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# Dynamic Analysis of Adsorption Heat Transformation: A Dimensionless Model Approach for Comparative Evaluation of Sorption Bed Designs

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## 1. ABSTRACT

This research has concentrated on examining the dynamic behaviour of the adsorption process through numerical techniques. It explores a distinctive approach that facilitates a comparative analysis across diverse sorption bed designs, such as diverse heat exchangers with varying geometric characteristics and different arrangements of sorptive material. By a dimensionless lumped parameter model, the research not only offers computational efficiency but also provides a versatile framework for comparing sorption bed designs under different operating conditions.

## 2. INTRODUCTION

In recent times, there has been significant interest in adsorption-based heat transformation, encompassing technologies such as air capture, as well as adsorption-based heating and cooling. Despite the increasing adoption of these technologies, challenges persist in this field. Beyond the thermodynamic considerations of adsorption heat transformation, focusing on the dynamics of these systems is crucial to further elevate their efficiency. Examining the dynamic aspects of Adsorption Heat Transformation (AHT) requires acknowledging that considering separately the adsorbent materials from the heat exchangers would lead to an inaccurate interpretation. Additionally, the operational conditions during the adsorption/desorption steps constitute another factor influencing the dynamics of the process. To address these considerations, the Large Temperature Jump (LTJ) has been suggested, which involves examining an actual representative small section of the adsorption bed [1]. Various types of LTJ experiments, like Volumetric, Gravimetric, and Thermal Response Method (TRM), are documented in the literature [2]. Each of these approaches aims to track the evolution of uptake over time within a quasi-isobaric vessel, employing sophisticated and accurate experimental instruments. As conducting these experiments is both time-consuming and expensive, reliable numerical models become highly beneficial to explore the impact of various parameters on heat and mass transfer within adsorption beds. To simulate heat and mass transfer in adsorption beds, there are two approaches: 1) lumped-parameter model and 2) distributed-parameter model [3]. The former tracks the variation of key parameters (temperature, uptake, and pressure) over time, while the latter enables precise monitoring for parameter variations at every point in space within the bed at any given time. Although the lumped-parameter model offers less accuracy, it is more computationally efficient, cost-effective and a valuable aid to the initial system design. In current investigation, to circumvent both time-consuming experimental approaches and expensive numerical methods, a

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dimensionless version of the lumped parameter model is formulated and numerically simulated. The novelty of this analysis lies in its ability to provide a comprehensive exploration of sorption dynamics through the formulation and numerical simulation of dimensionless parameters. This approach allows for a nuanced comparison of bed designs, emphasizing the unique contribution of dimensionless numbers in characterizing and understanding the dynamic behavior of adsorption processes.

## 3. Methodology

The dynamics of an adsorption process are primarily influenced by the coupled of heat and mass transfer phenomena within the adsorption bed. In the context of governing equations using an original lumped parameter model, the temperature is regulated through a transient energy balance applied to the entire adsorber bed, as indicated by equation (1). Moreover, in the absence of experimental data regarding the outflow temperature of the heat transfer carrier fluid, an expression signifying the comprehensive balance of the heat carrier fluid, can be employed as equation (2).

$$\left[\left(mc_p\right)_{HEX} + \left(mc_p\right)_{ads} + \left(m_{ads}.w.c_{p_{sat.liq}}\right)\right]\frac{dT_{bed}}{dt} = m_{ads}\frac{dw}{dt}\,\Delta H - \left(\dot{m}c_p\right)_{htf}(T_{out} - T_{inlet}) \tag{1}$$

$$T_{out} = T_{bed} + (T_{inlet} - T_{bed})\exp\left[\frac{-UA}{\left(\dot{m}C_p\right)_{htf}}\right] \tag{2}$$

In the equation (1), the left-hand side includes the sensible heat associated with the entire adsorption process, encompassing the heat exchanger metal, adsorbent material, and adsorbed adsorbate. Meanwhile, the right-hand side incorporates the non-sensible power needed for the adsorption process and the overall input power. Equations (1, 2), along with the adsorption isotherm equation (Specifically, the Toth equation [4], with its coefficients derived from experimentally fitted curves on Silica-gel RD, provides an accurate predictive isotherm model for silica-gel) which characterizes mass transfer within the adsorbent material under equilibrium conditions, collectively dictate the entire dynamic behaviour of the adsorption process. The efficacy of capturing the system's dynamics through the governing equations is contingent upon the specific material pairs, bed design, and operational conditions, as evident in the system. In order to broaden the applicability of the captured dynamics, a set of novel dimensionless parameters, outlined in equation (3), has been introduced. These parameters encompass key factors essential for numerically replicating the TRM.

$$\tau = \frac{\left(\dot{m}C_p\right)_{htf}}{\left(mc_p\right)_{eff}}t,\ \theta = \frac{T - T_{inlet}}{T_{ini} - T_{inlet}},\ w^* = \frac{w - w_{ini}}{w_{final} - w_{ini}} \tag{3}$$

In the given set of dimensionless parameters, $\tau$ symbolizes dimensionless time, while $\left(mc_p\right)_{eff}$ denotes the overall heat capacity of the sorption bed. TRM reveals the maximum theoretical temperature and uptake variation in the system, expressed through the defined parameters $\Delta T = T_{ini} - T_{inlet}$ and $\Delta w = w_{final} - w_{ini}$. By incorporating this set of parameters, denoted as equation (3), into the governing equation, we derive the nondimensional form of equations, represented as equations (4, 5).

$$\frac{d\theta_{bed}}{d\tau} = K.\frac{dw^*}{d\tau} - \theta_{out},\ K = \frac{m_{ads}.\Delta w.\Delta H_{ads}}{\left(mC_p\right)_{eff}.\Delta T} \tag{4}$$

$$\theta_{out} = \theta_{bed}[1 - \exp(-NTU)],\ NTU = \frac{UA}{\dot{m}C_p} \tag{5}$$

Equations 4 and 5 reveal that the dynamic characteristics of an adsorption system can be delineated by two nondimensional numbers: $K$ and $NTU$. Specifically, $K$ signifies the ratio of the maximum energy generated from adsorption to the maximum sensible energy stored in inert mass during a step temperature change utilizing TRM. Alternatively, $K$ can be viewed as a parameter discerning the nature of the adsorber, where a coated bed is anticipated to have a considerably low $K$, contrasting with a packed bed that tends to exhibit a higher $K$ value. Moreover, $NTU$ serves as a representation of the number of energy transfer units within the adsorber, offering insights into the design

aspects of a sorption bed. Together, the parameters $K$ and $NTU$ provide a comprehensive understanding of the dynamic behaviour and design considerations inherent in adsorption systems.

## 4. Results and discussion

The combination system of equations results in a complex system of equations, necessitating numerical methods for solution. A numerical technique known as the implicit two-stage Runge-Kutta method, alternatively referred to as the trapezoidal rule, was employed to discretize the system of equations. Subsequently, the dynamics of the system were captured through the implementation of the Newton-Raphson nonlinear solver, facilitated by the development of a customized numerical code in MATLAB. Figure (1) illustrates the variation in dimensionless uptake and bed temperature for Silica-gel Fuji RD under a specific TRM condition, corresponding to $K = 1$, across a discrete range of $NTU$ values. The findings suggest that increasing NTU in an adsorber, while maintaining constant operating conditions for TRM, has a noteworthy impact on the time required for the system to reach its final equilibrium state.

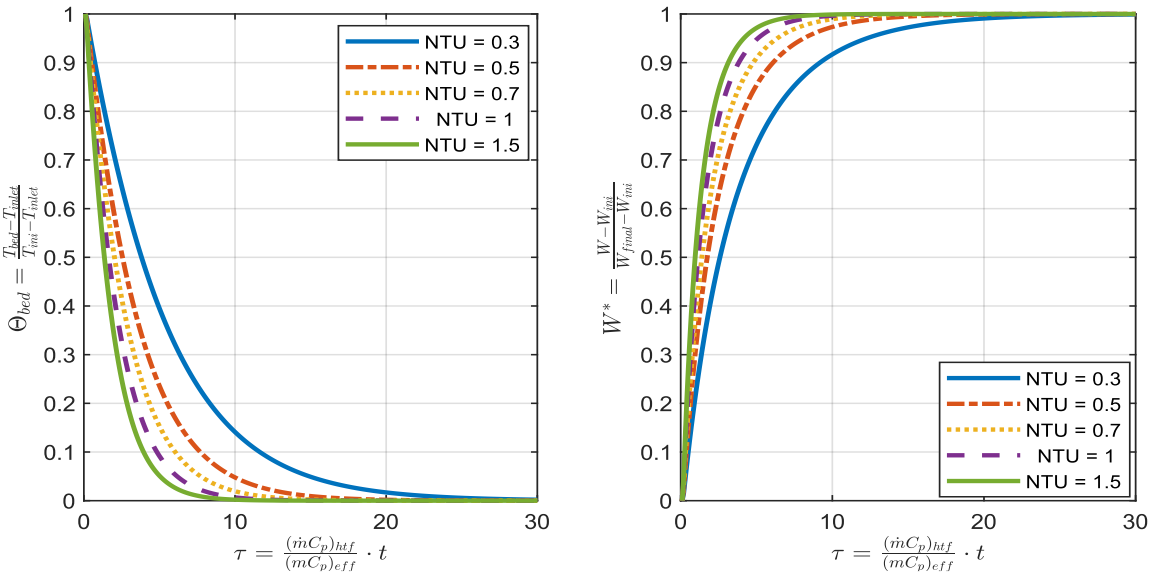


**Fig. 1:** Evolution of dimensionless temperature (right) and uptake (left) across dimensionless time.

## 5. Conclusion

This research introduces a numerical non-dimensional model utilizing innovative dimensionless parameters. This model facilitates a thorough comparative analysis from a design perspective on the dynamics of adsorption. In conclusion, the entire operational setup for TRM can be encapsulated within the parameter $K$. This allows for a comparison of bed designs by maintaining a constant value for $k$ while varying the $NTU$. To complete the current model in future works, the next step involves examining it as a predictive model through qualitative and quantitative assessments. This includes comparing it with a precise distributed parameter model, conducting experiments on sample adsorption beds, and studying the behaviour of sorbent materials.

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