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## A Mini-Review of Coupled Convection-Diffusion Equations in a Fixed-Bed Adsorption

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# A Mini-Review of Coupled Convection-Diffusion Equations in a Fixed-Bed Adsorption

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**Abstract.** Environmental contamination triggered by dyes has gained global attention. Industrial effluent of dye in high concentration into the rivers must be reduced to minimise the harmful effect on the quality of water that threatens human health. The removal of dye from wastewater is a significant step in addressing the problem of dye emission which can be achieved through adsorption separation technologies. In the most adsorption process, the adsorbent is in contact with fluid in a fixed bed. The performance of adsorptive separation of dye can be predicted through a fixed bed mathematical model which consists of coupled partial differential equations for optimizing the design and operating conditions. This paper presents a mini-review of mathematical modelling of fixed-bed adsorption of dye. The discussions are limited to the used of single component-dye separation in, convection-diffusion equations coupled with Langmuir isotherm. Besides, the numerical methods used for solving the convection-diffusion equations are also discussed in this paper.

## 1. Introduction

Pollution triggered by industrial wastewater has become a regular problem for many countries [1]. Dyes are the most common water pollutants that broadly exist in industrial waste streams [2]. The most significant sources of dyes released are from industries of cosmetics, textile, printing, plastics, paper production, leather and food industries [3]. Wastewater containing dyes has much impact on environmental protection that causes harm to aquatic life and humans [4]. A primary concern of increasing dye concentration and its effect on water quality has caused major environmental agencies and organisations effort including the United States Environmental Protection Agency (US EPA) to control and reduce the highly toxic and hazardous pollutants [5]. Therefore, it is essential to eliminate dyes from wastewater emitted by industries to avoid excess dyes discharge [4]. Various methods of treatment, for example chemical oxidation, electrochemical oxidation, coagulation, degradation, biological process and adsorption are increasingly been applied to reduce the presence of dye in wastewater [6].



Currently, the most extensively used technology for the elimination of dye from wastewater is adsorption [7] since it is taken into account as the best and most universal equilibrium separation method [8]. Besides, it was reported as an effective, efficient and economical method [7]. Generally, two types of adsorption can be categorised as static adsorption and dynamic adsorption. Static adsorption is known as batch adsorption that takes place in a closed system that only is used to treat the low volume of wastewater [9]. However, this process is not suitable in the case of column-mode operations [10]. Hence, fixed-bed adsorption is found to be more convenient over batch technique according to an industrial point of view as the adsorbent continuously remains in contact with fresh sorbate solution [8]. Fixed-bed adsorption is normally used for gas and liquid pollution control in flowing mode [9]. It is designed in such a way that the flowing polluted fluid encounters a fixed amount of adsorbent thereby creating room for treatment of a large volume of effluent fluid with less monitoring requirement [9]. Moreover, the system is easy to operate, low price and can easily be scaled up [9]. High selectivity and working capacity, as well as strong adsorption capability, is the key to choose a suitable adsorbent in the design of the dye adsorption process. As a result, a variety of adsorbents, such as alumina [11], silica gel [12], zeolites [13] and activated carbon [14] have been examined in recent years for this purpose. Many studies have chosen activated carbons in the elimination of different types of dyes since they are good materials but however, their use is limited and increase in cost [15]. Besides, it will become finished and are no longer be able to further adsorb the dyes. This has caused in attempts to prepare alternative adsorbents that are a low cost [16] from industrial waste, natural material, or agricultural by-products as these materials do not require any expensive additional pre-treatment step [17].

Determine the breakthrough curve is the main information needed in the design of appropriate column adsorption [18]. To gain the breakthrough curve of a given column adsorption system, two approaches that are widely used are direct experimentation or mathematical modelling [18]. A direct and brief breakthrough curve of a given system can be constructed from the experimental method. Nevertheless, it is regularly a time-consuming and economically is not always a desirable process, mostly for the trace pollutants and long amount of time that adsorbed molecules of dyes spend on the surface. Also, it greatly relies on the experimental condition, such as air temperature surrounding a component and modelling of residence time [18]. Comparatively, mathematical modelling is easy [18] and required in design and optimisation adsorption columns for representing and correlating the breakthrough curve data of the experiment [19]. Additionally, the number of experiments associated with new operating conditions can be minimised once mathematical modeling has been validated [20]. Attention among the researchers in the mathematical modelling process has increasingly attracted due to the reasons stated before.[18]. Therefore, the primary aim of this paper is to review recent research on the convection-diffusion equation and the numerical study used to simulate the behavior of the dye column adsorption system. Numerous methods for solving the mathematical equation for dye column-adsorption as well as different descriptions of the mass transfer mechanisms within the particle of adsorbent are reviewed.

## **2. Description of the Mathematical Equation**

### **2.1. Convection-Diffusion Equation Coupled with Source Term**

The fixed-bed adsorption system can be analysed and understood through the formulation and mathematical model. Mathematical model development plays a vital role in the prediction of breakthrough curve behavior [18]. The mathematical equations describing the fixed-bed adsorption are

partial differential equations that can be derived based on the mass conservation principle for fluid. The general form of a mass balance equation can be written as [21]

$$\text{Rate of material in} + \text{Rate of material out} = \text{Rate of accumulation of material} + \text{Rate of loss by adsorption}$$

The modelling of dye column adsorption has been divided into four basic parts: (1) liquid phase mass transfer including convective mass transfer and molecular diffusion, (2) interface diffusion between bulk solution and external surface of adsorbents and (3) intraparticle mass transfer including pore diffusion and surface diffusion. Liquid phase mass transfer is where the movement of molecules or ions in the column are in both axial and radial directions and usually is considered by other researchers in modelling of the fixed-bed adsorption process [6] [20] [22] [23] [24]. It is general to assume that homogeneous for all cross-sections and the movement is in axial as for simplification. Thus, radial movement can be neglected. Therefore, the equation for a mass balance that is acquired to represent the dynamic behavior of dye through fixed-bed is the convection-diffusion equation coupled with source term as shown in Equation (1) [6] [20] [22] [23] [23] [25]. This equation includes axial dispersion term, convection flow term, accumulation in the fluid phase and adsorption term.

$$-D_L \frac{\partial^2 c}{\partial z^2} + \frac{\partial}{\partial z}(vc) + \frac{\partial c}{\partial t} + \frac{(1-\varepsilon)}{\varepsilon} \frac{\partial \bar{q}}{\partial t} = 0 \quad (1)$$

Here,  $c$  is the concentration of the bulk solution,  $D_L$  is coefficient of axial dispersion,  $v$  is the superficial velocity,  $t$  is time,  $\varepsilon$  is the bed porosity,  $z$  is the distance to inlet and  $\bar{q}$  is the average adsorbed phase dye concentration [22]. Equation (1) is derived considering the assumptions as follows: (1) the system is in condition of isothermal, (2) no occurrence of chemical reaction in column, (3) radial dispersion is negligible, (4) the filling material is made of particles that are porous and uniform in size, (5) the flow rate is constant and (6) the equilibrium of adsorption is described by Langmuir isotherm. The next step is the interface diffusion between bulk solution and outer surface of adsorbent [18]. This is the first step in the adsorption process where the dye is transported from the fluid to the exterior surface of adsorbent across the boundary layer [6] [20] [22] [23] [24], and it is known as the film diffusion. It predominates the total uptake rate to some level and in some cases turn out to be the rate control step. The rate of mass transfer is stated as Equation (2) below;

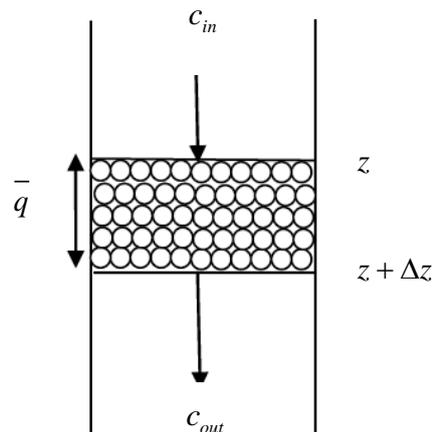
$$\frac{\partial \bar{q}}{\partial t} = k_f a (c - c_s) \quad (2)$$

where  $a$  is volumetric surface area,  $c_s$  is the dye concentration at the exterior surface of adsorbent and  $k_f$  is the coefficient of film diffusion. The second step in column adsorption is intrapellet diffusion.

The intraparticle or internal particle diffusion is a complicated step and plays a key role in the consideration of modelling column adsorption [6] [20] [22] [23] [24]. The diffusion of the dye occurs in the liquid within the pores of the adsorbent (pore diffusion) or along the pore walls (surface diffusion) are involved in intraparticle transfer simultaneously. Normally, Fick's law is used to describe the intraparticle diffusion of the dye inside the pores of adsorbent particles. However, to present the mass transfer into the pellets, some of the researchers [20] [22] [23] [24] apply a linear driving force to simplify the solution of the differential equations. It considers that the rate of mass transfer at a given point of the bed is proportional to the difference between the current of solute concentration on the adsorbent at a local level and that corresponding when the equilibrium with the bulk phase is achieved. The rate of uptake expression based on a linear driving force model is as shown [20]

$$\frac{\partial \bar{q}}{\partial t} = k_e (q - \bar{q}) \quad (3)$$

Where  $q$  is the loading of the dye at the exterior surface of the adsorbent and it is obtained from the Langmuir isotherm and  $k_e$  is the kinetic coefficient for intraparticle diffusion in the adsorbent. The process of dye flow through a packed bed based on Equation (1) is represented in Figure 1 [21].



**Figure 1.** Flowing of dye through a packed-bed

Another relationship is required to formally describe the fourth term on the left-hand side of Equation (1) as to relate the concentration of dye in the bulk with the adsorbed amount at the interface. This relationship is vital for the last step of adsorption process itself onto the surface and the relationship is given by the Langmuir isotherm as following [1] [16] [26] [27] [28];

$$q = \frac{q_m K c_s}{1 + K c_s} \quad (4)$$

where  $q$  is the equilibrium concentration in the solid phase,  $q_m$  is the maximum adsorption capacity of the adsorbent,  $K$  is the Langmuir isotherm constant and  $c_s$  is the concentration of solute in the liquid

phase inside the pores or equilibrium concentration in the liquid phase [18]. Choosing the isotherm style is a prerequisite in the modelling of the dynamic adsorption as it will directly affect the effect of mathematical modelling. The Langmuir isotherm assumes that the adsorption process occurs as a monolayer, homogeneous for the surface of the adsorbent and no interactions between the adsorbed molecules. No additional adsorption can occur at that site when once a site is occupied with dye molecule, it has been conclusively shown that the adsorption process is a monolayer in nature. Langmuir isotherm is frequently chosen by the researchers [6] [20] [22] [23] [24] due to its simple form and good-fitting performance [18]. Therefore, Langmuir isotherm has turn-into one of the most famous models in adsorption studies. Thus, Equation (1) along with Equation (4) gives a coupled system of differential equations due to the temperature-dependent in concentration and the adsorption rate [30]. Two dependent variables which make Equation (1) to be coupled are  $c$  and  $\bar{q}$ .

Proposing a general model is a difficult task but significant when considering the different components of the adsorption systems (dye and adsorbent), a variation of operation conditions and specific demands of accuracy and calculative simplicity since most models are derived from different assumptions. The differences in the mathematical models of adsorption processes arise from the different expressions of the mass transfer inside and outside the adsorbent particle and the equilibrium isotherm considered in convection-diffusion equation for the dye in a fixed-bed column [23]. Table 1 summarizes the main assumptions and considerations about the convection-diffusion equation for modelling the fixed-bed adsorption of dye reported in the literature.

**Table 1.** Summary of mathematical models based on convection-diffusion equations for fixed-bed adsorption of dye

Adsorbate	Adsorbent	Assumptions	Equation	Reference
Maxilon Goldgelb GL EC 400 % (MG-400) and Maxilon Schwarz FBL-01 300 % (MS-300).	Granular activated carbon and natural zeolite	<ul style="list-style-type: none"> <li>• Isothermal adsorption of a single component.</li> <li>• Negligible concentration gradient in the radial direction.</li> <li>• The Linear Driving Force (LDF) model is used.</li> <li>• The cross-section is constant and the properties of the adsorbent bed throughout the column are uniform.</li> </ul>	<p>Governing equation:</p> $v \frac{\partial c}{\partial z} + \frac{\partial c}{\partial t} + \frac{1-\varepsilon}{\varepsilon} \frac{d}{dt} (\varepsilon_p \bar{c} + \bar{q}) = D_L \frac{\partial^2 c}{\partial z^2}$ <p>Rate of mass transfer of dye from bulk fluid to the external surface of adsorbent:</p> $m = \frac{d}{dt} (\varepsilon_p \bar{c} + \bar{q})$ <p>In terms of external mass transfer, (LDF) model</p> $m = \frac{3k_f}{R_p} (c - c_s)$ <p>Rate of uptake equation based on the linear driving force (LDF) model for solid diffusion:</p> $m = \frac{15D_s}{R_p^2} (q - \bar{q})$ <p>Langmuir equation:</p>	[23]

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$q = \frac{q_m Kc_s}{1 + Kc_s}$			
Dye	Natural Zeolite	<ul style="list-style-type: none"> <li>• Isothermal adsorption of a single component.</li> <li>• Negligible concentration gradient in the radial direction.</li> <li>• The Linear Driving Force (LDF) model is used.</li> <li>• Constant cross-section and uniform properties of adsorbent bed throughout the column.</li> </ul>	<div style="text-align: right;">[22]</div> <p>Fluid phase mass balance equation:</p> $-D_L \frac{\partial^2 c}{\partial z^2} + \frac{\partial}{\partial z}(vc) + \frac{\partial c}{\partial t} + \left(\frac{1-\varepsilon}{\varepsilon}\right) \frac{\partial \bar{q}}{\partial t} = 0$ <p>Mass transfer rate of dye from bulk fluid to external adsorbent surface:</p> $m = \frac{d\bar{q}}{dt}$ <p>External mass transfer phase,</p> $m = \frac{3k_f}{R_p}(c - c_s)$ <p>Rate of uptake equation based on the LDF model for solid diffusion:</p> $m = \frac{15D_s}{R_p^2}(q - \bar{q})$ <p>Langmuir equation:</p> $q = \frac{q_m Kc_s}{1 + Kc_s}$
Basic Green 4	Activated carbon	<ul style="list-style-type: none"> <li>• The superficial velocity inside the column is constant.</li> <li>• The flow moves in the axial direction.</li> <li>• Isothermal system.</li> <li>• No chemical reaction occurs on the bed.</li> <li>• Dispersion in the radial direction is negligible.</li> </ul>	<div style="text-align: right;">[20]</div> <p>Conservation equation for dye:</p> $\frac{\partial c}{\partial t} + \left(\frac{1-\varepsilon}{\varepsilon}\right) \frac{\partial \bar{q}}{\partial t} + v \frac{\partial c}{\partial z} - D_L \frac{\partial^2 c}{\partial z^2} = 0$ <p>LDF model is applied to describe the adsorption rate process of the dye for the fluid phase of the adsorbent in terms of the global mass transfer of the fluid phase is shown below:</p> $\frac{\partial \bar{q}}{\partial t} = k_f a (q - \bar{q})$ <p>Langmuir isotherm:</p> $q = \frac{q_m Kc_s}{1 + Kc_s}$

		<ul style="list-style-type: none"> <li>The porosity of the bed inside the column is constant.</li> </ul>		
C.I Acid Blue 92	Exfoliated Graphite	<ul style="list-style-type: none"> <li>Implementing nonlinear isotherm.</li> <li>Linear driving force mass transfer.</li> <li>Axial dispersion</li> </ul>	<p>Applying mass conservation for dyestuff in the liquid phase:</p> $\left(\frac{\rho_b}{\varepsilon}\right) \frac{\partial \bar{q}}{\partial t} + \frac{\partial c}{\partial t} + u \frac{\partial c}{\partial z} - D_L \frac{\partial^2 c}{\partial z^2} = 0$ <p>Mass transfer resistance in the liquid phase is described by the LDF approximation:</p> $\frac{\partial \bar{q}}{\partial t} = k_f (c - c_s)$ <p>Langmuir isotherm:</p> $q = \frac{q_m K c_s}{1 + K c_s}$	[6]
Reactive blue 5G dye	Dowex Optipore SD-2	<ul style="list-style-type: none"> <li>Axial dispersion model.</li> <li>Homogeneously distributed adsorption particles.</li> <li>Isothermal and isobaric process.</li> <li>Constant physical properties of the bed and liquid phases.</li> </ul>	<p><b>Model 1</b></p> <p>Mass balance in the liquid phase:</p> $\frac{\partial c}{\partial t} + v \frac{\partial c}{\partial z} + \left(\frac{\rho_b}{\varepsilon}\right) \frac{\partial \bar{q}}{\partial t} - D_L \frac{\partial^2 c}{\partial z^2} = 0$ <p>External mass transfer resistance:</p> $\frac{\partial \bar{q}}{\partial t} = \frac{k_f \varepsilon}{\rho_B} (c - c_s)$ <p>Langmuir isotherm:</p> $q = \frac{q_m K c_s}{1 + K c_s}$ <p><b>Model 2</b></p> <p>Mass balance in the liquid phase:</p> $\frac{\partial c}{\partial t} + v \frac{\partial c}{\partial z} + \left(\frac{\rho_b}{\varepsilon}\right) \frac{\partial \bar{q}}{\partial t} - D_L \frac{\partial^2 c}{\partial z^2} = 0$ <p>LDF model is used for internal mass transfer resistance</p> $\frac{\partial \bar{q}}{\partial t} = -k_f (\bar{q} - q)$	[24]

Langmuir isotherm:

$$q = \frac{q_m K c_s}{1 + K c_s}$$

### Model 3

Mass balance in the liquid phase:

$$\frac{\partial c}{\partial t} + v \frac{\partial c}{\partial z} + \left( \frac{\rho_b}{\varepsilon} \right) \frac{\partial \bar{q}}{\partial t} - D_L \frac{\partial^2 c}{\partial z^2} = 0$$

Adsorption in the adsorbent sites described by pseudo second-order reaction rate law:

$$\frac{\partial \bar{q}}{\partial t} = k_a (q_m - \bar{q}) c - k_d \bar{q}$$

Reduces to Langmuir isotherm at equilibrium:

$$\frac{\partial \bar{q}}{\partial t} = k_a (q_m - \bar{q}) c - \frac{k_a}{K} \bar{q}$$

As can be seen from Table 1 (above), a number of researchers have proposed a few mathematical models to describe the dye column adsorption process, which can commonly be categorised into adsorption reaction models [24] and diffusion models [6] [20] [22] [23]. The kinetic process of adsorption can be described based on both models. However, both models are quite different. It has been noted that the construction of adsorption diffusion models are usually based on three different stages in a fixed-bed adsorption process such as external, internal mass transfer and adsorption in adsorbent sites where the main equation involved is the convection-diffusion equation, Equation (1) together with Equation (2), Equation (3) and Equation (4). However, Marin, Borba, Módenes, Espinoza-Quiñones, Oliveira and Kroumov [24] have used the adsorption reaction model in their research. This model originating from chemical reaction kinetics that is based on the entire process of adsorption without considering stages in the fixed-bed adsorption process. They describe the adsorption in the adsorbent site by using a pseudo-second-order reaction rate model. Generally speaking, this model [24] cannot offer valuable information to obtain a deep understanding of the adsorption mechanism and to design a system of fixed-bed and are therefore not representative of the real course of adsorption [30]. On the contrary, a real adsorption course can be represented more reasonably through the adsorption diffusion models that are based upon basic steps together with the convection-diffusion equation [30]. The mathematical models [6] [20] [23] [24] develop have considered the convection-diffusion equation together with mass transfers are shown to be suitable for the prediction of concentration of dye in the fixed-bed adsorption since they can represent a significant tool for the textile industry used. To solve the mathematical formulation, the numerical method is needed for the simulation of fixed-bed dynamics.

## 2.2. Numerical Method

The solution of the coupled convection-diffusion equation and their associated initial and boundary conditions play a significant role in the modelling of the breakthrough curve for a fixed-bed adsorption system of dye. Accurate prediction of the breakthrough curve is crucial to determine the operation and the dynamic behaviour of column adsorption. Very few partial differential equations have the analytical or exact solution due to the complexity and nonlinearity of mathematical. Even in linear and extremely simplified cases, analytical solutions are scarce and generally slowly converging. Hence, numerical methods are the only possible alternative to find an approximate solution of the convection-diffusion equation to simulate the breakthrough curve of the fixed-bed column [31].

Several sophisticated models have been successfully developed by researchers to solve equations by implementing numerical methods that are finite difference method (FDM) [6] [22] [23] and finite volume method (FVM) [20]. FDM is the oldest method used to replace the derivatives in the differential equations by finite difference approximations which give an algebraic system of equations to be solved in place of the differential equation [32]. The major advantages of FDM are that it is simple, efficient in solving parabolic equations and ease of varying initial and boundary conditions [31]. However, this method cannot directly be applied in curvilinear coordinates, without transforming into a Cartesian coordinate system [33]. Markovska, Meshko, Noveski and Marinkovski [23] have transformed the coupled convection-diffusion equation into a set of an ordinary differential equation using FDM and then solve using SPEEDUP software for adsorption of Maxilon Goldgelb GL EC 400 % (MG-400) and Maxilon Schwarz FBL-01 300 % (MS-300) onto granular activated carbon and natural zeolite. The result appeared a satisfying agreement between the experimental and the simulation of breakthrough curves. However, the model is not quite fulfilled for these experiments as some deviations are found between the experimental and predicted data. This denotes especially to the assumption of a constant coefficient of solid diffusion. The values of the solid diffusion coefficient, the coefficient of axial dispersion and the coefficient of external mass transfer are required to be manipulated to obtain satisfactory agreement between the simulated and the experimental breakthrough curves.

Babu and Gupta also [22] considered solving the equations simultaneously using the explicit finite difference method and simulating the solution using MATLAB. The simulations are carried out to understand the influence of axial dispersion, external film resistance and solid diffusion resistance on adsorption of dye on natural zeolite. However, they found the axial dispersion, coefficient of solid diffusion and external mass transfer need to be adjusted to give the best-fit curve. Goshadrou and Moheb [6] also applied FDM in discretization and simulate the behavior by ODE integrator subroutine of MATLAB for C.I Acid Blue 92 dye adsorption on exfoliated graphite. The breakthrough curves obtained from modeling and experimental work are compared showing a very good agreement.

FVM used a discretization technique for partial differential equations based on the integral form of the conservation laws, rather than their differential form [34]. This method is particularly useful for direct discretization in the physical space [33]. Thus, there are no problems with any kind of transformation between the physical and the computational coordinate system. Souza, Peruzzo and de Souza [20] obtain a discretized form of the coupled convection-diffusion equation and showed a good agreement with the experimental data. Model [20] based on the Basic Green 4 dye on granular activated carbons shown to be convenient for the prediction of the mass transfer process. Downhill simplex optimization method is used to solve the coupled convection-diffusion equations. The mass transfer limiting step of reactive Blue 5G dye is identified through the simulation result using Maple software for removal process in a fixed-bed column packed with Dowex Optipore SD-2 adsorbent.

### 3. Conclusion

Mathematical modelling and simulation processes are the essential tools in the design and understanding of the fixed-bed adsorption system performance under various conditions to improve operation. A review of mathematical modelling of fixed-bed adsorption of dye conducted by various researchers is provided in this study. Most of the model reviewed here include mass transfer rate, resulting in a theoretical represent that more closely approximates an actual process. Recently, researchers have shown an increased interest in solving a convection-diffusion equation together with mass transfer rate and Langmuir isotherm for modelling and design of a column adsorption process. So far, however, there has been little discussion about solving the convection-diffusion equation for dye fixed-bed column adsorption. The solution of the convection-diffusion equation requires a numerical method to solve the equation. The convection-diffusion equation has been solved by many researchers mostly using FDM and FVM. There are two main obstacles may be faced in the simulation of convection-diffusion equations using numerical methods. This is due to the coupling between convection-diffusion equations with the adsorption isotherm. The used of a reduced mathematical model is recommended in getting the simulation results since it can aid in the identification of mass transfer mechanism, interpretation and analysis of experimental data, prediction of responses due to changes in the operational condition and process optimisation [24]. Simplify the representation of mass transfer phenomena within the adsorbent particles is one of the alternatives in facilitating the fixed-bed adsorption calculation. To represent numerical data realistically, it is suggested to solve the convection-diffusion equation with the combination of other numerical methods or improved methods [31] to accurately represent the dye adsorption onto a fixed-bed column and thus, several experiments associated with new operating conditions can be reduced.

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