Analysis and Measurement of Ink Media Interactions in Inkjet Printing

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ABSTRACT

A study is presented of various effects involved in the interactions of pigmented ink with porous media in conventional inkjet printing applications. The study involves the use of two different numerical models, one for predicting the absorption of ink in porous media and another for predicting the flocculation of pigment during absorption. Specifically, computational fluid dynamic (CFD) analysis is used to predict the absorption of an impacting droplet on a porous substrate taking into account the velocity, viscosity and surface tension of the droplet and the porosity and permeability of the media. A population balance model is used to study flocculation of pigments. The models are demonstrated via application to conventional inks and media.

***Keywords*:** Inkjet Printing, Ink media interactions, Flocculation, Ink pigment aggregation, ink absorption, Population balance modeling of particle aggregation, porosity of ink jet paper, permeability of inkjet paper.

1 INTRODUCTION

The commercialization of a modern inkjet printing system is a complex undertaking that requires an interdisciplinary team to address numerous critical and fundamental issues encountered throughout the product development cycle. An inkjet development effort spans a broad range of diverse yet coupled activities that include the rational design of ink formulations, design and optimization of a droplet generator, precision control of a high-throughput deposition of droplets onto a moving media and modeling and characterization of various ink media interactions, e.g. spreading, absorption and coalescence of droplets, to achieve high image quality. The focus of this presentation is on ink media interactions (Fig.1), which directly impact inkjet print quality and speed. We present and demonstrate two models for predicting ink media interactions, a CFD-based approach for predicting the absorption and spreading of droplets upon impact with porous media, and a population balance approach for predicting the flocculation of colloidal ink pigments during the ink deposition process. The CFD analysis takes into account the physical properties of the media such as porosity, permeability and contact, and critical properties of the ink including surface tension and viscosity, as well as the size and velocity of the incident droplet. The population balance model, which is based on Smoluchowski kinetics and DLVO theory, is used to predict the flocculation of ink pigments taking into account the initial size distribution and surface potential of the particles and the ionic strength of the ink [1-2]. Theoretical and experimental results are presented to quantify these processes. The challenges associated with the quantifying ink media interactions are also discussed.

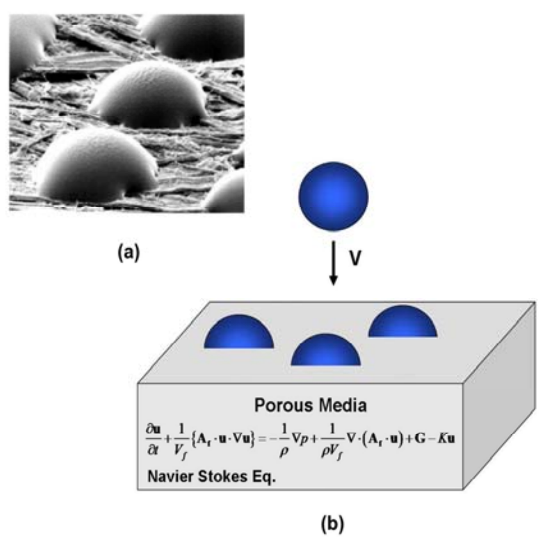


Figure 1: Ink media interactions: (a) ink drops on a porous media, (b) illustration of a CFD model used to predict ink absorption.

2 MODELING AND RESULTS

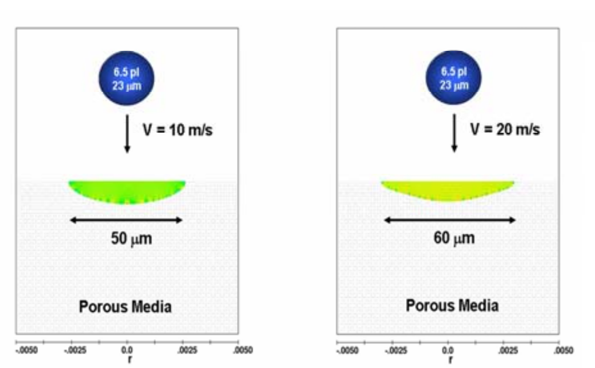
We use two different and complimentary models to study ink media interactions, a CFD-based model for ink absorption and a population balance model to predict pigment flocculation.

2.1 Ink Absorption

We use CFD analysis to study drop spreading as a function of surface and fluid properties. The volume of fluid method (VOF) as implemented in the FLOW3D software (www.flow3d.com) was used for this analysis The Navier-Stokes equation with a distributed resistance term is implemented for this analysis

$$\frac{\delta \mathbf{u}}{\delta t}+\frac{1}{V_f}\left\{\mathbf{A_f}\cdot\mathbf{u}\cdot\nabla\mathbf{u}\right\}=-\frac{1}{\rho}\nabla p+\frac{1}{\rho V_f}\nabla\cdot\left(A_f\cdot\mathbf{u}\right)+\mathbf{G}-\boldsymbol{K}\mathbf{u} \quad (1)$$

where **u** and p ate the velocity and pressure in the fluid, V_f is the volume fraction (porosity) of a computational cell, A_f is the diagonal tensor area fractions of a cell. ***K*** is a drag coefficient that accounts for the flow resistance in the porous medium. We performed parametric analysis of ink absorption as a function ink and media properties that are characteristic of commercial inks and papers. Examples of this analysis are shown in Fig. 2. In this analysis the volume of drop is 6.5pl. The ink has a viscosity of 2.5 cp and its surface tension is 40 dyne/cm. We assume an ink-media contact angle of 45 degrees. The porosity of media is 50%. The capillary pressure of the media is computed using Eq. (2), and the drag coefficient of media is



(a) **(b)**

Figure 2. CFD analysis of ink absorption, a 6.5pl droplet impacting a porous media at two different velocities: (a) v = 10 m/s, (b) v = 20m/s.

evaluated using Eq. (3),

$$p_{cap}=\frac{4\sigma\cos(\theta)}{d} \quad (2)$$

$$K=\frac{\mu\phi}{\rho\kappa} \quad (3)$$

In these equations d, ϕ μ, ρ and k are the average pore size, porosity, viscosity, density and permeability of the media, respectively. The analysis of Fig. 2 shows that if the drop hits the media at 5 m/s, it spreads to a spot size of approximately 50 μm in diameter, and this increases to 60 μm at an impact velocity of 10 m/s. The CFD analysis can be used to study this process in detail.

2.2 Pigment Flocculation

In order to model pigment flocculation (aggregation) one needs to quantify the aggregation kernels or aggregation rate constant for the particulate system in question. The key factors affecting the aggregation rate constant are the inter-particle forces and stability ratio derived from the properties of the kernels [1-3]. The two major contributions to the inter-particle interaction are the electrostatic repulsive forces and the Van der Waals attraction force. The total interaction potential energy V_T between two particles is found by simple arithmetic addition of repulsive V_R and attractive V_A potentials associated with these forces,

$$V_T(H)=V_R(H)+V_A(H) \quad (4)$$

$$V_A(H)=-\frac{A}{6}\left[\frac{2a_1a_2}{h^2+2a_1h+2a_2h}+\frac{2a_1a_2}{h^2+2a_1h+2a_2h+4a_1a_2}+\ln\left(\frac{h^2+2a_1h+2a_2h}{h^2+2a_1h+2a_2h+4a_1a_2}\right)\right] \quad (5)$$

$$V_R(H)=\frac{\varepsilon_0 a_1 a_2\left(\psi_1^2+\psi_2^2\right)}{4\left(a_1+a_2\right)}\times\left[\frac{2\psi_1\psi_2}{\left(\psi_1^2+\psi_2^2\right)}\ln\left(\frac{1+\exp(-\kappa H)}{1-\exp(-\kappa H)}\right)+\ln\left(1-\exp(-2\kappa H)\right)\right] \quad (6)$$

where a_1 and a_2 are the radii of the particles, and H and h are the surface-to-surface and center-to-center distance between them, respectively. The accuracy of the stability ratio depends on the validity of the inter-particle forces used for their calculations. In our model, Van der Waals force is modeled using Hamaker theory [4]. Hamaker derived the attractive potential energy between unequal spheres and separated by distance h by equation (5). The value of effective haymaker constant for carbon black is 0.79×10^{20}. Electrostatic repulsive potential is estimated using the solution of Poisson Boltzmann equation derived by Hogg, Healy and Fuerstenau [5]. Equation (6) is used to evaluate electrostatic repulsive potential for two dissimilar spheres and unequal surface potential but the validity of the equation is limited to $\kappa a > 5$ and values of the surface potential up to 70mV.

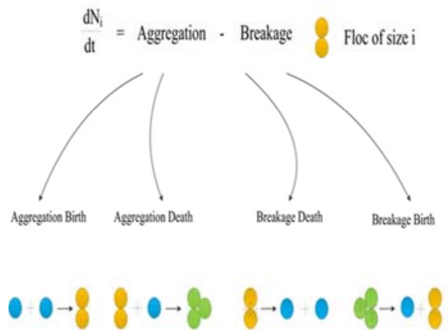


Figure 3. Population balance: illustration of aggregation birth and aggregation death of particles.

The aggregation kernel is defined in terms of a continuous population balance model for aggregation. The aggregation coefficient beta is effectively the rate constant of aggregation for two particles. For our model the aggregation coefficient is given by Eq (7), where k_f is the rate of aggregation derived from the appropriate collision mechanism and $W_{i,j}$ is the stability ratio calculated from the models for inter-particle forces. The collision

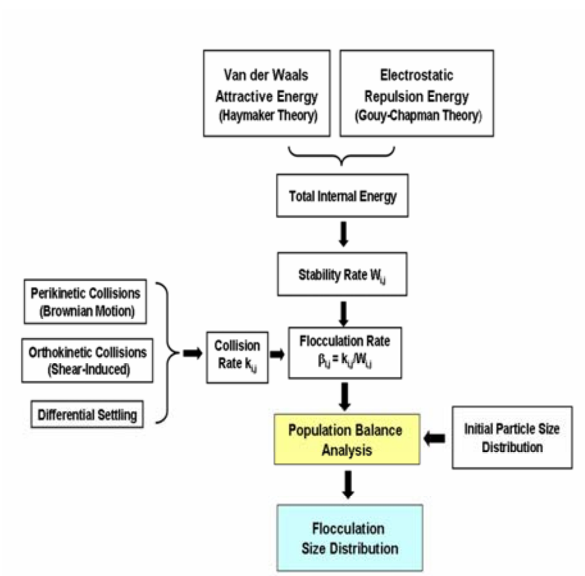


Figure 4. Flow chart of population balance model.

mechanism accounts for the manner in which collision occurs (assuming no inter-particle forces), and the stability ratio accounts for any deviations from this idealized case due to the presence of inter-particle force. There are three types of collision mechanisms that can influence particle aggregation, namely perikinetic, orthokinetic and sedimentation. In our application, the perikinetic collision mechanism dominates the orthokinetic mechanism and sedimentation settling. The perikinetic collision rate constant $k_{i,j}$ is determined by Eq. (8)

$$\beta_{i,j} = \frac{k_f}{W_{i,j}} \tag{7}$$

$$k_{i,j} = \frac{2kT}{3\mu}\frac{(a_i + a_j)^2}{a_i a_j} \tag{8}$$

The stability ratio W for colloidal aggregation is calculated using Eq. (9), where $V_T(l)$ is the total interaction potential of two particles. The computational time in evaluating W can be greatly reduced, while still maintaining accuracy, by using an efficient integration technique such as Gaussian quadrature [6]. In this method, the integral in Eq. (9) is partitioned into integrals over a number of smaller intervals as shown in Eq. 10, and the resulting integrations are converted into simple arithmetic operations as indicated in Eq. 11,

$$W = (a_i + a_j)\int_{(a_i+a_j)}^{\infty} \frac{\exp\left(\frac{V_T(l)}{kT}\right)}{l^2}dl \tag{9}$$

$$\int_a^b f(x)dx = \int_a^{a+h} f(x)dx + \sum_{i=1}^{\infty}\int_{L_{i-1}}^{L_i} f(x)dx \tag{10}$$

$$L_i = a + h\sum_{j=0}^{i} r_g^j \tag{11}$$

The population balance for the pigments is governed by Eq. (12). Figure (3) illustrates the various mechanisms that factor into the population balance analysis. Particle birth and death functions are defined in Eqs. (13) and (14), respectively. These equations describe a continuous batch operation, which cannot be directly used in our mathematical model. Instead, we discretize the theory and use a series of bins to define a finite set of particle sizes that span the distribution of sizes for the flocculation process. Equation (15) is used to define the particle bins, where q is an adjustable discretizing parameter. The rate of change of particle number within the i'th bin is calculated using Eq. (16),

$$\frac{dn(L)}{dt} = B(L) - D(L) \tag{12}$$

$$B(L) = \frac{L^2}{2}\int_0^L \frac{\beta\left[(L^3-\lambda^3)^{1/3},\lambda\right] n\left[\left((L^3-\lambda^3)^{1/3},\lambda\right)\right] n(\lambda)d\lambda}{(L^3-\lambda^3)^{2/3}} \tag{13}$$

$$D(L) = n(L)\int_0^{\infty}\beta(L,\lambda)n(\lambda)d\lambda \tag{14}$$

$$\frac{V_{i+1}}{V_i} = 2^{1/q} \tag{15}$$

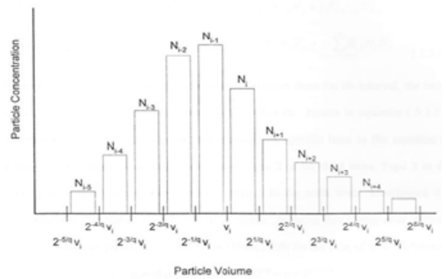


Figure 5: Discretization of particle size bins used in the population balance model.

$$\frac{dN_i}{dt} = \sum_{j=1}^{1-S(1)} \beta_{i-1,j} N_{i-1} N_j \left(\frac{2^{(j-1+1)/q}}{2^{1/q}-1} \right)$$
$$+ \sum_{k=1}^{q} \sum_{j=i-S(k-1)}^{1-S(k)} \beta_{i-k,j} N_{i-k} N_j \left(\frac{2^{(j-1+1)/q} - 1 + 2^{-(k-1)/q}}{2^{1/q}-1} \right)$$
$$+ \frac{1}{2} \beta_{i-q,j-q} N_{i-q}^2 + \sum_{k=1}^{q-1} \sum_{j=i+1-S(k)}^{1+1-S(k+1)} \beta_{i-k,j} N_{i-k} N_j \left(\frac{-2^{(j-1+1)/q} + 2^{1/q} - 2^{-(k-1)/q}}{2^{1/q}-1} \right)$$
$$- \sum_{j=1}^{1-S(1)+1} \beta_{i,j} N_i N_j \left(\frac{2^{(j-1)/q}}{2^{1/q}-1} \right) - \sum_{j=1-S(1)+2}^{\infty} \beta_{i,j} N_i N_j \qquad (16)$$

The discretization method is set forth by Grebard, Seinfeld, Landgrebe and Pratsinis [7] where no integration within intervals is necessary. The implementation of the discretization method presented above, results in a set of ordinary differential equation, one differential equation for each discretization bin is used. The equations are solved using Runge-Kutta-Fehlberg integration technique in MATLAB R2007b. This model was used to predict the growth in the average particle size given an initial size distribution of pigments. Figure 6 shows the results of a simulation. Starting with a monodisperse concentration of 132 nm carbon black particles, the average particle size increases to 200 nm in 250 seconds using a 100mNM concentration of NaCl.

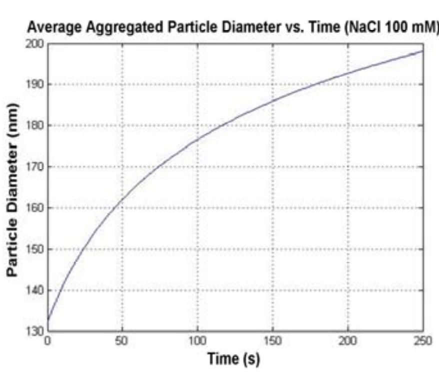


Figure 6: Plot of particle diameter (nm) as function of time for NaCl with concentration of 100 mM.

3 CONCLUSIONS

Image quality in conventional inkjet printing technology is critically dependent on various interactions that occur at the ink media interface during the deposition and absorption of droplets onto porous paper. Many factors govern these processes including various ink and media properties. For pigmented inks, image quality is also a function of the local density of deposited pigments, which in turn depends of the flocculation of the pigments during absorption. In this presentation we have described and demonstrated modeling techniques that can be used to advance understanding of ink media interactions and enable rational design of ink jet printing systems for optimum image quality. The models involve the use of continuum CFD analysis to study ink absorption and a population balance model to predict pigment flocculation. These models should prove useful for the development of conventional inkjet systems as well as novel systems for printing functional materials.

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