Modeling and Simulation of Nitrogen Generation by Pressure Swing Adsorption for Power-to-Ammonia: Supplementary Material

Marcus J. Schytt[a], Lorenz T. Biegler[b], and John B. Jørgensen[a]*

[a] Technical University of Denmark, DTU Compute,
Kongens Lyngby, Capital Region, Denmark
[b] Carnegie Mellon University, Department of Chemical Engineering,
Pittsburgh, Pennsylvania, USA
* Corresponding Author: jbjo@dtu.dk.

January 2026

1 Adsorbent parameters

We study the kinetic separation of air $\mathcal{C} = \{\mathrm{N}_2, \mathrm{O}_2, \mathrm{Ar}\}$ over a bed of carbon molecular sieve (CMS) pellets. We consider the commercial Takeda 3A CMS adsorbent studied in [1, 3, 4]. Parameters describing the adsorbent are given in Table 1.

Table 1: Adsorbent parameters.

CMS-T3A		
Bed porosity, ε [–]	0.3	[1, 3, 4]
Particle diameter, d_p [m]	$5.66{\cdot}10^{-3}$	[4]
Particle density, ρ_p [kg/m^3]	900	[1, 3, 4]
Particle heat capacity, $c_{p,p}$ [MJ/(kg·K)]	$1.05{\cdot}10^{-3}$	[4]
Particle porosity, ε_p [–]	0.3	[3]

2 Adsorption rate parameters

2.1 Adsorption equilibria

Following [3], we consider the modified Langmuir (ML) isotherm

$$q^*_\alpha = q_{\max,\alpha} \frac{b_\alpha P_\alpha}{1 + \sum_{\beta \in \mathcal{C}} b_\beta P_\beta},$$

given $\alpha \in \mathcal{C}$. The necessary component parameters were estimated in [3] based on the data in [1, 2] provided at temperatures $T \in [293, 313]$ [K] across pressures $P \in [1, 15]$ [atm]. Originally, in [3], the saturation capacity is reported on a mass basis with units $q_\alpha^{\max}$. To get the saturation capacity on a volumetric basis, we multiply it by the particle density $q_\alpha^{\max} \to \rho_p q_\alpha^{\max}$. The Langmuir parameters were fit to temperature-dependent correlations

$$q_{\alpha,\max}(T) = k_{1,\alpha} - k_{2,\alpha} T, \tag{1}$$

$$b_\alpha(T) = k_{3,\alpha} \exp\left(\frac{k_{4,\alpha}}{T}\right), \tag{2}$$

$$n_\alpha(T) = k_{5,\alpha} - \frac{k_{6,\alpha}}{T}. \tag{3}$$

The component-wise parameters are reported (with original units) in Table 2. From the measured equilibrium capacities in [1, 2], the component-wise heat of adsorption ΔH can be experimentally computed from the Clausius-Clapeyron relation [1, 5]. We consider the averages reported in [3] seen in Table 3.

Table 2: Equilibrium isotherm parameters [3].

	N_2	O_2	Ar
k_1 [kmol/kg]	$1.13 \cdot 10^{-2}$	$5.817 \cdot 10^{-3}$	$9.556 \cdot 10^{-3}$
k_2 [kmol/(kg·K)]	$2.8 \cdot 10^{-5}$	$7.512 \cdot 10^{-6}$	$2.101 \cdot 10^{-5}$
k_3 [1/kPa]	$3.089 \cdot 10^{-4}$	$7.948 \cdot 10^{-6}$	$6.566 \cdot 10^{-5}$
k_4 [K]	359.7	1381	773.8

Table 3: Component-wise heat of adsorption [3].

	N_2	O_2	Ar
ΔH [MJ/kmol]	-13.39	-13.81	-14.23

2.2 Rate constants

Pressure-dependent models of the apparent time constants D_α / r_p^2 are introduced in [1] and fitted in [3], against the data in [2, 1]. We employ the supercritical-structural-Langmuir (SSL) model

$$\frac{D_\alpha}{r_p^2} = k_\alpha \sqrt{P_{r,\alpha}} \left(1 + b_\alpha P_\alpha\right)^2. \tag{4}$$

specified by the reduced pressure $P_{r,\alpha} = P_\alpha / P_{c,\alpha}$. The remaining parameters are specified in Table 4.

Table 4: Rate parameters [3, 6].

	N_2	O_2	Ar
k [1/s]	$9.0 \cdot 10^{-5}$	$2.4 \cdot 10^{-2}$	$4.7 \cdot 10^{-5}$
P_c [kPa]	3398	5043	4898

References

[1] Y. S. Bae and C. H. Lee, *Sorption kinetics of eight gases on a carbon molecular sieve at elevated pressure*, Carbon, 43 (2005), pp. 95–107.

[2] Y.-S. Bae, J.-H. Moon, H. Ahn, and C.-H. Lee, *Effects of adsorbate properties on adsorption mechanism in a carbon molecular sieve*, Korean Journal of Chemical Engineering, 21 (2004), pp. 712–720.

[3] J.-G. Jee, M.-B. Kim, and C.-H. Lee, *Pressure swing adsorption processes to purify oxygen using a carbon molecular sieve*, Chemical Engineering Science, 60 (2005), pp. 869–882.

[4] J.-G. Jee, S.-J. Lee, H.-M. Moon, and C.-H. Lee, *Adsorption Dynamics of Air on Zeolite 13X and CMS Beds for Separation and Purification*, Adsorption, 11 (2005), pp. 415–420.

[5] Y.-J. Park, S.-J. Lee, J.-H. Moon, D.-K. Choi, and C.-H. Lee, *Adsorption Equilibria of O2, N2, and Ar on Carbon Molecular Sieve and Zeolites 10X, 13X, and LiX*, Journal of Chemical & Engineering Data, 51 (2006), pp. 1001–1008.

[6] B. E. Poling, J. M. Prausnitz, and J. O'Connell, *The properties of gases and liquids*, McGraw-Hill Professional, 5th ed., 2000.