Proceedings of the 2005 Winter Simulation Conference
M. E. Kuhl, N. M. Steiger, F. B. Armstrong, and J. A. Joines, eds.

NUMERICAL SIMULATION OF DYEBATH AND THE INFLUENCE OF DISPERSION FACTOR ON DYE TRANSPORT

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ABSTRACT

In order to model the mass transfer in a fluid, a “dispersion” model is frequently used. When the flow behavior does not drastically deviate from plug flow, the model performs well. The dispersive flow properties of liquids within fibrous textile assemblies however, have not been fully explored. In the mass transfer model, the dispersive flow is assumed to reduce the concentration gradient of dye liquor flowing through the package. This paper illustrates the influence of dispersion term on dye transport based on numerical simulation of dyebath. The transfer of dye through the package is described by a set of time-dependent partial differential equations, which govern convection, dispersion, and adsorption of dyes in the dyebath and across the yarn package. The simulation results prove, theoretically, that the inclusion of the dispersion term in the dyeing model improves the results of the dyeing process in terms of dye uptake and levelness.

1 INTRODUCTION

Uniform deposition of chemicals and reagents within the system is often of great importance. This is a critical requirement for the dyeing process where variations in deposition could lead to different colour tones and shades, often synonymous with the rejection of the dyed articles.

In order to model the mass transfer in a fluid system, a “dispersion” model is frequently used to represent flow characteristics in packed-bed reactors. In real systems where the flow behavior does not drastically deviate from plug flow, the model performs well (Greenkorn 1983). However, the dispersive flow properties of liquids within fibrous textile assemblies have not been fully explored.

In the mass transfer model, the dispersion factor is assumed to reduce the concentration gradient of dye liquor flowing through the package, resulting in a more even distribution of dye in the liquor within the package (Vosoughi 1993). Little has been published describing the influence of dispersion factor on dyeing rate. For example, although Burley (Burley et al 1985) included the dispersive transport of dye into formal mathematical equations in their model of textile dyeing processes, by containing the dispersion model parameter – denoted as the dispersion coefficient. However, the degree of significance of the effect of dispersion factor on dyeing was not clearly shown.

In addition, for modeling the mass transfer in real systems, a clear definition of dispersion is essential, as there are different descriptions among the different workers and within different fields, which often causes confusion.

2 THEORY

The flow of a fluid through a packed bed with a given velocity is quite complex, and the solution even in one-dimension with fluids of uniform properties are difficult. This is due to the fact that the mixing takes place both longitudinally (in the direction of flow) and transversely (perpendicular to the flow). There are three different phenomena involved in this process:

- Diffusion, a random process due to molecular motion, which is flow velocity independent.
- Dispersion, occurring in flow in which layers of different velocity exist, which is flow velocity dependent.
- Convection, the movement of molecules due to the flow.

2.1 Diffusion

The most fundamental process for dispersion is molecular *diffusion*, which is a special case of dispersion when the velocity of the fluid is zero. Molecules in the liquid state are not stationary, even if the bulk fluid velocity is zero, because the molecules are in continuous motion. The flux due to the random molecular motion can be represented by equation (1) below: (Crank 1975)

$$j_{dif} = -D_{dif} \frac{\partial c}{\partial x} \tag{1}$$

where D_{dif} is diffusion coefficient, c the concentration of diffusant, and x the distance. If the direction after each molecular collision is random, then the mean square distance traveled is proportional to time and the proportionality constant is the molecular diffusivity. In mathematical terms, this is known as Fick's 2nd law (named after the German physical chemist Fick):

$$\frac{\partial c}{\partial t} = D_{dif} \frac{\partial^2 c}{\partial x^2} \tag{2}$$

That is, the change in concentration over time, at a given point, is proportional to the slope of the concentration gradient, with movement from areas of high concentration to areas of low concentration. This law is simply a mathematical description of the macroscopic consequence of random motion.

2.2 Dispersion

Dispersion occurs in any kind of flow in which layers of different velocity exist. It is a process of distributing or spreading out of concentration profiles due to mechanisms in which the flux is proportional to the concentration gradient (Burley et al 1991).

$$j_{dis} = -D_{dis} \frac{\partial c}{\partial x} \tag{3}$$

where D_{dis} is dispersion coefficient, which is flow velocity dependent, c the concentration of chemicals, and x the distance. In the context of this work, the term 'dispersion' means the process of distributing or spreading out of concentration profiles due to mechanisms in which the flux is proportional to the concentration gradient. It does not relate to the particle size distribution of dyes or pigments, which is another commonly used term in coloration technology.

It is important to note that dispersion is a process in which the mass of the species is conserved. The species mass conservation equation includes a term with the divergence of the flux of the species. If the flux depends on the concentration gradient, then the conservation equation will have second order spatial derivatives of concentration. Thus, dispersion will add second order spatial derivatives of concentration (or saturation) to the conservation equation.

$$\frac{\partial c}{\partial t} = D_{dis} \frac{\partial^2 c}{\partial x^2} \tag{4}$$

In this model, similarity to Fick's Law of diffusion is used whereby a dispersion coefficient, D_{dis}, is defined and employed to present the macroscopic transport of material instead of Fick's molecular diffusion coefficient.

2.3 Convection

Convection is the process in which chemicals are transported due to bulk movement of the fluid, and which is assumed the fastest form of chemical transport in liquor. The flux due to the bulk flow is

$$J_c = vc \tag{5}$$

where v is the average velocity of the bulk flow. As a result, the concentration decreases in the direction of fluid movement.

$$\frac{\partial c}{\partial t} = -v \frac{\partial c}{\partial x} \tag{6}$$

These three phenomena of diffusion, dispersion, and convection are assumed to be additive and independent [6]. The presence of the cross-flow does not bias the probability that the molecule will take a diffusive step to the right or the left; it just adds something to that step. Therefore, the total flux of dissolved solute can be shown as:

$$\begin{gathered} J = j_c + j_{dis} + j_{dif} \\ J = vc - D_{dif} \frac{\partial c}{\partial x} - D_{dis} \frac{\partial c}{\partial x} \end{gathered} \tag{7}$$

or, by combining the last two terms

$$J = vc - D \frac{\partial c}{\partial x} \tag{8}$$

where "D" in this equation is the mathematical representation of diffusion, but it is greater than what would be observed by diffusion alone. It is called the dispersion coefficient, but it should be emphasized that it includes both convective and diffusive mechanisms. If the dispersion is seen to increase with velocity, it is often given as a composite term: $D_{dis} = \alpha v$, where α is the dispersivity, a fundamental property for a system.

Based on Equation 8 and the conservation of mass for chemical transport in a fluid system, a convection-dispersion-sorption equation can be derived (Zhao 2004) as:

$$\varepsilon\frac{\partial C_p}{\partial t}+(1-\varepsilon)\frac{\partial C_f}{\partial t}=-\nabla\cdot(UC_p)+\nabla\cdot(D\nabla C_p) \tag{9}$$

where C_p and C_f are concentration of dye in liquor and on fibres within the system, respectively, ε is the porosity of the package, and U is interstitial velocity of flow within the package.

It should be noted that in many of the previous researchers publications, the term (D) in equation (9) was intermittently defined as either dispersion or diffusion. In the context of this work, dispersion is used to describe this phenomenon, whereby the diffusion is a special case of dispersion when the velocity of the fluid is zero.

3 SOLUTION AND DISCUSSION

3.1 Basic Assumptions and System Geometry

The following assumption were used in the design of the numerical simulation model.

1. The density of dye liquor is considered constant under isothermal conditions.
2. The dye liquor is assumed as a Newtonian fluid, the viscosity is constant.
3. The influence of external volume force field, such as gravity is ignored.

The dye-liquor is assumed to circulate through the package. The direction of the flow is reversible either from out-to-in or in-to-out. Due to the symmetry of the package, the geometry of the system can be simplified to that shown in Figure 1. The symmetric line was treated as the left boundary of the system.

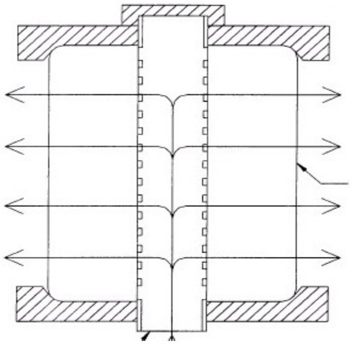

Figure 1: Geometry of the System

3.2 Parameters

The common parameter values used in the model are given below:

• *Package* inner radius	0.018m
• *Package* outer radius	0.056m
• *Package* height	0.136m

3.3 The Role of Dispersion Factor

Based on the model equations and numerical methods, the results of computer simulation of dyeings of textile packages can be presented and discussed. The results are mainly presented in graphical forms.

To evaluate dyeing quality, two aspects of dyeing should be considered: the dye uptake rate on fibres and the levelness of dye distribution throughout the package. The concentration of dye at the end line (flow exit face) of the package (CDEP) with time could be used to represent the rate of dye uptake providing no-reversal of flow is employed during the dyeing. The simulation results obtained provide the opportunity to formulate a dimensionless criterion for the prediction of the levelness of dyeing of a cylindrical fibrous package. This criterion can be named as dye distribution factor (DDF), which is the ratio of the lowest to the highest concentration of dye on fibres in the package at the time at which the levelness is examined.

Figures 2 and 3 present the simulation results of both CDEP and DDF against time, where the dispersion coefficients are $1.25\text{x}10^{-4}$, $1.25\text{x}10^{-5}$, and 0 (no adsorption term), respectively.

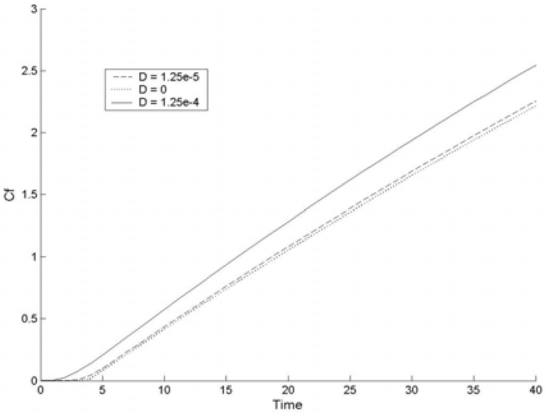

Figure 2: CDEP against Time for Different Dispersion Coefficients.

Figure 2 shows that an increase in dispersion coefficient does not significantly change the rate of dye uptake on fibres after a very short time period (5 time unit), although it slightly increases the value of CDEP during the process. The effect however, is minimal since an increase of 10 times in dispersion coefficient only causes an increase of 13.4% in CDEP. When the dispersion coefficient is zero, which means the dispersion term is ignored within the system, the final value of CDEP is only slightly less than that compared to a system where the dispersion coefficient is $1.25x10^{-5}$. This simulation result implies that the dispersion term does not play an important role during the dyeing in terms of influencing the rate of dye uptake.

It can be seen from Figure 3 that the effect of dispersion coefficient on the levelness of dye distribution across the package is similar to the effect of dispersion on the dye uptake rate. In other words, the DDF is increased as the dispersion coefficient is increased, which is consistent with that well accepted assumption stating that dispersion factor can influence even distribution of dye in the liquor within the package by reducing the concentration gradient of dye liquor flowing through the package.

When the dyeing systems were of the Freundlich and Langmuir adsorption isotherm types, similar results were obtained for both CDEP and DDF, further demonstrating that a higher dispersion coefficient leads to a higher dye uptake and a better levelness of dye distribution across the package, though the effect was not large.

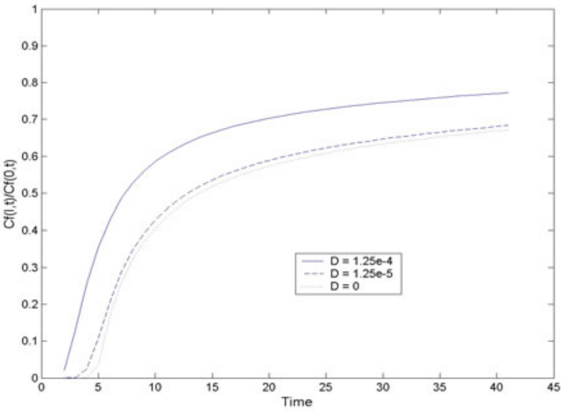

Figure 3: DDF against Time for Different Dispersion Coefficients using a Nernst Type Adsorption Isotherm.

The results proved in theory that the inclusion of dispersion term is favorable for dyeing, in terms of both dye uptake and levelness, compared with the results obtained from the dyeing when the dispersion term is ignored.

4 CONCLUSIONS

The use of computational methods to simulate the dyeing process provides a powerful tool to facilitate the understanding of the kinetics of mass transfer in aqueous solutions during the dyeing process. In this study, the transfer of dye through the package was described by a set of time-dependent partial differential equations, which govern convection, dispersion, and adsorption of dyes in the dyebath and across the yarn package. The study leads to a precise knowledge of the kinetics of dyeing during the process which can lead to improving process control, reliability and, perhaps most importantly, the environmental impact of the dyeing process.

The simulation results prove, theoretically, that the inclusion of the dispersion term in the dyeing model improves the results of the dyeing process in terms of dye uptake and levelness. Increasing the size of the dispersion coefficients in simulations resulted in increased dye uptakes and improved degrees of dye distribution across the package. However, the recorded difference in simulated results was minimal. Therefore, in order to simplify the dye transfer model it may be reasonable to ignore the dispersion effect.

These results of these simulations can be used to further the understanding of the dispersion phenomena and its role in the dyeing process. They could also aid in introduction of novel approach to design the package dyeing process control.

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