: An Open-Source IDAES Framework for Simulating Inductively Heated Adsorption Processes

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ADSORPTION ISOTHERM DATA

The isotherm data for both carbon dioxide and nitrogen were extracted from Bellusci *et al.* [2,4] using WebPlotDigitizer, across 298 - 403K and 0.01 - 100kPa. The extracted raw data are provided in Tables S1-S2. These served as the training dataset for pyAPEP [5] to determine binary Sips parameters via nonlinear least square minimization (`scipy.optimize.curve_fit`).

Table S1. Carbon Dioxide Isotherm data for Fe_3O_4@HKUST-1

Carbon Dioxide Isotherm data - Fe_3O_4@HKUST-1							
Temp_273K		Temp_298K		Temp_308K		Temp_403K	
Pressure (kPa)	Gas_uptake (mmol/g)	Pressure (kPa)	Gas_uptake (mmol/g)	Pressure (kPa)	Gas_uptake (mmol/g)	Pressure (kPa)	Gas_uptake (mmol/g)
0.17	0.01	1.18	0.05	0.84	0.00	0.67	0.00
0.84	0.13	2.86	0.13	2.52	0.06	3.36	0.02
1.85	0.21	3.87	0.16	4.37	0.10	5.71	0.02
2.86	0.30	5.04	0.21	5.88	0.16	7.39	0.02
3.87	0.40	6.39	0.28	7.56	0.21	9.08	0.02
5.38	0.54	7.90	0.34	8.74	0.26	10.76	0.05
6.89	0.67	9.24	0.38	10.59	0.35	20.34	0.06
7.90	0.75	10.59	0.44	20.50	0.68	30.42	0.11
8.74	0.83	19.83	0.77	30.08	0.85	40.50	0.12
10.08	0.93	30.25	1.13	40.50	1.10	50.42	0.16
20.67	1.67	40.17	1.43	50.76	1.34	60.67	0.17
29.75	2.25	50.25	1.74	60.84	1.58	70.76	0.21
40.50	2.81	60.50	2.01	71.09	1.79	80.84	0.24
50.92	3.32	70.76	2.27	80.84	1.99	91.09	0.27
60.84	3.77	80.50	2.49	90.92	2.18	99.66	0.30
70.92	4.13	90.92	2.73	99.66	2.35		
80.84	4.45	99.66	2.93				
91.09	4.78						

99.50	5.03	

Table S2. Nitrogen Isotherm data for Fe_3O_4@HKUST-1

Nitrogen Isotherm data - Fe_3O_4HKUST-1					
Temp_273K		Temp_298K		Temp_308K	
Pressure (kPa)	Gas_uptake (mmol/g)	Pressure (kPa)	Gas_uptake (mmol/g)	Pressure (kPa)	Gas_uptake (mmol/g)
0.01	0.00	0.35	0.00	0.71	0.00
1.95	0.01	2.83	0.01	3.36	0.01
4.60	0.02	6.02	0.01	5.66	0.01
6.90	0.02	9.03	0.02	8.14	0.01
9.20	0.03	10.80	0.02	10.62	0.02
10.80	0.04	20.00	0.04	20.35	0.04
20.18	0.07	30.44	0.06	30.44	0.06
30.09	0.11	40.35	0.09	40.71	0.07
40.18	0.14	50.27	0.10	50.62	0.09
50.27	0.18	60.35	0.13	60.53	0.11
60.35	0.21	70.62	0.15	71.15	0.13
70.62	0.24	80.88	0.17	81.24	0.15
80.88	0.28	90.97	0.19	91.15	0.16
90.80	0.31	99.47	0.20	99.47	0.18
99.47	0.33				

CONSERVATION EQUATIONS DERIVATIONS

Gas Phase Mass Balance

Derivation from First Principles

Consider a differential control volume of length Δx at position x. For species i in the gas phase:

$$Accum. = In - Out - Consumption\ by\ Adsorption \quad (1)$$

Rate of change of moles in the void volume:

$$Accumulation = \frac{\partial(A_b \cdot \varepsilon_b \cdot \Delta x \cdot \rho_{mol} \cdot y_i)}{\partial t} \quad (2)$$

Convective inflow at x:

$$In = F_{mol,i}(x,t) = u \cdot A_b \cdot \rho_{mol} \cdot y_i|_x \quad (3)$$

Convective Outflow at $x + \Delta x$:

$$Out = F_{mol,i}(x + \Delta x, t) = u \cdot A_b \cdot \rho_{mol} \cdot y_i|_{x+\Delta x} \quad (4)$$

Consumption by Adsorption:

$$Consumption = A_s \cdot \Delta x \cdot \rho_p \cdot r_{ads,i} \quad (5)$$

where $A_{solid} = A_{bed}(1 - \varepsilon_b)$. Combining equations (1) to (5), we get the following gas phase species balance equation:

$$\frac{\partial(A_b \cdot \varepsilon_b \cdot \Delta x \cdot \rho_{mol} \cdot y_i)}{\partial t} = F_{mol,i}(x,t) - F_{mol,i}(x + \Delta x, t) - A_s \cdot \Delta x \cdot \rho_p \cdot r_{ads,i} \quad (6)$$

Taking the limit as $\Delta x \to 0$, dividing by Δx and taking the limit, final gas phase mass balance becomes:

$$A_b \cdot \varepsilon_b \frac{\partial(\rho_{mol} \cdot y_i)}{\partial t} = -\frac{\partial(F_{mol,i})}{\partial x} - A_s \cdot \rho_p \cdot r_{ads,i} \quad (7)$$

Gas Phase Energy Balance

Derivation from First Principles

For the gas phase in differential control volume of length Δx:

$$\frac{\partial}{\partial t}(H_g) = H_{in} - H_{out} + Q_{\text{in}} \quad (8)$$

Accumulation:

$$H_g = A_b \cdot \varepsilon_b \cdot \Delta x \cdot \rho_{mol} \cdot h_{mol,g} \quad (9)$$

Convective enthalpy Flow rate:

$$\Delta H_g = u \cdot A_b \cdot \rho_{mol} \cdot h_{mol,g} \quad (10)$$

Gas-Solid Heat Transfer: The gas-solid heat transfer rate per unit length is:

$$Q_{in/out} = -h_{gs} \cdot \frac{6}{d_p} \cdot A_s \cdot (T_g - T_s) \quad (11)$$

When $T_s > T_g$, heat flows FROM solid TO gas, so gas gains energy.
Final Gas Phase energy balance:

$$A_b \cdot \varepsilon_b \cdot \frac{\partial}{\partial t}(\rho_{mol} \cdot h_{mol,g}) = -\frac{\partial}{\partial x} H_g - \frac{6h_{gs}}{d_p} \cdot A_s \cdot (T_g - T_s) \quad (12)$$

Sign Convention: MINUS sign means gas loses heat to solid when $T_g > T_s$.

Pure Component Molar Enthalpy:

$$h_i(T) = \Delta h_{f,i} + \int_{T_{ref}}^{T} c_{p,i}(T) \cdot dT \quad (13)$$

Where:

$\Delta h_{f,i}$ = standard heat of formation at T_{ref} = 298.15 K (J/mol)

$c_{p,i}(T)$ = temperature-dependent molar heat capacity [J/mol/K].

The heats of formation for CO_2 and N_2 are $\Delta h_{f,CO_2}$ = −393, 509 J/mol and $\Delta h_{f,N_2}$ = 0 J/mol (reference state), respectively. The correlations used to compute the molar enthalpy are the Shomate equations (NIST webbook: https://webbook.nist.gov/

Momentum Balance (Ergun Equation)

The momentum balance is given by Ergun equation which is a combination of viscous and inertial pressure drop term given as follows:

$$-\frac{\partial P_g}{\partial x} = \frac{150 \cdot \mu_g \cdot (1-\varepsilon_b)^2}{\varepsilon_b^3 \cdot d_p^2} \cdot u + \frac{1.75 \cdot \rho_g \cdot (1-\varepsilon_b)}{\varepsilon_b^3 \cdot d_p} \cdot u^2 \quad (14)$$

Solid Phase Mass Balance

Derivation from First Principles

Here, conservation is applied to the Solid Phase. For species i adsorbed on solid:

$$Accumulation\ in\ solid = Transfer\ from\ gas \quad (15)$$

Total moles adsorbed by solid particles:

$$N_{i,ads} = A_{solid} \cdot \rho_p \cdot \frac{\partial q_i}{\partial t} \quad (16)$$

Where q_i = adsorbed loading of species i. The transfer rate from gas equals:

$$Transfer\ rate = A_s \cdot \rho_p \cdot r_{ads,i} \quad (17)$$

The final solid species balance is given by combining equations:

$$A_s \cdot \rho_p \cdot \frac{\partial q_i}{\partial t} = A_s \cdot \rho_p \cdot r_{ads,i} \quad (18)$$

The LHS is the rate of change of adsorbed amount per unit mass adsorbent. The RHS is the adsorption rate from Linear Driving Force (LDF) kinetics.

Final Solid Phase Species Balance

$$\frac{\partial q_i}{\partial t} = r_{ads,i} \quad (19)$$

Solid Phase Energy Balance

Derivation from First Principles

$$\frac{\partial H_s}{\partial t} = Q_{gs} + Q_{ads} + Q_{induction} - Q_{wall\ loss} \quad (20)$$

Accumulation:

$$\frac{\partial H_s}{\partial t} = A_s \cdot \rho_p \cdot c_{p,s} \frac{\partial T_s}{\partial t} \quad (21)$$

Gas-Solid Convection:

From the solid perspective, when $T_g > T_s$, solid gains heat from gas:

$$Q_{gs} = h_{gs} \cdot \frac{6}{d_p} \cdot A_s \cdot (T_g - T_s) \quad (22)$$

where h_{gs} is the heat transfer coefficient calculated through Nusselt number.

Heat of Adsorption:

Adsorption is exothermic: $\Delta H_{ads,i} < 0$. When CO_2 adsorbs ($r_{ads,i} > 0$), chemical potential energy converts to thermal energy as follows:

$$Q_{ads} = -\sum_i A_s \cdot \rho_p \cdot r_{ads,i} \cdot \Delta H_{ads,i} \quad (23)$$

Since $\Delta H_{ads,i} < 0$ and $r_{ads,i} > 0$ during adsorption:

$$-r_{ads,i} \cdot \Delta H_{ads,i} = -(positive) \cdot (negative) = positive \quad (24)$$

So, heat is released (exothermic)and this increases T_s.

Inductive Heating:

The duty of direct volumetric heating of magnetic particles is:

$$\dot{Q}_{ind} = Q_{ind} \cdot A_s \quad (25)$$

where:

$$Q_{ind} = L(B) \cdot \rho_p \quad (26)$$

The Specific Power Loss or Specific Adsorption Rate follows quadratic field dependence:

$$L(B) = L_{ref} \left(\frac{B}{B_{ref}}\right)^2 \quad (27)$$

Wall Heat Loss:

The heat loss through the reactor wall to the ambient surroundings is:

$$Q_{wall} = h_{wall} \cdot \pi \cdot d_{bed} \cdot (T_s - T_{ambient}) \quad (28)$$

Final Solid Phase Energy Balance:

$$A_s \cdot \rho_p \cdot c_{p,s} \cdot \frac{\partial T_s}{\partial t} = \frac{6h_{gs}}{d_p} \cdot A_s \cdot (T_g - T_s) - A_s \cdot \rho_p \sum_i [\Delta H_{ads,i} \cdot r_{ads,i}] + Q_{ind} \cdot A_s - Q_{wall} \quad (29)$$

Heat Transfer Coefficients

Reynolds Number

$$Re = \frac{u_g \rho_g d_p}{\mu_g} \quad (30)$$

Prandtl Number

$$\mathrm{Pr} = \frac{c_{p,g} \mu_g}{k_g} \quad (31)$$

Nusselt Number

$$Nu_p = 2 + 1.1\, Pr^{1/3} Re^{0.6} \quad (32)$$

Heat Transfer Coefficient

$$h_{gs} = \frac{Nu_p k_g}{d_p} \quad (33)$$

NOMENCLATURE

Greek Symbols

Symbol	Description	Units
$\Delta H_{ads,i}$	Heat of adsorption for species i	J/mol
$\Delta H_{b,i}$	Isosteric heat of adsorption for species i	J/mol
$\Delta h_{f,i}$	Standard heat of formation at T_{ref}	J/mol
Δx	Differential length element	m
ε_b	Bed porosity (void fraction)	$-$
μ_g	Gas viscosity	$Pa \cdot s$
ρ_g	Gas mass density	$kg/m\text{^}3$
ρ_{mol}	Gas molar density	$mol/m\text{^}3$
ρ_p	Particle density	$kg/m\text{^}3$

Latin Symbols

Symbol	Description	Units
A_b	Bed cross-sectional area	m^2
A_s	Solid cross-sectional area (= $(1-\varepsilon_b)A_b$)	m^2
B	Applied magnetic field amplitude	mT
B_{ref}	Reference magnetic field amplitude	mT
$b_i(T)$	Temperature-dependent affinity parameter	Pa^{-1}
$b_{ref,i}$	Affinity parameter at T_{ref}	Pa^{-1}
c_i	Heterogeneity parameter	$-$
$c_{p,s}$	Solid heat capacity	$J/(kg \cdot K)$
$c_{p,i}$	Molar heat capacity of component i	$J/(mol \cdot K)$
d_b	Bed diameter	m
d_p	Particle diameter	m
f	Magnetic field frequency	kHz
$F_{mol,i}$	Molar flow rate of species i	mol/s
$h_{mol,g}$	Gas molar specific enthalpy	J/mol
h_{gs}	Gas-solid heat transfer coefficient	$W/(m^2 \cdot K)$
h_i	Molar enthalpy of component i	J/mol
H_{wall}	Wall heat transfer coefficient	$W/(m^2 \cdot K)$
H_g	Gas enthalpy flow rate	W
H_s	Solid enthalpy	J
k_g	Gas thermal conductivity	$W/(m \cdot K)$
k_i	LDF Mass transfer coefficient for species i	s^{-1}
L	Bed length	m
$L(B)$	SAR as function of magnetic field	W/g
L_{ref}	Reference SAR at B_{ref}	W/g
$n_{\infty,i}$	Saturation capacity for species i	mol/kg
P_g	Gas absolute pressure	Pa
P_i	Partial pressure of species i	Pa, kPa
q_i	Adsorbed loading of species i	mol/kg
$q_{eq,i}$	Equilibrium loading of species i	mol/kg
Q_{ads}	Heat release from adsorption	W
Q_{gs}	Gas-solid heat transfer rate	W
Q_{ind}	Volumetric inductive heating rate	W/m^3
Q_{wall}	Wall heat loss per unit length	W/m
$r_{ads,i}$	Adsorption rate of species i	$mol/(kg \cdot s)$
R	Universal gas constant	$J/(mol \cdot K)$
R^2	Coefficient of determination	$-$
$RMSE$	Root mean square error	mol/kg
t	Time	s
T_g	Gas temperature	K
T_s	Solid temperature	K
T_{ref}	Reference temperature (298 K)	K
$T_{ambient}$	Ambient temperature	K
u	Superficial velocity	m/s
x	Axial position coordinate	m
y_i	Mole fraction of species i	$-$

Subscripts and Superscripts

Symbol	Description
i	Component index (CO_2, N_2)
ads	Adsorption
amb	Ambient
b	Bed
eq	Equilibrium
exp	Experimental

g	Gas phase
gs	Gas-solid interface
in	Inlet
ind	Inductive heating
mol	Molar basis
out	Outlet
p	Particle
ref	Reference condition
s	Solid phase
$wall$	Reactor wall

Abbreviations

Abbreviation	Description
CO_2	Carbon dioxide
DAE	Differential Algebraic Equation
HKUST-1	Hong Kong University of Science and Technology-1 ($Cu_3(BTC)_2$)
IDAES	Institute for the Design of Advanced Energy Systems
LDF	Linear Driving Force
MISA	Magnetic Inductive Swing Adsorption
MOF	Metal Organic Framework
N_2	Nitrogen
PDE	Partial Differential Equation
PSA	Pressure Swing Adsorption
pyAPEP	Python Adsorption Parameter Estimation Package
SAR	Specific Absorption Rate (also SPL - Specific Power Loss)
TSA	Temperature Swing Adsorption