



Multidimensional numerical analysis of coupled heat and mass transfer for energy-efficient desiccant bed regeneration

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ARTICLE INFO

Keywords:

Thermal regeneration
Desiccant bed
Coupled heat and mass transfer
Radial transport
Energy optimization
Zeolite 13X

ABSTRACT

This work implements a multi-dimensional numerical scheme to capture the time-dependent thermal and moisture migration occurring inside zeolite 13X packed columns over cyclic sorption and desorption stages. By integrating implicitly coupled user-defined functions with linear driving force (LDF) kinetics and the Sips equilibrium isotherm, a two-dimensional axisymmetric computational fluid dynamics (CFD) model ensures stable numerical convergence for both capture and release steps. Unlike traditional one-dimensional formulations that overlook spatial variations, the present model effectively captures radial gradients in temperature, gas-phase concentration, and solid loading arising from external heat transfer and column wall thermal inertia. A comparison with the one-dimensional model showed that cross-sectional averaging underestimates the required regeneration time by 12.0–15.3% for 50% moisture removal and by 21.3–30.4% for 75% moisture removal. To avoid the inefficient tailing regime near equilibrium, a practical regeneration criterion of 90% moisture removal was adopted. The desorption driving force is significantly amplified by elevating the regeneration thermal input, which subsequently curtails the required purge-gas flow rate. In the high-efficiency regime where the mass-flow-rate ratio was below unity, increasing the regeneration temperature from 453K to 463K and 473K reduced the total regeneration power consumption by approximately 8% and 15%, respectively. The lowest power consumption was achieved at 473K. These results demonstrate the importance of multidimensional transport analysis for accurate regeneration prediction and energy-efficient desiccant bed operation.

1. Introduction

Temperature swing adsorption (TSA) processes play a vital role in gas purification, industrial dehumidification, and thermochemical energy storage systems where effective desiccant regeneration is paramount [1–3]. Due to its outstanding moisture affinity and superior capacity at low partial pressures, zeolite 13X is frequently selected as the working adsorbent. High-fidelity performance forecasting of these columns necessitates a comprehensive mathematical formulation that tightly couples multi-phase transport with intrinsic adsorption kinetics [4].

To minimize computational expense, conventional literature has predominantly relied on one-dimensional (1D) lumped representations [5–8]. While such simplified models capture the macro-scale axial movement of concentration and thermal waves, they fail to resolve localized multi-dimensional phenomena. In practical packed beds, cross-sectional distributions of velocity, temperature, and moisture are rarely uniform, as they are strongly modulated by external ambient cooling, non-isothermal flow profiles, and the heat capacity of the desiccant column itself. These multidimensional effects strongly

influence local adsorption equilibrium and mass transfer characteristics, highlighting the necessity of multidimensional computational fluid dynamics (CFD) analysis for accurate prediction of practical desiccant bed behavior [9–13].

Despite these advantages, implementing multidimensional CFD models for adsorption systems remains numerically challenging because adsorption kinetics are highly nonlinear and strongly coupled with heat and mass transport [14,15]. In commercial CFD solvers, adsorption kinetics are generally incorporated through User-Defined Functions (UDFs) as source terms in the governing equations [16]. When treated explicitly, these source terms frequently induce numerical instability and non-physical oscillations, particularly during the initial adsorption stage where the mass transfer driving force becomes large [17,18]. Therefore, stable implicit coupling strategies are required to ensure reliable transient simulations without excessively small time-step requirements [14,19,20].

Similar numerical challenges have also been reported in non-equilibrium phase-change and mixture-based heat and mass transfer problems, where latent heat release, finite-rate mass transfer, relaxation effects, and local thermodynamic imbalance produce strongly

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<https://doi.org/10.1016/j.icheatmasstransfer.2026.112062>

Nomenclature**Variables**

b	Isotherm affinity parameter [Pa^{-1}]
$C_{p,a}$	Specific heat capacity of adsorbed phase [$\text{J}/(\text{kg K})$]
$C_{p,g}$	Specific heat capacity of gas [$\text{J}/(\text{kg K})$]
$C_{p,s}$	Specific heat capacity of adsorbent [$\text{J}/(\text{kg K})$]
$C_{p,w}$	Specific heat capacity of wall [$\text{J}/(\text{kg K})$]
c	Molar concentration [mol/m^3]
D	Diffusivity [m^2/s]
d	Sips isotherm parameter [–]
d_p	Adsorbent particle diameter [m]
$e_{\max}$	Local relative error [–]
h_o	External heat transfer coefficient [$\text{W}/(\text{m}^2 \text{K})$]
ΔH	Isosteric heat of adsorption [J/mol]
$\mathbf{I}$	Identity matrix [–]
K	Permeability [m^2]
k_{LDF}	Linear driving force mass transfer coefficient [s^{-1}]
k_g	Thermal conductivity of gas [$\text{W}/(\text{m K})$]
k_w	Thermal conductivity of wall [$\text{W}/(\text{m K})$]
L	Column length [m]
M	Molecular weight [kg/mol]
$\dot{m}$	Mass flow rate [kg/s]
n	Isotherm exponent [–]
N_r	Number of radial nodes [–]
N_x	Number of axial nodes [–]
p	Pressure [Pa]
P_{heat}	Heating power [W]
P_{pump}	Pumping power [W]
P_s	Saturation pressure [Pa]
P_{total}	Total power [W]
q	Adsorbed amount [mol/kg]
q^*	Equilibrium adsorption capacity [mol/kg]
q_m	Maximum adsorption capacity [mol/kg]
Q_{vol}	Volumetric flow rate [m^3/s]
R	Universal gas constant [$\text{J}/(\text{mol K})$]
r_i	Inner radius of the column [m]
r_o	Outer radius of the column [m]
S	Source term [$\text{kg}/(\text{m}^3 \text{s})$]
T	Temperature [K]
T_{in}	Inlet temperature [K]
T_{∞}	Ambient temperature [K]
t	Time [s]
t_w	Wall thickness [m]
$\mathbf{u}$	Velocity [m/s]
u_c	Concentration wave velocity [m/s]
Y	Mass fraction [–]

Greek Symbols

ϵ	External void fraction [–]
κ_{eff}	Effective thermal conductivity [$\text{W}/(\text{m K})$]
μ	Gas viscosity [Pa s]
ρ_g	Gas density [kg/m^3]
ρ_s	Adsorbent density [kg/m^3]

$(\rho C_p)_{\text{eff}}$	Effective density and specific heat [$\text{J}/(\text{m}^3 \text{K})$]
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Subscripts

ads	Adsorption
eff	Effective
T	Total
v	Water vapor
z	Axial

Superscripts

T	Transpose
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coupled source terms. Recent studies on non-equilibrium condensation in moist-air and wet-steam flows have demonstrated the importance of robust numerical treatment for predicting coupled heat and mass transfer, thermodynamic losses, and energy-system performance [21,22]. Although the present study deals with moisture adsorption/desorption in a porous desiccant bed rather than condensation in transonic flows, these studies provide useful methodological context for the implicit treatment of nonlinear source terms adopted in this work.

In addition to numerical stability, the thermal regeneration stage represents the dominant energy consumption process in TSA systems [23–26]. Many previous studies have evaluated regeneration performance under the assumption of complete desorption. However, practical industrial systems generally operate under fixed cycle times to maintain continuous upstream and downstream processes [27,28]. Under such constraints, attempting complete moisture removal leads to excessive energy consumption because desorption progressively slows in the low-concentration regime, producing a severe tailing effect caused by the steep equilibrium isotherm slope. Consequently, regeneration performance should be evaluated based on realistic operational constraints and overall energy efficiency rather than complete desorption alone [29–31].

In this study, a multidimensional numerical framework based on a two-dimensional (2D) axisymmetric CFD model is developed to investigate coupled heat and mass transfer during adsorption and thermal regeneration in a zeolite 13X desiccant bed. The adsorption kinetics are implemented using implicitly coupled source terms incorporating the Linear Driving Force (LDF) model and the Sips isotherm, enabling stable transient simulations without non-physical concentration oscillations. The proposed model is applied to analyze radial heat and mass transfer characteristics, wall-induced thermal lag, and their influence on regeneration prediction, which are inherently neglected in conventional 1D approaches. To avoid the excessive energy penalty associated with the tailing region, a practical regeneration criterion based on 90% moisture removal under fixed-cycle operation is introduced. The total regeneration power consumption is evaluated by considering both pumping power and thermal heating power, and the trade-off between regeneration temperature and purge-gas flow rate is systematically analyzed to identify energy-efficient operating conditions [32–35].

The main contributions of this study are summarized as follows: (i) development of an implicitly coupled multidimensional CFD framework for zeolite 13X adsorption and regeneration, (ii) quantitative assessment of radial transport effects and the limitations of 1D modeling, and (iii) optimization of thermal regeneration conditions based on a practical fixed-cycle moisture-removal criterion.

2. Numerical analysis**2.1. Computational domain**

A 2D axisymmetric computational domain was employed to simulate the adsorption and thermal regeneration processes in a cylindrical

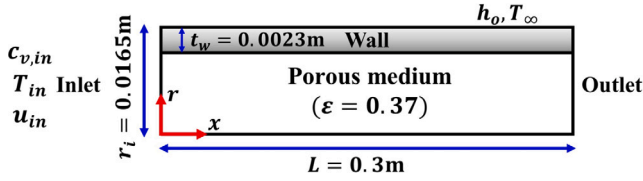


Fig. 1. Computational domain.

desiccant bed, as illustrated in Fig. 1. The desiccant bed consisted of a uniformly packed zeolite 13X porous bed with a porosity of 0.37. The axisymmetric formulation was adopted to capture radial heat and mass transfer characteristics while maintaining computational efficiency for long-term transient simulations.

The governing equations were numerically integrated via the commercial software ANSYS Fluent. Ideal gas behavior was assumed for the working fluid consisting of a nitrogen and water vapor mixture. Fluid flow throughout the porous bed was restricted to an unsteady, laminar regime. The inlet boundary was defined by prescribing the fluid velocity, temperature, and species fraction, while the downstream boundary condition utilized a fixed pressure outlet. Ambient heat dissipation through the column casing was incorporated via an external convective boundary layer. This modeling approach successfully captured the cross-sectional thermal fields and wall-induced thermal lag across both cyclic operations.

2.2. Governing equations

The adsorption and regeneration processes within the porous desiccant bed were modeled using a transient 2D axisymmetric CFD framework.

The physical system is governed by a fully coupled set of conservation laws comprising continuity, momentum equations for porous media, species transport, and energy balance equations. The transient migration of moisture is tracked via the gas-phase mass fraction. The governing equations are expressed as follows:

$$\frac{\partial \epsilon \rho_g}{\partial t} + \nabla \cdot (\epsilon \rho_g \mathbf{u}) + (1 - \epsilon) \frac{\partial q}{\partial t} M_v = 0 \quad (1)$$

$$\frac{\partial \epsilon \rho_g \mathbf{u}}{\partial t} + \nabla \cdot (\epsilon \rho_g \mathbf{u} \mathbf{u}) = -\epsilon \nabla p + \nabla \cdot \mu \left[\nabla \epsilon \mathbf{u} + (\nabla \epsilon \mathbf{u})^T - \frac{2}{3} (\nabla \cdot \epsilon \mathbf{u}) \mathbf{I} \right] + \epsilon \frac{\mu}{K} \mathbf{u} \quad (2)$$

$$\frac{\partial \epsilon \rho_g Y_v}{\partial t} + \nabla \cdot (\epsilon \rho_g \mathbf{u} Y_v) = \nabla \cdot (\rho_g \epsilon D \nabla Y_v) - (1 - \epsilon) \frac{\partial q}{\partial t} M_v \quad (3)$$

$$(\rho C_p)_{\text{eff}} \frac{\partial T}{\partial t} + \nabla \cdot (\epsilon \rho_g C_{p,g} \mathbf{u} T) = \nabla \cdot [\kappa_{\text{eff}} \nabla T] - (1 - \epsilon) \frac{\partial q}{\partial t} (\Delta H + RT) \quad (4)$$

where

$$(\rho C_p)_{\text{eff}} = \epsilon \rho_g C_{p,g} + (1 - \epsilon) \rho_s C_{p,s} \quad (5)$$

$$\kappa_{\text{eff}} = \epsilon k_g + (1 - \epsilon) k_s \quad (6)$$

Here, ϵ is the bed porosity, ρ_g is the gas density, $\mathbf{u}$ is the superficial velocity vector, Y is the vapor mass fraction, D is the vapor diffusivity, K is the permeability of the porous medium, and q is the adsorbed amount of water vapor. The source terms in the continuity, species, and energy equations account for adsorption and desorption occurring within the porous adsorbent. The effective thermal conductivity was used to represent heat conduction within the porous medium, while the adsorption heat source term was incorporated through the heat of adsorption ΔH . These governing equations were solved in a fully coupled manner to capture the transient interaction between flow, heat transfer, mass transport, and adsorption kinetics during both adsorption and regeneration processes.

2.3. Adsorption equilibrium and kinetics

The adsorption and desorption kinetics of water vapor within the zeolite 13X bed were described using the Linear Driving Force (LDF) model. The temporal evolution of the adsorbed amount q was calculated as

$$\frac{\partial q}{\partial t} = k_{\text{LDF}} (q^* - q) \quad (7)$$

where k_{LDF} is the effective mass transfer coefficient and q^* is the equilibrium adsorption capacity. This lumped parameter approach offers an elegant and computationally economical alternative to resolving detailed intra-pellet diffusion profiles by consolidating the total transport resistance into a single effective mass transfer coefficient [36–38].

The equilibrium adsorption capacity was determined using the modified Sips isotherm model [39]:

$$q^* = \rho_s \frac{q_m (b R T c_v)^n}{[1 + (b R T c_v)^n] \left(1 - \frac{R T c_v}{P_s}\right)^d} \quad (8)$$

where q_m is the maximum adsorption capacity, b , d , and n are empirical isotherm parameters, c_v is the vapor molar concentration, P_s is the saturation pressure, and ρ_s is the adsorbent density. The modified Sips model was adopted because it accurately represents the adsorption equilibrium behavior of zeolite 13X over a wide humidity range, including high relative humidity conditions [39].

The adsorption source terms used in the continuity, species, and energy equations were directly calculated from the adsorption rate $\frac{\partial q}{\partial t}$. The kinetic and equilibrium models were fully coupled with the CFD framework to capture the transient interaction between adsorption, heat transfer, and vapor transport during both adsorption and regeneration processes.

2.4. Numerical implementation

The adsorption source terms appearing in the continuity, species, and energy equations were implemented in ANSYS Fluent through User-Defined Functions (UDFs). Because the adsorption kinetics are strongly coupled with transient heat and mass transfer, explicit treatment of the source terms can lead to numerical instability and non-physical oscillations, particularly during the initial adsorption stage where the concentration gradient becomes large [9,14,15].

To improve numerical stability, the adsorption source term in the species transport equation was treated implicitly by linearizing the adsorption rate with respect to the vapor mass fraction. The water-vapor source term can be written as

$$S = -(1 - \epsilon) k_{\text{LDF}} (q^* - q) M_v \quad (9)$$

where q^* is the equilibrium adsorption capacity obtained from the Sips isotherm. Because the Sips isotherm introduces a nonlinear dependence of q^* on the local vapor molar concentration c_v , a local pseudo-Jacobian was introduced for numerical stabilization as

$$\frac{dS}{dY_v} = \frac{dS}{dc_v} \frac{dc_v}{dY_v} \approx \left[-(1 - \epsilon) M_v k_{\text{LDF}} \left(\frac{q^*}{c_v} \right) M_v (q^* - q) \right] \left[\frac{\rho_g}{M_v} \right]. \quad (10)$$

Here, the local molar concentration c_v is defined as

$$c_v = \frac{\rho_g Y_v}{M_v} \quad (11)$$

It should be emphasized that (q^*/c_v) in Eq. (10) is not intended to represent the exact analytical derivative of the Sips isotherm. Instead, it is introduced as a local linearization coefficient for the implicit source-term treatment in the CFD solver. The original adsorption source term, given by Eq. (9), is still evaluated from the LDF model and the Sips equilibrium isotherm at each time step. Thus, the pseudo-Jacobian does not replace or modify the physical adsorption kinetics.

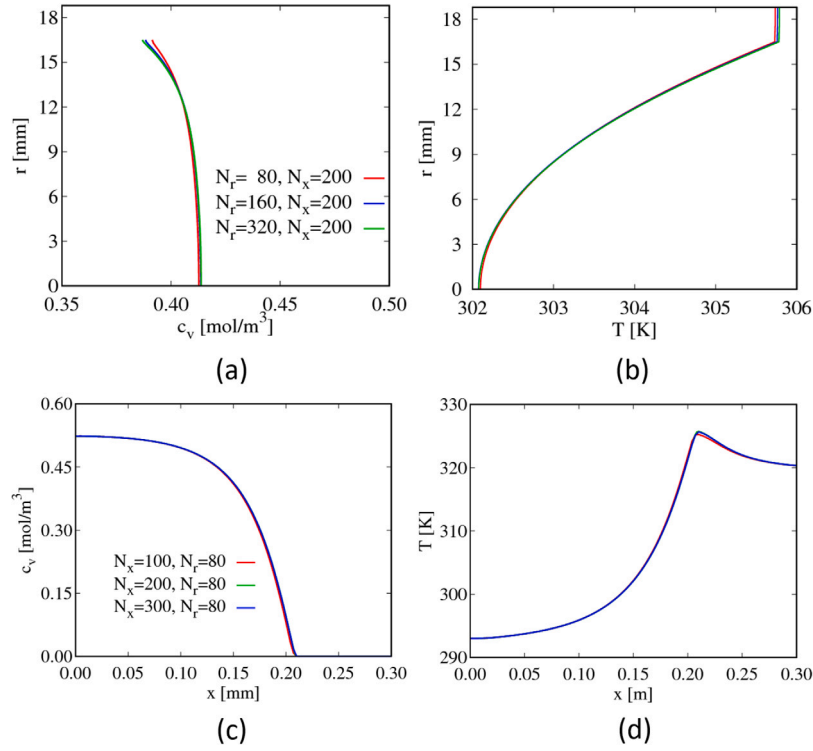


Fig. 2. Grid resolution test at $t = 15,000$ s showing the sensitivity of (a) radial c_v , (b) radial T , (c) axial c_v , and (d) axial T profiles.

The role of the local pseudo-Jacobian is to improve the diagonal dominance of the discretized species equation and to guide the convergence of the inner iterations within each transient time step. After the prescribed residual tolerance of 10^{-6} is satisfied for the conservation equations, the accepted solution is governed by the original nonlinear adsorption source term and equilibrium relation. Therefore, the proposed implicit stabilization improves numerical robustness and suppresses non-physical oscillations without altering the underlying LDF-Sips adsorption model.

This implicit source-term treatment suppressed non-physical concentration oscillations and enabled stable convergence under larger time-step conditions compared with an explicit implementation. Consequently, this stable formulation establishes an economically viable computational architecture for the long-term prediction of simultaneous heat and species transport within desiccant packed matrices.

2.5. One-dimensional formulation

For comparison with the multidimensional CFD framework, a simplified one-dimensional (1D) benchmark model was formulated based on the governing equations of the 2D model. The 1D formulation assumes ideal plug flow, $u = u(x)$, and instantaneous cross-sectional thermal equilibrium between the fluid and wall, $T_f = T_w$. It should be emphasized that the assumption ($T_f = T_w$) does not imply that the wall thermal inertia is physically negligible in the actual desiccant bed. Rather, this assumption represents a conventional lumped one-dimensional approximation in which the fluid, porous bed, and column wall are assumed to be instantaneously equilibrated over each cross-section. In this formulation, the thermal capacity and conductivity of the wall are included through effective properties, but a separate wall temperature and finite radial thermal response are not resolved. Therefore, the 1D model should be interpreted as a simplified reference case corresponding to the limiting condition of infinitely fast cross-sectional thermal equilibration. Under these assumptions, radial variations in velocity, temperature, and vapor concentration are neglected, allowing the transport behavior to be described only along the axial direction.

The 1D model consists of the reduced total mass balance, vapor species transport equation, and thermal energy conservation equation. The total mass balance was used to update the axial variation of the gas velocity, while the species equation describes vapor transport coupled with adsorption and desorption kinetics. The energy equation includes axial heat conduction, convective heat transport, adsorption heat effects, and external heat loss through the column wall ($r = r_o$). The pressure drop across the packed bed was calculated using the Ergun equation [6].

This formulation retains the same variables and material parameters as the 2D model to ensure a consistent comparison between the two approaches. Therefore, the 1D model is used not as an equivalent high-fidelity model, but as a lumped reference model to evaluate the prediction errors introduced by neglecting radial heat and mass transfer, finite wall thermal response, and near-wall moisture retention, which are explicitly captured by the 2D CFD framework. The governing equations of the 1D model are given as follows:

$$\frac{\partial(\epsilon \rho_g)}{\partial t} + \frac{\partial(\epsilon \rho_g u)}{\partial x} + (1 - \epsilon) \frac{\partial q}{\partial t} M_v = 0 \quad (12)$$

$$\frac{\partial(\epsilon \rho_g Y_v)}{\partial t} + \frac{\partial(\epsilon \rho_g u Y_v)}{\partial x} = \frac{\partial}{\partial x} \left(\rho_g \epsilon D \frac{\partial Y_v}{\partial x} \right) - (1 - \epsilon) \frac{\partial q}{\partial t} M_v \quad (13)$$

$$\begin{aligned} & (\rho C_p)_{\text{eff}} \frac{\partial T}{\partial t} + \frac{\partial(\epsilon \rho_g C_{p,g} u T)}{\partial x} \\ & = \frac{\partial}{\partial x} \kappa_{\text{eff}} \frac{\partial T}{\partial x} - \frac{2h_o r_o}{r_i^2} (T - T_\infty) - (1 - \epsilon) \frac{\partial q}{\partial t} (\Delta H + RT) \end{aligned} \quad (14)$$

$$-\frac{dp}{dx} = \frac{150\mu \cdot u \cdot (1 - \epsilon)^2}{d_p^2 \epsilon^2} + \frac{1.75(1 - \epsilon)\rho_g \cdot u \cdot |u|}{d_p \epsilon} \quad (15)$$

where

$$(\rho C_p)_{\text{eff}} = \epsilon \rho_g C_{p,g} + (1 - \epsilon) \rho_s C_{p,s} + \frac{r_o^2 - r_i^2}{r_i^2} \rho_w C_{p,w} \quad (16)$$

$$\kappa_{\text{eff}} = \epsilon k_g + (1 - \epsilon) k_s + \frac{r_o^2 - r_i^2}{r_i^2} k_w \quad (17)$$

Table 1
Parameters used for the present analysis.

Column parameters	
Length, L [m]	0.3
Inner radius, r_i [m]	0.0165
Wall thickness, t_w [m]	0.0023
External void fraction, ϵ [–]	0.37
Density of wall, ρ_w [kg/m ³]	8000
Specific heat capacity of wall, $C_{p,w}$ [J/kg K]	500
Thermal conductivity of wall, k_w [W/m K]	17
External heat transfer coefficient, h_o [W/m ² K]	1.71
Gas and adsorbed phase parameters	
Diffusivity, D [m ² /s]	2.581×10^{-5} (ads)/ 4.864×10^{-5} (des)
Thermal conductivity of gas, k_g [W/m K]	0.025
Specific heat capacity of gas, $C_{p,g}$ [J/kg K]	1047
Specific heat capacity of adsorbed phase, $C_{p,a}$ [J/kg K]	2392.6
Gas viscosity, μ [Pa s]	1.8×10^{-5}
Zeolite 13X pellet parameters	
Adsorbent density, ρ_s [kg/m ³]	1100
Specific heat capacity, $C_{p,s}$ [J/kg K]	920
Thermal conductivity of particle, k_p [W/m K]	0.4
Particle diameter, d_p [mm]	4.0
k_{LDF} [s ⁻¹]	5.0×10^{-4} (ads)/ 1.0×10^{-3} (des)
Universal gas constant, R [J/mol K]	8.314
Saturation pressure, P_s [Pa]	$610.94 \exp \left[\frac{17.625(T-273.15)}{T-30.11} \right]$
Sips isotherm parameters	
q_m [mol/kg]	14.9
b [Pa ⁻¹]	2.91×10^{-7}
n [–]	0.288
d [–]	0.02772
Isosteric heat, $-\Delta H$ [J/mol]	6.27×10^4
Boundary and initial conditions	
Inlet temperature in adsorption [K]	293
Inlet temperature in desorption [K]	403–473
Inlet concentration in adsorption [mol/m ³]	0.523
Initial concentration in adsorption [mol/m ³]	1×10^{-5}
Inlet flow rate in adsorption [Nm ³ /s]	1.5×10^{-4}

2.6. Computational conditions

The computational parameters and operating conditions used in the present simulations are summarized in Table 1. The material properties and adsorption parameters were selected based on previously reported experimental data for zeolite 13X adsorption systems [5,39]. The adsorption process was performed at 293 K, while the regeneration temperature was varied from 393 K to 473 K to evaluate the influence of thermal conditions on desorption performance and energy consumption.

During adsorption, humidified nitrogen with a prescribed vapor concentration and flow rate was supplied at the inlet boundary. During thermal regeneration, dry purge gas was introduced under elevated temperature conditions. To encapsulate ambient heat dissipation, a convective boundary layer was prescribed along the outer surface of the column shell [6]. The desorption simulation was initialized using the final state obtained from the adsorption process to ensure physical continuity throughout the cyclic operation. This initialization approach allows the residual adsorbed loading and thermal distributions at the end of adsorption to serve directly as the initial conditions for the subsequent regeneration process.

Different k_{LDF} values were applied for the adsorption and desorption processes, as listed in Table 1. A larger k_{LDF} value was assigned during regeneration to account for the fact that the increase in temperature leads to higher intra-particle diffusivity and subsequently enhances the lumped mass transfer coefficient. In the present study, the diffusivity and k_{LDF} values for the desorption process were specifically evaluated at a reference temperature of 423 K. The transient simulations were conducted under fixed operating conditions to evaluate the regeneration performance and total energy consumption for practical industrial operation.

3. Results and discussion

3.1. Grid resolution test

To guarantee mesh-independent numerical results, a systematic grid sensitivity evaluation was conducted at $t = 15,000$ s. The spatial resolution effects were isolated by separately varying the node counts in the cross-sectional and flow directions. Specifically, three radial configurations including $N_r = 80, 160$, and 320 nodes were examined under a constant axial resolution of $N_x = 200$ nodes, alongside three axial grids from $N_x = 100$ to $N_x = 300$ with a fixed radial resolution of $N_r = 80$. As shown in Fig. 2, local vapor concentration and temperature profiles were plotted across the bed to identify convergence thresholds. Both transport variables exhibit negligible variations beyond specific refinement levels.

To supplement the visual comparison and provide a quantitative assessment of grid independence, a profile-wide error analysis was performed using three mesh levels: medium ($N_r \times N_x = 80 \times 200$), selected (160×200), and fine (320×300). The selected mesh was used as the reference for evaluating the changes caused by coarsening and further refinement. The root mean square error (RMSE) and the maximum local relative error ($e_{\max}$) were calculated for the spatial profiles of vapor concentration (c_v) and temperature (T) during the high-flux desorption stage.

As shown in Table 2, the medium mesh produced a maximum local relative error of 2.18% for the vapor concentration profile, indicating that the grid was not sufficiently refined. In contrast, further refinement from the selected mesh to the fine mesh resulted in much smaller differences. The RMSE values were 6.12×10^{-4} mol/m⁻³ for vapor concentration and 0.28 K for temperature, and the corresponding $e_{\max}$

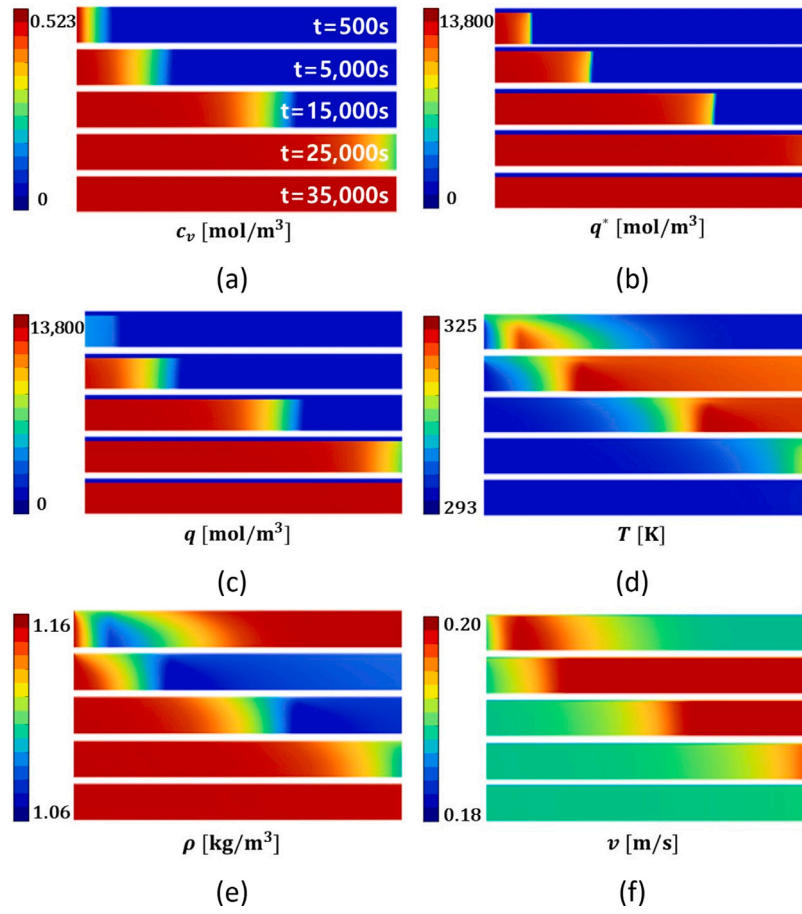


Fig. 3. Transient distributions of transport variables during adsorption at $c_{v,in} = 0.523 \text{ mol/m}^3$, $u_{in} = 0.188 \text{ m/s}$, $T_{in} = 293 \text{ K}$: (a) vapor concentration, (b) equilibrium adsorption capacity q^* , (c) adsorbed amount q , (d) temperature, (e) gas density and (f) velocity magnitude. The domain dimensions are identical to those shown in Fig. 1.

Table 2
Quantitative grid-independence analysis relative to the selected mesh.

Mesh level	Grid dimensions ($N_r \times N_x$)	Vapor concentration profile (c_v)		Temperature profile (T)	
		RMSE [mol/m³]	e_{max} [%]	RMSE [K]	e_{max} [%]
Medium	80×200	4.25×10^{-3}	2.18	1.85	0.59
Selected (reference)	160×200	–	–	–	–
Fine	320×300	6.12×10^{-4}	0.32	0.28	0.15

values were 0.32% and 0.15%, respectively. Since these errors are below the prescribed tolerance of 1.0%, the selected mesh ($N_r \times N_x = 160 \times 200$) was adopted for the remaining transient simulations as a balance between numerical accuracy and computational cost.

3.2. Model validation for adsorption

To validate the proposed numerical framework, the adsorption process was first investigated under the operating conditions summarized in Table 1. Fig. 3 presents the transient spatial distributions of the key transport variables during adsorption. As the inlet moisture front propagates through the packed bed, a distinct mass transfer zone develops and gradually moves toward the outlet, accompanied by a significant increase in the local vapor concentration within the active adsorption region, as shown in Fig. 3(a). According to the Sips isotherm, the increase in vapor concentration leads to a corresponding increase in the equilibrium adsorption capacity q^* , as illustrated in Fig. 3(b). The adsorbed amount q subsequently increases while following the advancing adsorption front, indicating progressive saturation of the desiccant bed along the axial direction, as shown in Fig. 3(c). The

adsorption process is strongly coupled with heat transfer due to the exothermic nature of water vapor adsorption. The resulting thermal response is presented in Fig. 3(d), where the local temperature rises substantially within the active adsorption region due to the exothermic adsorption of water vapor, reaching approximately 325 K during the peak adsorption period.

The gas density distribution in Fig. 3(e) reflects the coupled thermal and concentration effects within the porous medium. As adsorption proceeds, the local temperature rise and vapor uptake modify the gas-phase composition, leading to noticeable density gradients near the active adsorption front. The velocity field shown in Fig. 3(f) exhibits a moderate increase near the active adsorption region where the temperature rises due to exothermic adsorption. This behavior is primarily attributed to the local reduction in gas density associated with thermal expansion. Under the imposed flow condition, the decrease in density leads to a corresponding increase in the superficial gas velocity to satisfy mass conservation.

The reliability of the proposed CFD framework was quantitatively validated through comparison with experimental breakthrough data, as presented in Fig. 4. The predicted normalized vapor concentration

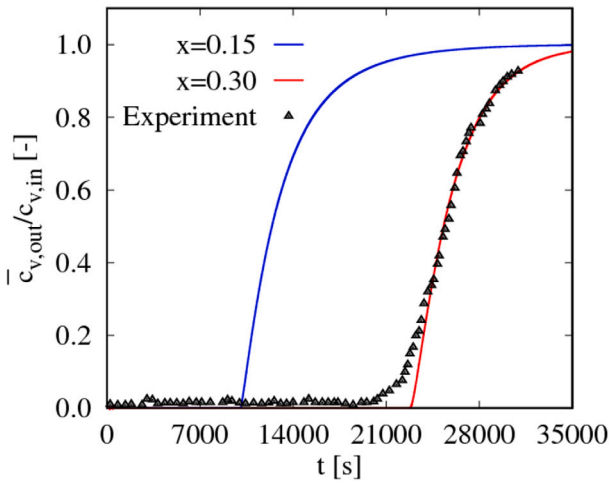


Fig. 4. Validation of the proposed CFD model through comparison with experimental breakthrough data during adsorption at $c_{v,in} = 0.523 \text{ mol/m}^3$, $u_{in} = 0.188 \text{ m/s}$, $T_{in} = 293 \text{ K}$: normalized outlet vapor concentration at different axial positions.

at $x = 0.30 \text{ m}$ shows good agreement with the experimental measurements, accurately reproducing both the breakthrough time and the characteristic S-shaped saturation behavior. In addition, the numerical result at $x = 0.15 \text{ m}$ illustrates the transient propagation of the adsorption front along the packed bed, demonstrating the capability of the present model to capture the axial transport dynamics during adsorption.

The close agreement between the numerical predictions and experimental data confirms that the present 2D CFD framework, incorporating the implicitly coupled LDF kinetics and Sips isotherm, can reliably predict the coupled heat and mass transfer behavior in desiccant beds. The validated model therefore provides a reliable foundation for subsequent analyses of multidimensional transport phenomena and thermal regeneration characteristics.

3.3. Radial heat and mass transfer characteristics

The radial distributions of the key transport variables at the axial midpoint $x = 0.15 \text{ m}$ are presented in Fig. 5 to provide a detailed view of the transient multidimensional transport phenomena during adsorption. The vapor concentration in Fig. 5(a) and the adsorbed amount in Fig. 5(b) exhibit radial non-uniformity during the active adsorption period. These distributions are closely associated with the axial velocity field. Due to the no-slip condition at the column wall, the axial velocity decreases in the near-wall region, resulting in a delayed convective transport of water vapor compared with the central region. Consequently, the adsorption front propagates more rapidly along the bed center, while the near-wall region experiences slower moisture penetration and delayed adsorption dynamics. This behavior produces the observed radial variations in both vapor concentration and adsorbed amount during the transient adsorption process.

The radial temperature difference relative to the bed center ($T - T_{r=0}$) is illustrated in Fig. 5(c) to reveal the transient thermal behavior associated with the exothermic adsorption process. During the early stages ($t = 500 \text{ s}$ and 5000 s), the near-wall region remains cooler than the core region, exhibiting negative temperature transfer gradients due to external cooling and wall thermal inertia. As adsorption progresses to the intermediate stage ($t = 15,000 \text{ s}$), a thermal inversion occurs where the wall-adjacent zone becomes up to 3.7 K hotter than the bed center. This inversion arises because the core region approaches local saturation and undergoes thermal dissipation, whereas the structural mass of the wall retains the accumulated exothermic heat. Eventually,

as the entire bed reaches complete saturation ($t = 35,000 \text{ s}$), these localized thermal gradients diminish toward a uniform thermal state.

The radial transport characteristics are also influenced by the velocity distribution shown in Fig. 5(d). Owing to the no-slip condition at the column wall, the axial velocity decreases near the wall region. More importantly, the velocity near the bed center exhibits a transient increase during the active adsorption period. As the gas temperature increases in the central region due to the exothermic heat of adsorption, the gas density decreases via thermal expansion. To satisfy total mass conservation under the imposed flow condition, the localized superficial gas velocity increases proportionally. As the desiccant approaches saturation, local heat generation ceases and the gas density recovers, returning the velocity profile to its baseline distribution.

The transient evolution of the cross-sectionally averaged fluid and wall temperatures at $x = 0.15 \text{ m}$ and $x = 0.30 \text{ m}$ is presented in Fig. 5(e). The fluid temperature rapidly increases during the initial adsorption stage due to the exothermic heat release, whereas the wall temperature rises more gradually. This clear thermal lag verifies that the column wall acts as a structural thermal buffer, creating localized equilibrium discrepancies between the fluid and solid phases. Furthermore, the delayed temperature peaks between $x = 0.15 \text{ m}$ and $x = 0.30 \text{ m}$ trace the macro-transport propagation of the thermal front through the porous matrix.

The present results demonstrate that radial heat transfer and structural thermal inertia introduce severe spatial non-uniformities that conventional 1D models cannot resolve. By enforcing instantaneous cross-sectional equilibrium and effectively assuming infinite radial thermal conductivity, a 1D formulation smooths out these localized thermal inversions and transport bottlenecks. The multi-dimensional CFD framework successfully captures these coupled radial phenomena, proving essential for the realistic representation of industrial desiccant systems.

3.4. Desorption transport dynamics under thermal regeneration

Following the adsorption analysis, the desorption behavior under thermal regeneration conditions was investigated to evaluate the transient transport dynamics within the desiccant bed. Fig. 6 presents the transient spatial distributions of the key transport variables during low-temperature regeneration at $T_{in} = 293 \text{ K}$. As the dry purge gas enters the bed, the vapor concentration c_v shown in Fig. 6(a) gradually decreases from the inlet region and propagates downstream. This reduction in gas-phase moisture concentration shifts the local equilibrium adsorption capacity q^* shown in Fig. 6(b) according to the Sips isotherm. However, because the regeneration temperature remains relatively low, the equilibrium adsorption capacity is only weakly reduced during the process. Consequently, the adsorbed amount q in Fig. 6(c) decreases slowly, indicating limited moisture removal under low-temperature regeneration conditions.

The thermal profiles depicted in Fig. 6(d) further substantiate how the regeneration step acts as a localized heat sink. During regeneration, thermal energy is consumed for moisture desorption, resulting in a local temperature decrease below the initial bed temperature within the active desorption region. This cooling effect generates a thermal front that gradually propagates downstream along the bed. The gas density distribution shown in Fig. 6(e) reflects the coupled influence of temperature variation and vapor release during desorption. In addition, the velocity field shown in Fig. 6(f) exhibits only slight local variations associated with the corresponding density changes. Nevertheless, the overall flow structure remains relatively uniform throughout the porous bed.

These results indicate that regeneration at 293 K does not provide a sufficiently strong thermodynamic driving force to effectively reduce the adsorption equilibrium of zeolite 13X. As a result, moisture removal remains limited and the desorption process proceeds slowly under low-temperature conditions.

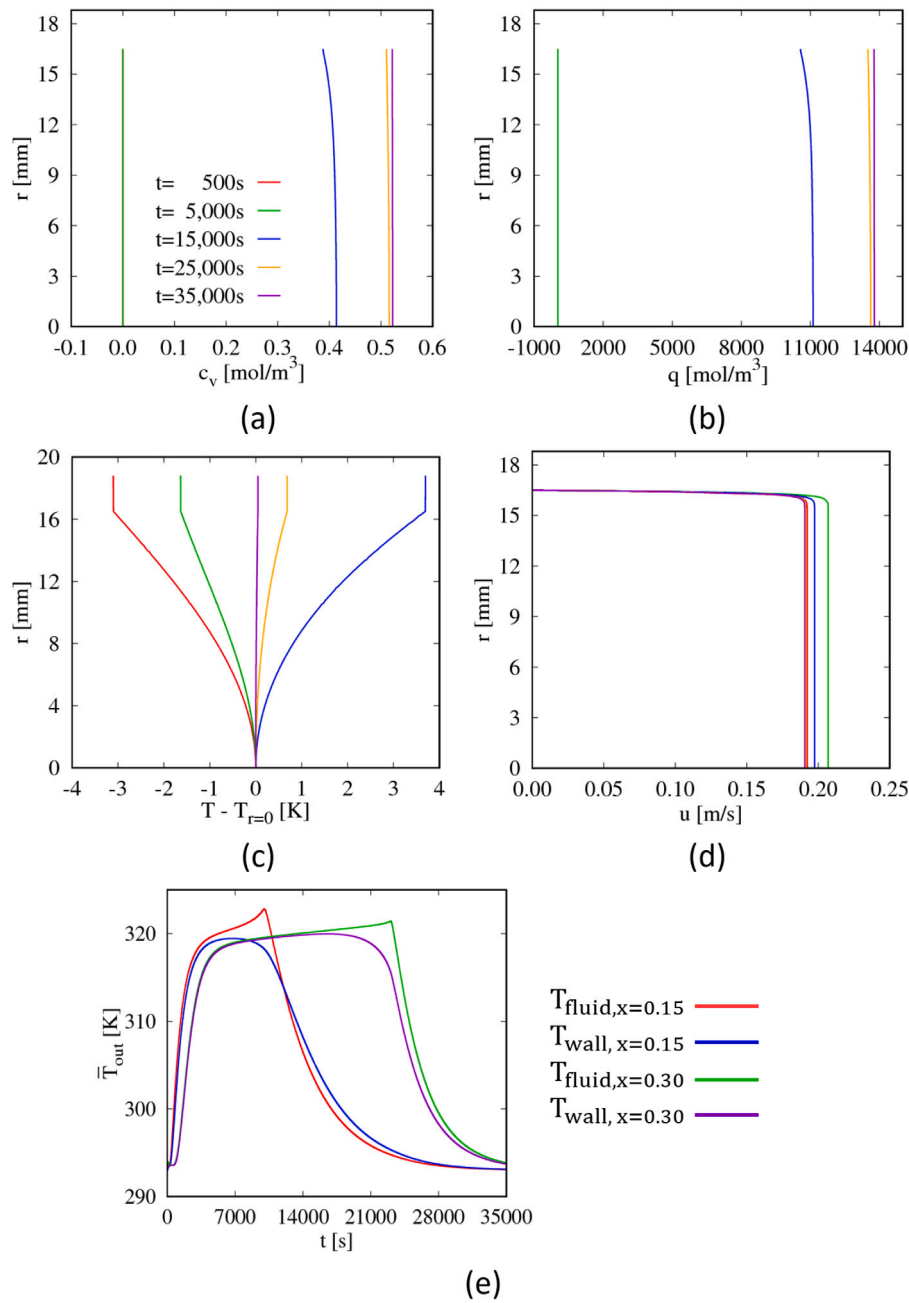


Fig. 5. Radial distributions of transport variables at the desiccant center ($x = 0.15$ m) during adsorption at $c_{v,in} = 0.523$ mol/m³, $u_{in} = 0.188$ m/s, $T_{in} = 293$ K: (a) vapor concentration, (b) adsorbed amount, (c) temperature difference, (d) axial velocity, (e) Transient spatially averaged fluid and wall temperatures at the bed center and outlet.

To investigate the influence of elevated regeneration temperature, additional desorption simulations were conducted at $T_{in} = 423$ K, as presented in Fig. 7. Compared with the low-temperature case, high-temperature regeneration produces substantially enhanced heat and mass transfer characteristics. As shown in Fig. 7(a), the vapor concentration front propagates rapidly through the bed due to accelerated moisture release. Correspondingly, the equilibrium adsorption capacity q^* shown in Fig. 7(b) decreases significantly because the elevated temperature strongly suppresses the adsorption equilibrium predicted by the Sips isotherm. Consequently, the adsorbed amount q in Fig. 7(c) decreases rapidly, demonstrating substantially enhanced desorption kinetics under high-temperature conditions.

The thermal field shown in Fig. 7(d) captures the propagation of the heating front through the porous bed. During regeneration, the supplied thermal energy is consumed both for heating the porous matrix and for

supporting the endothermic desorption process, resulting in a transient delay in the temperature rise during the early stage of regeneration. Nevertheless, the elevated thermal input rapidly increases the bed temperature and promotes effective moisture desorption throughout the bed. The gas density distribution shown in Fig. 7(e) reflects the combined effects of thermal expansion and vapor release under high-temperature conditions. Correspondingly, the velocity field in Fig. 7(f) exhibits moderate local variations associated with the thermally induced density changes. However, the overall flow structure remains stable during the regeneration process.

These findings demonstrate that elevated regeneration temperature significantly enhances the desorption performance by increasing the thermodynamic driving force for moisture removal. Compared with the low-temperature case, regeneration at 423 K achieves substantially

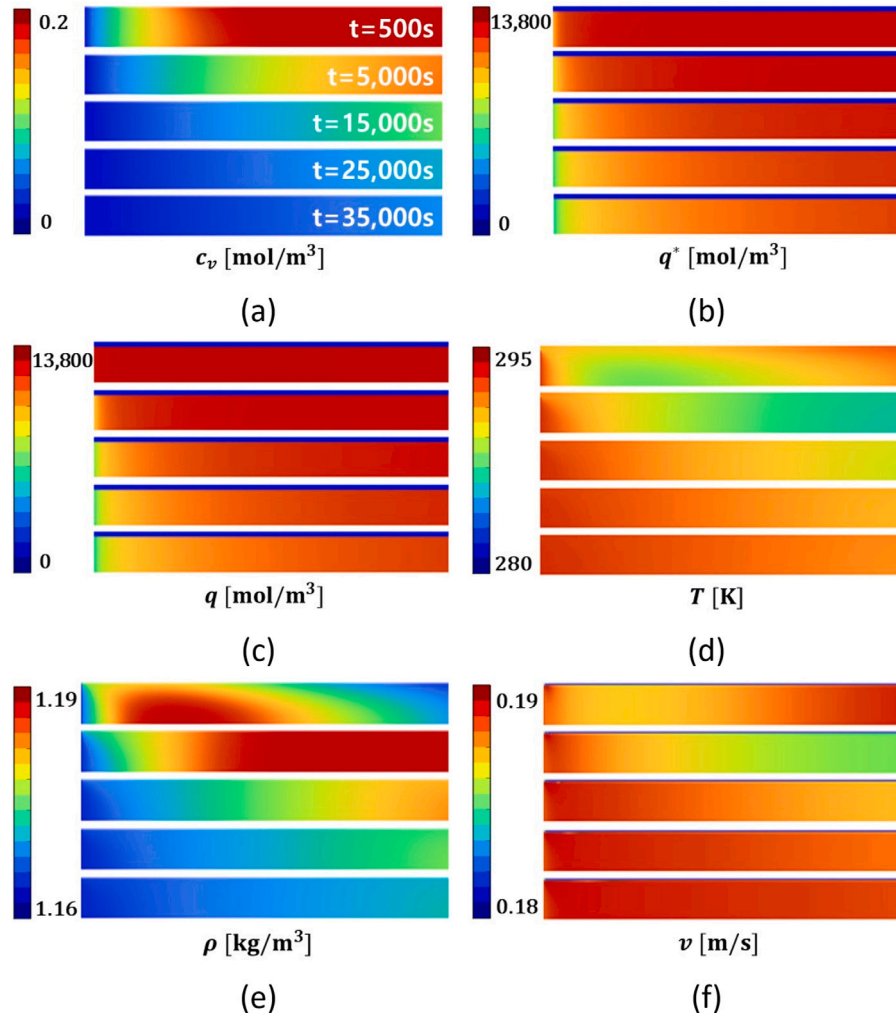


Fig. 6. Transient spatial distributions of transport variables during low-temperature desorption at $c_{v,in} = 0 \text{ mol/m}^3$, $u_{in} = 0.188 \text{ m/s}$, $T_{in} = 293 \text{ K}$: (a) vapor concentration, (b) equilibrium adsorption capacity q^* , (c) adsorbed amount q , (d) temperature, (e) gas density and (f) velocity magnitude. The domain dimensions are identical to those shown in Fig. 1.

faster and more effective moisture desorption, highlighting the importance of thermal management in practical desiccant regeneration systems.

The radial distributions of the key transport variables at the axial midpoint $x = 0.15 \text{ m}$ are presented in Fig. 8 to provide a detailed understanding of the multidimensional transport behavior during high-temperature regeneration. The vapor concentration profiles shown in Fig. 8(a) and the residual adsorbed amount shown in Fig. 8(b) illustrate the transient transport behavior. During the early stage of regeneration ($t = 500 \text{ s}$), the vapor concentration increases first near the bed center as the desorbed moisture released from the inlet region is transported downstream by the purge flow. Because the axial velocity is slightly higher in the core region, the downstream propagation of the vapor front occurs more rapidly near the bed center than near the wall region, resulting in a distinct radial concentration gradient where c_v reaches its peak at $r = 0.00 \text{ mm}$. As regeneration proceeds, the radial non-uniformity of the vapor concentration gradually diminishes. Correspondingly, the residual adsorbed amount shown in Fig. 8(b) decreases progressively over the entire radial direction during the desorption process, maintaining a slightly higher moisture loading near the cooler wall boundary.

The radial temperature difference relative to the bed center ($T - T_{r=0}$) is illustrated in Fig. 8(c). Throughout the entire regeneration process, the near-wall region remains continuously cooler than the core region, as indicated by the persistent negative values of the temperature

difference. This thermal deficit expands to a maximum gap of -3.2 K at the intermediate stage ($t = 5000 \text{ s}$) due to the structural thermal inertia of the wall and external heat dissipation. Consequently, moisture release and vapor transport proceed more rapidly in the hotter core region. As regeneration progresses toward the late stages ($t = 25,000 \text{ s}$ and $35,000 \text{ s}$), the thermal energy gradually penetrates into the peripheral layers, causing the radial temperature difference to contract back toward a more uniform thermal state.

The radial velocity profiles shown in Fig. 8(d) also exhibit transient radial variation during regeneration. In the hotter core region, the gas density decreases because of thermal expansion, resulting in a moderate increase in the axial velocity under the imposed flow condition to satisfy mass conservation. Consequently, the central region exhibits slightly faster downstream vapor transport than the near-wall region, while the no-slip condition maintains lower velocity near the wall boundary. These results demonstrate that radial thermal gradients and wall thermal inertia play important roles in determining the multidimensional regeneration characteristics of practical desiccant systems, establishing transport bottlenecks that are inherently neglected in simplified one-dimensional frameworks.

Fig. 9 compares the axial vapor concentration and temperature profiles predicted by the 1D and 2D models during regeneration. The vapor concentration profiles are shown at $t = 500, 15,000$, and $35,000 \text{ s}$ in Fig. 9(a)–(c), while the corresponding temperature profiles are presented in Fig. 9(d)–(f). At $t = 500 \text{ s}$, both models capture the overall axial

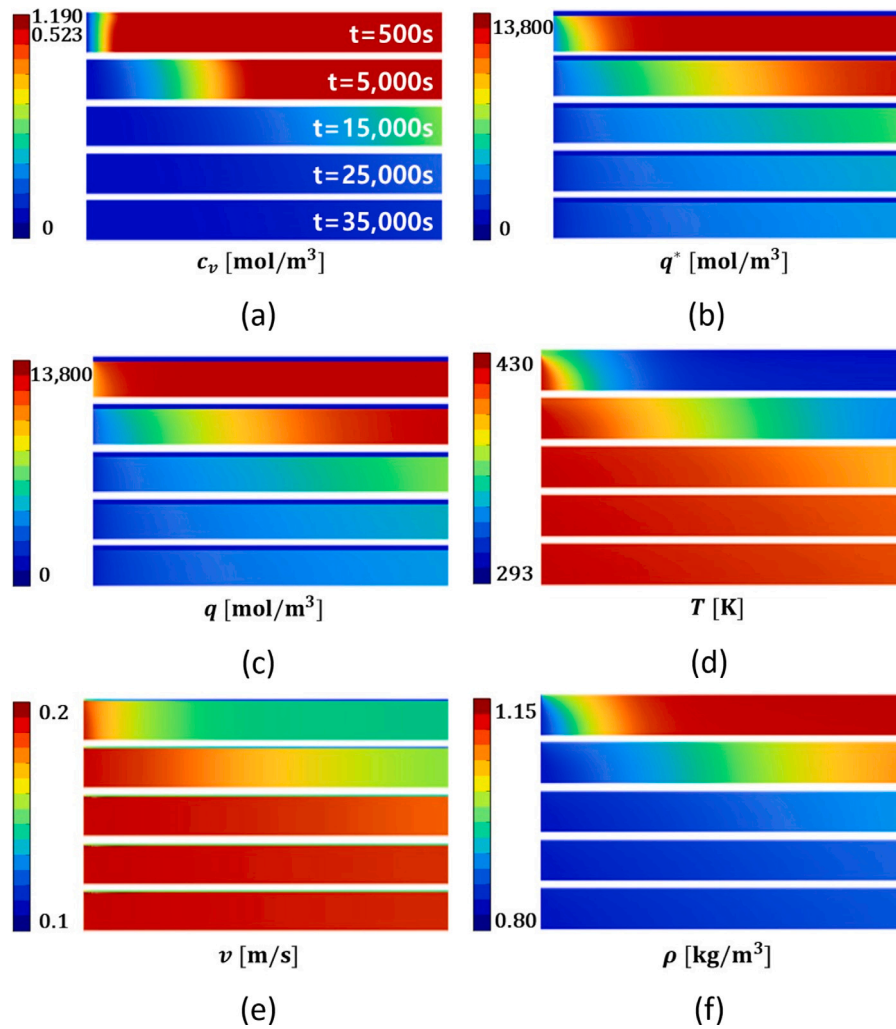


Fig. 7. Transient spatial distributions of transport variables during high-temperature desorption at $c_{v,in} = 0 \text{ mol/m}^3$, $u_{in} = 0.188 \text{ m/s}$, $T_{in} = 423 \text{ K}$: (a) vapor concentration, (b) equilibrium adsorption capacity q^* , (c) adsorbed amount q , (d) temperature, (e) gas density and (f) velocity magnitude. The domain dimensions are identical to those shown in Fig. 1.

propagation of the regeneration front. However, the 1D model overpredicts the vapor concentration peak and the thermal-front propagation speed because it enforces instantaneous cross-sectional equilibration. The 2D model, by contrast, resolves radial variations in which the bed core heats and desorbs faster, while the near-wall region exhibits delayed thermal response and weaker vapor release due to wall thermal inertia and finite radial transport resistance. As regeneration proceeds to $t = 15,000$ and $35,000 \text{ s}$, the global axial profiles of the two models become qualitatively similar, but noticeable quantitative discrepancies remain. The 1D model tends to overpredict the bed temperature and underpredict the vapor concentration because it cannot represent localized thermal lag and moisture retention near the wall. These results demonstrate that radial transport effects, although partially masked in cross-sectionally averaged trends, play an important role in predicting the tailing behavior and completion time of bed regeneration.

The transient evolution of the vapor concentration and temperature during high-temperature regeneration at $T_{in} = 423 \text{ K}$ is shown in Fig. 10. Fig. 10(a) presents the cross-sectionally averaged vapor concentration at the bed center ($x = 0.15 \text{ m}$) and outlet ($x = 0.30 \text{ m}$). A sharp concentration peak appears during the early stage of regeneration owing to rapid moisture release induced by the hot purge gas. The peak occurs earlier at the bed center, whereas the outlet shows a delayed but larger peak because the desorbed moisture is accumulated and transported downstream as the regeneration front propagates through the bed.

Fig. 10(b) shows the corresponding fluid and wall temperature histories at the same axial locations. The fluid temperature rises faster than the wall temperature because the hot purge gas directly heats the fluid region, while the column wall responds more slowly due to its thermal inertia. In addition, the upstream position reaches the regeneration temperature earlier than the outlet, indicating the axial propagation of the heating front. These results demonstrate that regeneration is governed by the coupled evolution of vapor release, downstream moisture transport, and wall-induced thermal lag.

To evaluate the effect of purge-gas humidity on regeneration performance, desorption was simulated using humid purge gas with $c_{v,in} = 0.523 \text{ mol/m}^3$, as shown in Fig. 11. Unlike the dry purge-gas case, the vapor concentration remains finite throughout the bed during regeneration because of the non-zero inlet moisture content. As a result, the equilibrium adsorption capacity q^* remains at a finite level even at the elevated regeneration temperature of $T_{in} = 423 \text{ K}$, as predicted by the Sips isotherm. Consequently, the adsorbed amount q decreases only until a new thermodynamic equilibrium state is approached, leaving residual moisture in the zeolite 13X bed.

The temperature field in Fig. 11(d) shows the propagation of the heating front, which is qualitatively similar to the dry purge-gas case. However, the presence of moisture in the purge gas limits the reduction in equilibrium adsorption capacity and therefore restricts the attainable degree of desorption. The density and velocity fields in Fig. 11(e)

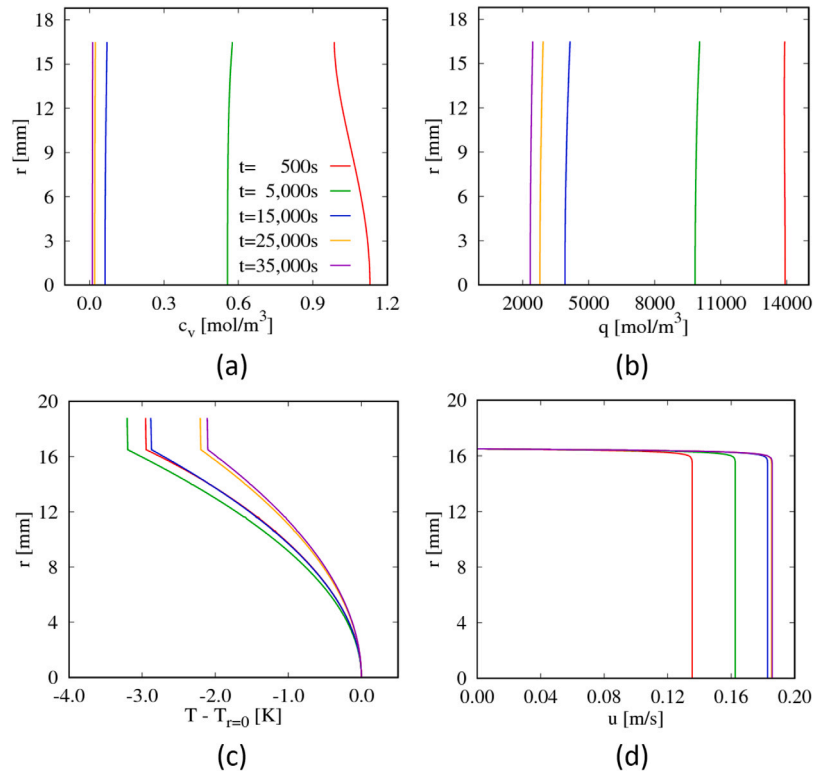


Fig. 8. Radial distributions of transport variables at the desiccant bed center ($x = 0.15$ m) during desorption at $c_{v,in} = 0$ mol/m³, $u_{in} = 0.188$ m/s, $T_{in} = 423$ K: (a) vapor concentration, (b) adsorbed amount, (c) temperature difference, (d) axial velocity.

and (f) mainly reflect the combined effects of heating, vapor content, and gas expansion during regeneration. These results demonstrate that regeneration performance is governed not only by the regeneration temperature but also by the inlet moisture concentration of the purge gas. Therefore, reducing purge-gas humidity is essential for improving moisture removal and cyclic adsorption capacity in practical desiccant systems.

Fig. 12 compares the temporal evolution of the spatially averaged adsorbed amount for dry and humid purge-gas conditions during regeneration. In both cases, the adsorbed amount decreases rapidly during the early stage of regeneration because of the elevated regeneration temperature. However, the dry purge-gas case ($c_{v,in} = 0$) exhibits a continuous decrease in the adsorbed amount throughout the regeneration process, whereas the humid purge-gas case ($c_{v,in} = 0.523$ mol/m³) approaches a higher residual equilibrium loading. This difference indicates that the humidity of the purge gas significantly influences the achievable regeneration level by modifying the equilibrium adsorption capacity during desorption. Although elevated temperature enhances the desorption kinetics, the presence of moisture in the purge gas limits the ultimate extent of moisture removal. These results highlight the importance of purge-gas humidity control for improving the cyclic regeneration performance of practical desiccant systems.

The present simulations were performed under well-defined inlet-gas conditions using a nitrogen–water vapor mixture to isolate the fundamental heat and mass transfer behavior of the zeolite 13X bed. In practical desiccant air-drying systems, however, the inlet humidity, temperature, flow rate, and contaminant concentration may fluctuate during cyclic operation. Because the present implicit source-term treatment is evaluated locally from the instantaneous vapor concentration, temperature, and adsorbed loading, the numerical framework can be extended to time-dependent boundary conditions by updating the local adsorption equilibrium and kinetic source terms at each time step. Nevertheless, additional validation is required for strongly fluctuating industrial operating conditions.

In addition, practical moist air may contain airborne pollutants, such as oil vapor, volatile organic compounds, aerosols, or fine particles. Recent studies on polluted moist air have shown that particulate matter and inlet humidity can significantly influence coupled heat and mass transfer and system performance in moist-air energy systems [40]. In desiccant beds, such contaminants may alter the local thermodynamic driving force for water adsorption by competing for adsorption sites, modifying the effective adsorption equilibrium, blocking micropores, or degrading the adsorbent over repeated cycles. These effects may reduce the cyclic adsorption capacity and change the regeneration requirement. The present model does not include multi-component competitive adsorption or pollutant-induced adsorbent degradation, and these effects should be addressed in future work by incorporating multi-species transport, competitive isotherms, and time-dependent adsorbent properties.

Fig. 13 compares the regeneration predictions of the 1D and 2D models under identical operating conditions. As shown in Fig. 13(a), the 1D model consistently underestimates the desorption time required to reach the target moisture-removal levels. The underprediction ranges from 12.0% to 15.3% for 50% moisture removal and from 21.3% to 30.4% for 75% moisture removal. This discrepancy arises because the 1D formulation assumes instantaneous cross-sectional equilibration and therefore neglects radial transport resistance, wall thermal inertia, and delayed near-wall desorption.

The temperature histories in Fig. 13(b) further show that the 1D model overpredicts the bed temperature, with relative errors of 4.7% at $x = 0.15$ m and 3.3% at $x = 0.30$ m. In contrast, the 2D model captures localized thermal lag near the wall, which reduces the local desorption driving force and delays moisture removal. These results indicate that radial heat and mass transfer effects become increasingly important as regeneration proceeds toward deeper moisture removal, where the tailing behavior strongly influences the required regeneration time.

The above discrepancy is directly related to the lumped thermal-equilibrium assumption used in the 1D reference model. Because ($T_f =$

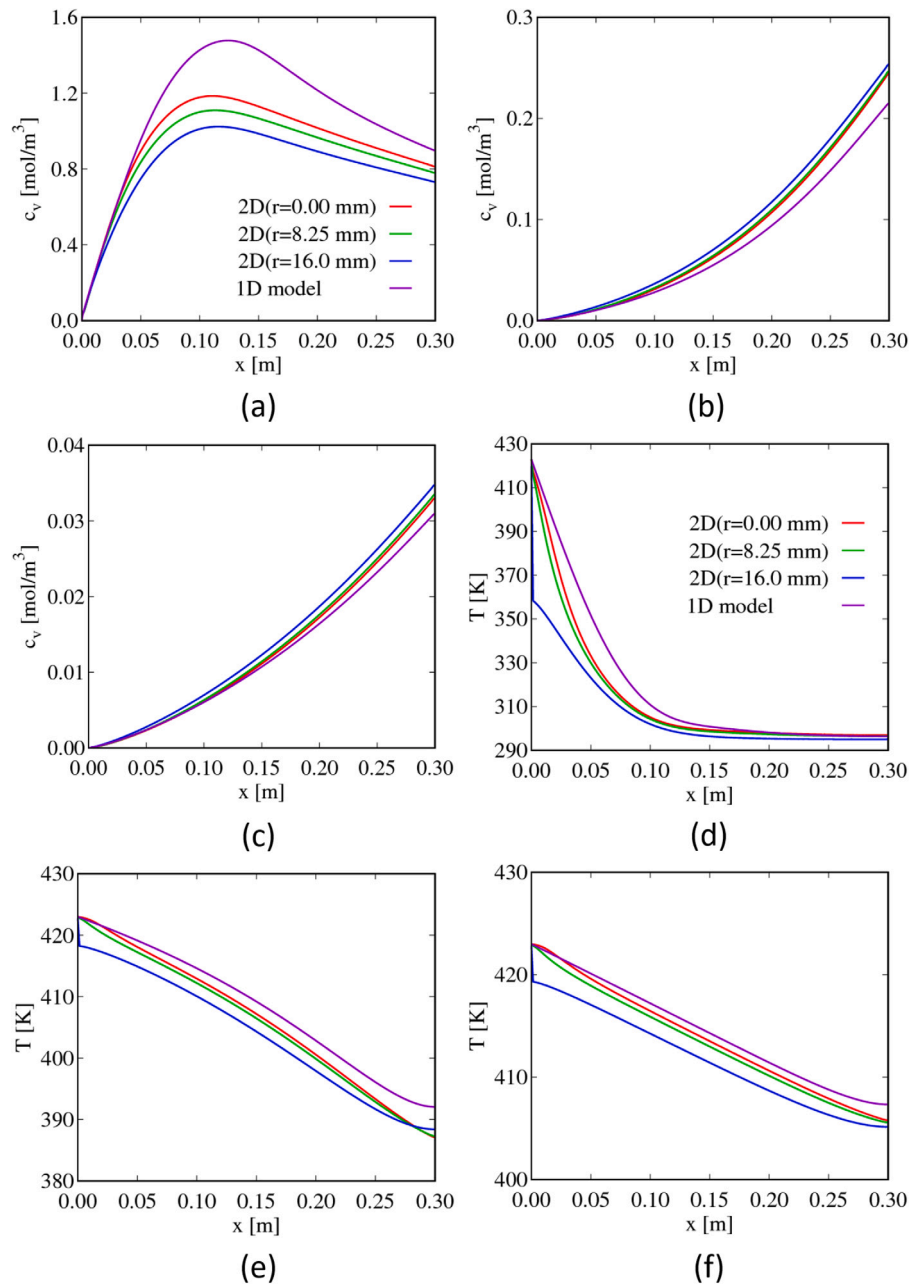


Fig. 9. Comparison of axial vapor concentration and temperature profiles predicted by the 1D and 2D models at different radial positions during regeneration: vapor concentration c_v at (a) $t = 500$ s, (b) $t = 15,000$ s, and (c) $t = 35,000$ s; temperature T at (d) $t = 500$ s, (e) $t = 15,000$ s, and (f) $t = 35,000$ s.

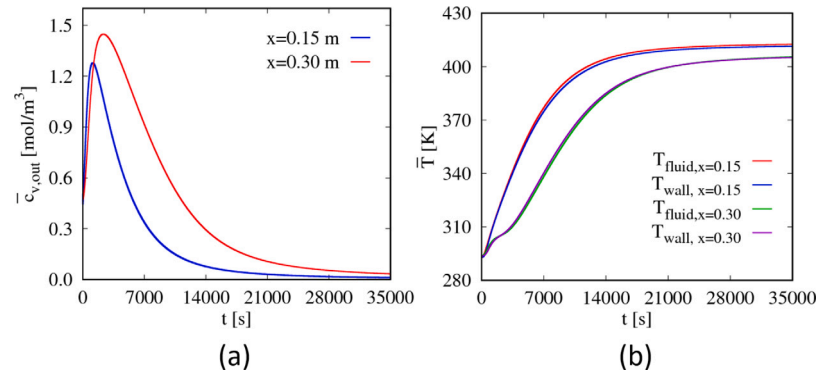


Fig. 10. Transient profiles during high-temperature desorption at $c_{v,in} = 0$ mol/m³, $u_{in} = 0.188$ m/s, $T_{in} = 423$ K: (a) outlet vapor concentration and (b) fluid and wall temperatures at different axial positions in the desiccant bed.

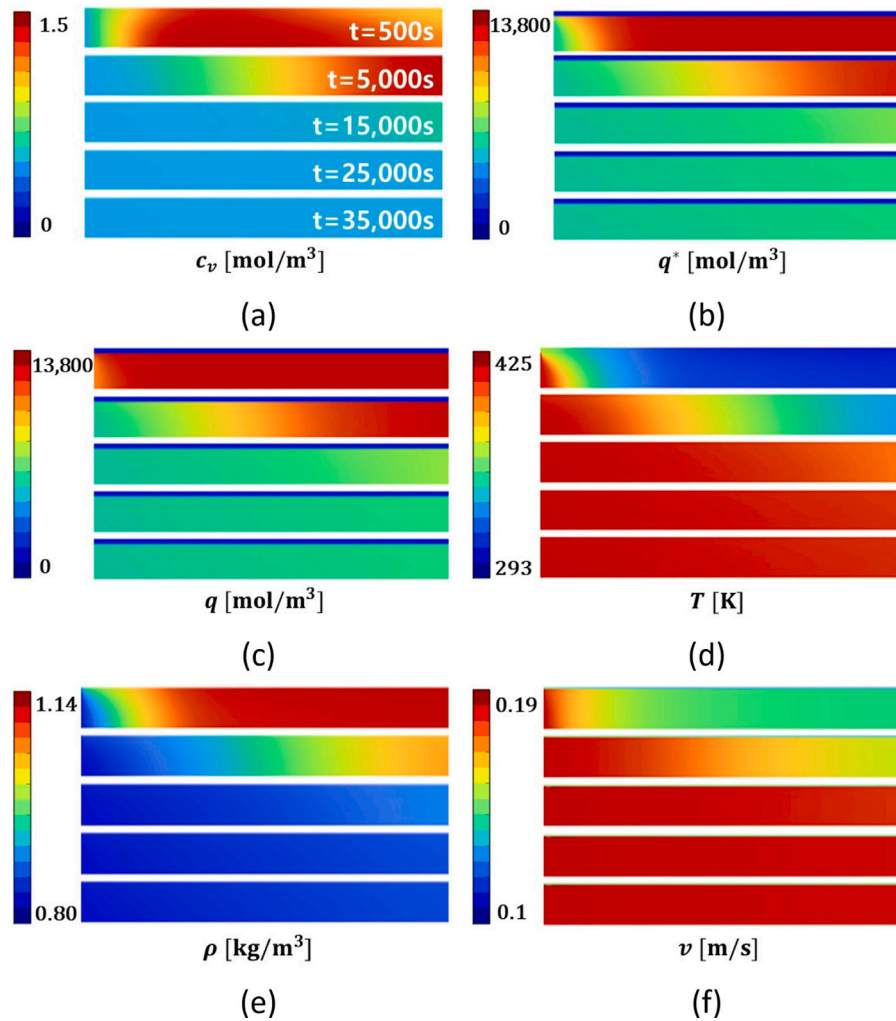


Fig. 11. Transient spatial distributions of transport variables during humid purge-gas desorption at $c_{v,in} = 0.523 \text{ mol/m}^3$, $u_{in} = 0.188 \text{ m/s}$, $T_{in} = 423 \text{ K}$: (a) vapor concentration, (b) equilibrium adsorption capacity q^* , (c) adsorbed amount q , (d) temperature, (e) gas density and (f) velocity magnitude. The domain dimensions are identical to those shown in Fig. 1.

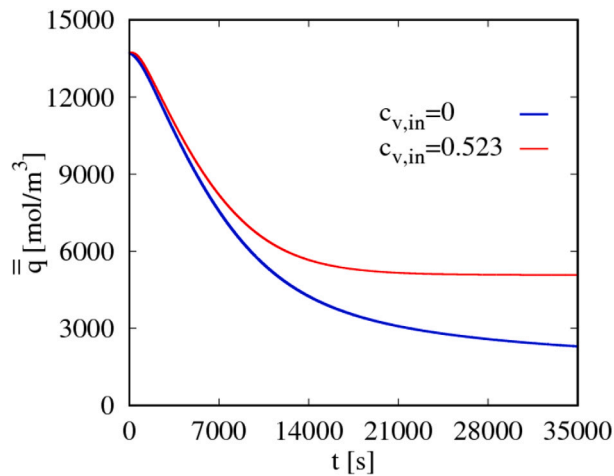


Fig. 12. Comparison of the average adsorbed amount over time for different inlet water vapor concentrations during the desorption process.

T_w) enforces instantaneous cross-sectional thermal equilibration, the 1D model cannot represent the delayed wall response or the cooler near-wall region observed in the 2D calculation. As a result, the 1D model tends to predict a higher effective bed temperature and a stronger local desorption driving force than the 2D model. The purpose of the 1D–2D comparison is therefore not to validate one model against the other, but to quantify the consequence of applying a conventional lumped 1D assumption to a system where wall thermal inertia and radial transport resistance are important.

3.5. Energy optimization of desiccant regeneration

To identify energy-efficient regeneration conditions, the required inlet operating conditions were determined for different regeneration temperatures. In all cases, the regeneration process was designed to achieve 90% moisture removal, corresponding to a normalized average adsorbed amount of $\bar{q}/q_{ref} = 10\%$, within $t = 35,000 \text{ s}$. Complete regeneration was not considered because the final stage of desorption is accompanied by severe thermodynamic tailing, resulting in extremely slow moisture removal and inefficient energy utilization. According to equilibrium-wave theory, the propagation velocity of the concentration wave front u_c is inversely related to the local slope of the adsorption

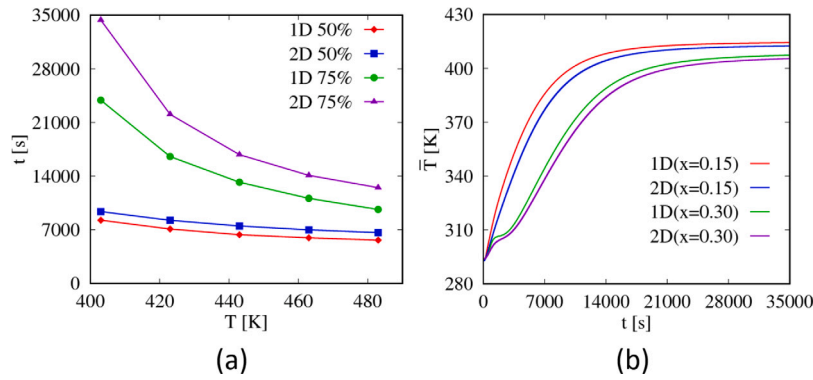


Fig. 13. Comparison of 1D and 2D model predictions during thermal regeneration: (a) required desorption time to achieve 50% and 75% moisture removal as a function of regeneration temperature and (b) temporal evolution of average bed temperatures at $x = 0.15$ m and $x = 0.30$ m.

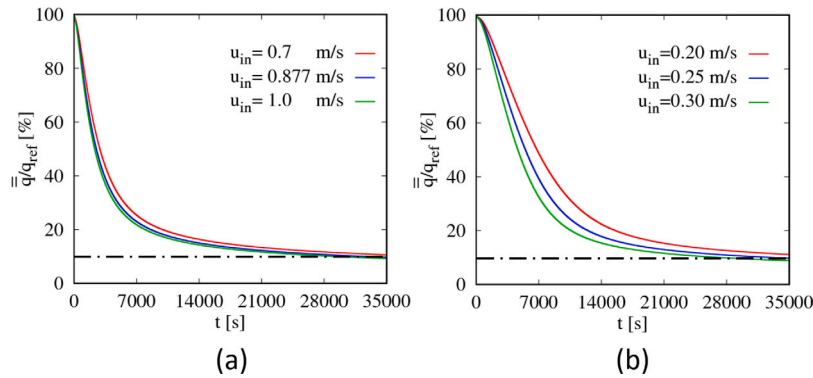


Fig. 14. Comparisons of normalized average adsorbed amounts during desorption for different inlet velocities at two regeneration temperatures: (a) $T_{in} = 413$ K and (b) $T_{in} = 453$ K.

isotherm and can be expressed as follows [6]:

$$u_c = \frac{u}{1 + \frac{1-\epsilon}{\epsilon} \rho_s \frac{\partial q}{\partial c}} \quad (18)$$

For zeolite 13X, the isotherm slope becomes very large in the low-concentration region, significantly reducing the desorption-front velocity near equilibrium conditions. Therefore, a practical regeneration criterion of 90% moisture removal was adopted to avoid the inefficient tailing regime during thermal regeneration.

Under this fixed-performance criterion, the inlet velocities required to achieve 90% regeneration within $t = 35,000$ s were determined for different regeneration temperatures. As shown in Fig. 14, the normalized average adsorbed amount was evaluated using the reference loading q_{ref} , corresponding to the fully saturated average adsorbed amount after adsorption. For each regeneration temperature, the inlet velocity was adjusted until $\bar{q}/q_{ref}$ reached 10% at $t = 35,000$ s. At $T_{in} = 413$ K, relatively high inlet velocities were required to meet the 90% regeneration criterion, whereas at $T_{in} = 453$ K, the same target was achieved with much lower purge-gas velocities. This indicates that increasing the regeneration temperature enhances the desorption driving force and reduces the required purge-gas flow rate. Thus, Fig. 14 provides the basis for determining the minimum purge-gas flow rate required at each regeneration temperature before evaluating the total regeneration power consumption.

The transient regeneration responses under different operating conditions are presented in Fig. 15. Although all cases achieved the target regeneration level within $t = 35,000$ s, the transient desorption behavior varied depending on the regeneration temperature and inlet flow rate. As shown in Fig. 15(a), the low-temperature case at 403 K exhibits the most rapid initial decrease in the normalized adsorbed amount because of the relatively high purge-gas velocity required to satisfy

the regeneration criterion. In contrast, the high-temperature case at 463 K shows a slower initial response due to the lower inlet velocity, although the elevated temperature provides a stronger thermodynamic driving force for desorption. As regeneration proceeds, the higher-temperature cases maintain more gradual and sustained desorption behavior, whereas the lower-temperature case approaches the tailing region more rapidly.

The outlet vapor concentration profiles shown in Fig. 15(b) further illustrate the influence of the regeneration conditions. At lower regeneration temperature, the large purge-gas flow rate results in relatively diluted outlet vapor concentration despite the rapid moisture removal. In contrast, the higher-temperature cases produce larger outlet vapor concentration peaks because the desorbed moisture is transported by a smaller purge-gas flow rate. The thermal responses shown in Fig. 15(c) reflect the combined effects of convective heat transfer and endothermic desorption. The low-temperature case exhibits a relatively rapid temperature increase because of the larger inlet flow rate, whereas the higher-temperature cases show slower thermal response due to the reduced convective transport and increased thermal consumption during desorption. Consequently, the thermal lag becomes more pronounced as the regeneration temperature increases.

These results demonstrate the trade-off between regeneration temperature and required purge-gas flow rate for achieving the target regeneration performance. Lower regeneration temperatures require substantially larger flow rates to compensate for the weaker desorption driving force, whereas higher temperatures reduce the required purge-gas flow rate by enhancing the desorption process.

The total regeneration power consumption was evaluated by considering both the pumping power P_{pump} and the thermal heating power P_{heat} :

$$P_{pump} = \Delta p \cdot Q_{vol} \quad (19)$$

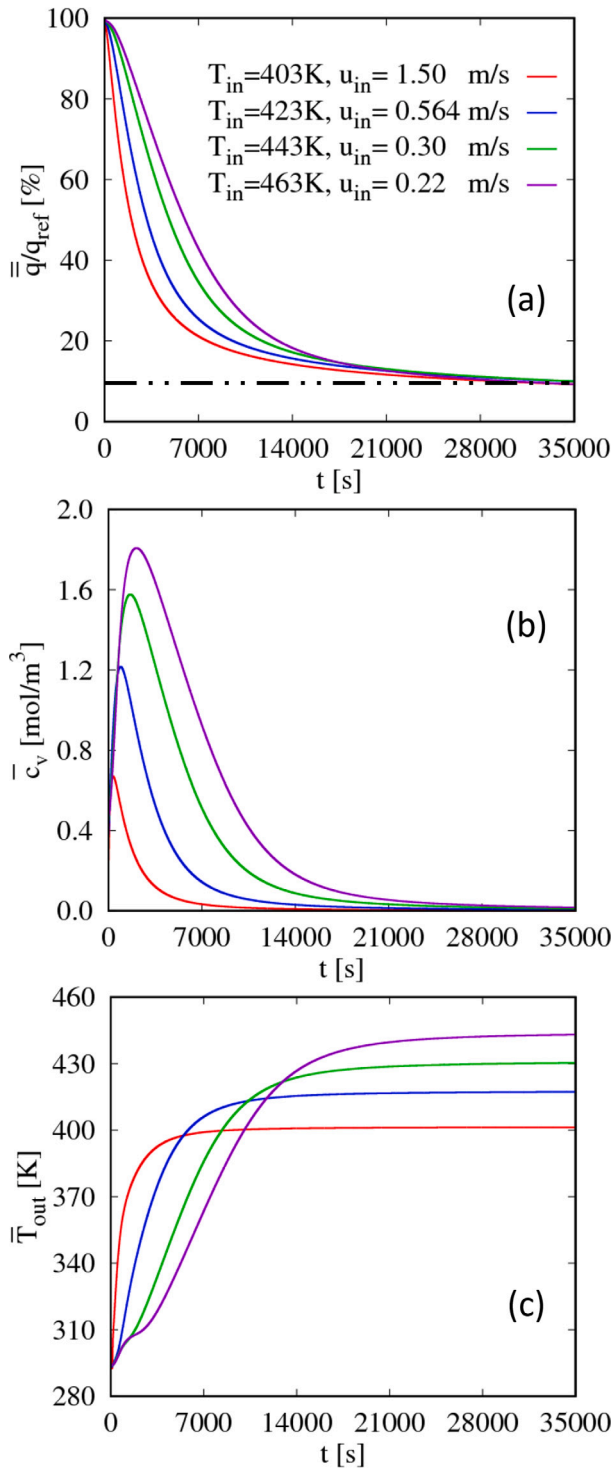


Fig. 15. Transient responses under different regeneration temperatures and corresponding inlet velocities satisfying the 90% moisture removal criterion: (a) normalized bed-averaged adsorbed amount, (b) average outlet vapor concentration, and (c) average outlet temperature.

$$P_{heat} = \dot{m}_{air} C_p (T_{in} - T_{\infty}) \quad (20)$$

The resulting power characteristics are summarized in Fig. 16. As shown in Fig. 16(a), the required purge-gas mass flow rate decreases significantly with increasing regeneration temperature because the elevated temperature enhances the desorption driving force and lowers the

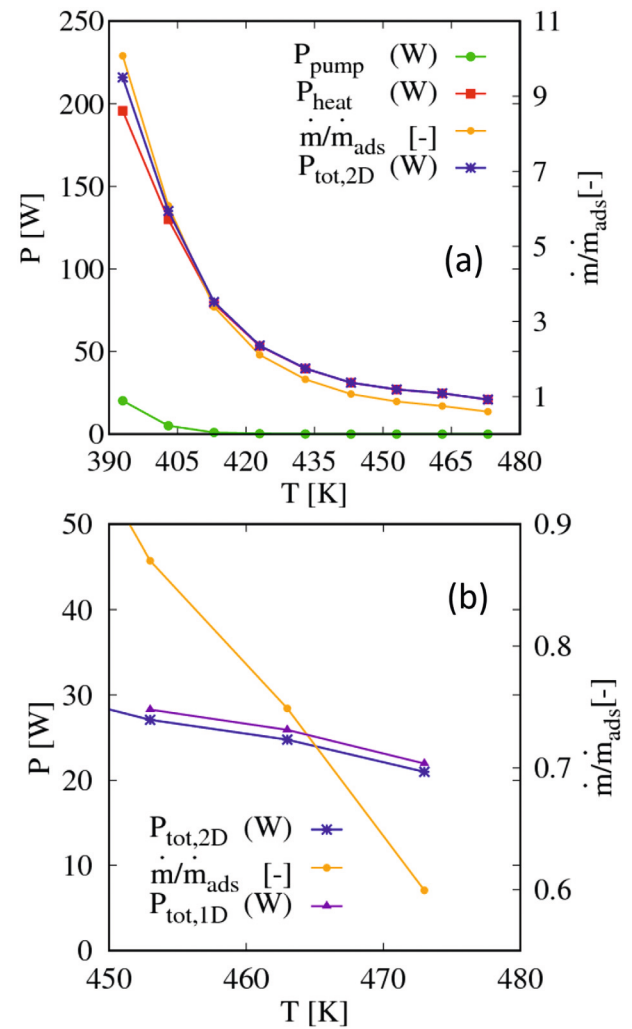


Fig. 16. Effects of regeneration temperature on the energy consumption and required mass flow ratio for desiccant regeneration: (a) overall trends and (b) enlarged view of the high-efficiency regime ($\dot{m}/\dot{m}_{ads} < 1$).

equilibrium adsorption capacity. The mass-flow-rate ratio $\dot{m}/\dot{m}_{ads}$ was introduced to evaluate the practical purge-gas requirement relative to the adsorption process. A value below unity indicates that the purge-gas flow rate required for regeneration is smaller than the dry-air flow rate used during adsorption. The ratio continuously decreases with increasing regeneration temperature and falls below unity in the high-temperature regime.

Fig. 16(b) provides an enlarged view of the high-efficiency regime where $\dot{m}/\dot{m}_{ads} < 1$. In this range, increasing the regeneration temperature from 453 K to 463 K and 473 K reduces the total regeneration power consumption by approximately 8% and 15%, respectively. This reduction occurs because the decrease in purge-gas flow rate and pumping power outweighs the additional thermal heating requirement. Among the investigated conditions, the lowest total regeneration power consumption is achieved at 473 K.

The comparison between the 1D and 2D models shows that the 1D model slightly overestimates the total regeneration power in this high-temperature regime, with discrepancies of 4.4%, 4.6%, and 4.6% at 453 K, 463 K, and 473 K, respectively. This difference arises because the 1D formulation enforces cross-sectional equilibration and cannot resolve radial thermal lag and residual moisture retention near the column wall. Consequently, the 1D model requires a slightly higher purge-gas flow rate to satisfy the same moisture-removal target. In contrast,

the 2D framework captures the balance between faster core desorption and delayed near-wall regeneration, providing a more realistic estimate of the regeneration power requirement.

It should be noted that the present power evaluation is based on the macroscopic pressure drop across the packed bed and the thermal energy required to heat the purge gas. This treatment is appropriate for the low-velocity porous-medium conditions considered in this study, where the bed-scale pressure drop is the pressure-loss contribution considered in the pumping-power estimate. However, practical regeneration systems may involve additional loss mechanisms, including entrance and exit losses, manifold and valve losses, flow maldistribution, local acceleration and deceleration associated with thermal expansion and density variation, and turbulence-related dissipation. These effects were not explicitly resolved in the present laminar porous-bed model.

In more complex internal flows involving non-equilibrium phase change, turbulence modeling can significantly influence the predicted flow structure, heat and mass transfer, and loss characteristics [41]. In contrast to such high-speed internal-flow problems, the present study focuses on coupled heat and mass transfer inside a low-velocity desiccant packed bed. Therefore, the calculated pumping power should be interpreted as a bed-scale estimate rather than a complete system-level power requirement.

Beyond the specific desiccant-bed configuration considered here, the present energy analysis suggests that fixed-performance optimization can be useful for other compressed-air energy systems where heat and mass transfer, flow requirement, and energy loss are strongly coupled. In compressed air energy storage systems, for example, compressor performance can be affected by moisture-related phase change, flow losses, and thermal-efficiency variations, and multidimensional numerical analysis has been used to guide compressor-operation optimization [42]. Although the present study deals with adsorption/desorption in a porous desiccant bed rather than condensation in compressor passages, both cases highlight the importance of resolving coupled transport processes when evaluating energy-efficient operation. Future work will extend the present framework to include detailed system components and additional flow-loss models for practical dryer modules.

4. Conclusions

A two-dimensional axisymmetric CFD model was developed to simulate adsorption and thermal regeneration in a zeolite 13X desiccant packed bed. The model incorporated LDF adsorption kinetics, a Sips equilibrium isotherm, conjugate heat transfer between the porous bed and column wall, and an implicit source-term treatment using a local pseudo-Jacobian. The proposed formulation improved numerical stability for strongly coupled heat and mass transfer without modifying the original LDF-Sips adsorption source term.

The comparison between the one-dimensional reference model and the two-dimensional CFD model showed that radial transport and wall thermal inertia strongly affect the predicted adsorption and regeneration dynamics. The one-dimensional model, which assumes instantaneous cross-sectional thermal equilibrium, underpredicted the regeneration time because it could not resolve the delayed near-wall desorption and wall-induced thermal lag. This result demonstrates the importance of multidimensional transport analysis for accurate prediction of desiccant-bed regeneration.

The energy analysis further showed that regeneration temperature significantly affects the balance between heating power, purge-gas requirement, and pumping power. Under a fixed regeneration time of 9.7 h and a 90% desorption target, increasing the regeneration temperature reduced the required purge-gas flow rate and lowered the total power consumption in the investigated operating range. The high-efficiency regime was identified when the purge-gas flow rate became lower than the adsorption flow rate, indicating that higher-temperature regeneration can be advantageous when the reduction in flow requirement outweighs the increase in heating demand.

Overall, the present results demonstrate that a two-dimensional CFD framework provides a more realistic basis for predicting desiccant-bed regeneration and identifying energy-efficient operating conditions. Future work will extend the present model toward practical dryer-module optimization by considering time-dependent boundary fluctuations, additional system-level flow losses, polluted moist air, and multi-component competitive adsorption.

CRedit authorship contribution statement

Minjun Kim: Writing – original draft, Software, Investigation, Conceptualization. **Gihun Son:** Writing – review & editing, Supervision, Methodology, Conceptualization.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Acknowledgments

This study was conducted with the support of the Korea Institute of Energy Technology Evaluation and Planning (KETEP) with funding from the government (Ministry of Trade, Industry and Energy) in 2026 (Project No. RS-2024-00423446).

Data availability

Data will be made available on request.

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