# Impact of Ink Evaporation on Drop Volume and Velocity

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## Abstract

A model has been developed to predict the impact on drop volume and velocity of selective evaporation of certain components of a multi-component ink from ink jet channels to ambient. The analysis consists of three steps: 1) changes in ink concentration along channels due to evaporation, 2) resulting spatial and temporal changes in ink viscosity leading to viscous plugs near nozzles, and 3) impact of this viscosity distribution on drop ejection process, i.e., drop volume and velocity. In the first step, an evaporation model which uses a number of analytical and numerical tools is developed to quantify the effects of channel geometry, material properties and ambient conditions. The second step essentially comes from measurements or data found in the literature. Finally the results from the first two steps are integrated into a numerical drop ejection model to determine the impact of evaporation on the hydrodynamic behavior of the system. The model has been found to agree very successfully with available experimental data covering a range of waiting (evaporation) time from 0 to 40 seconds.

## Introduction

The selective evaporation of certain components of a multi-component ink from the thermal ink jet (TIJ) channels to the surrounding atmosphere during non-operating periods poses a challenging problem in the design of printheads. For a typical water-based ink formulation, water has by far the largest volume fraction and it is commonly accompanied by smaller amounts of other non-volatile components. The volatile components diffuse out into the surrounding air establishing a net bulk motion in the channel from the reservoir towards the nozzle. This results in accumulation of the non-volatile components near the nozzle. The concentration profiles in the channel change until steady-state is reached at which point the convective transport of the non-volatile components is balanced by diffusion back towards the reservoir. Unless a protective cap is employed, the water concentration in the nozzle region can drop to very small values leading to a local ink composition totally different from the operating design point. Due to altered concentration and possibly pH, the die may precipitate out of the solution forming a plug or a crust at the nozzle. Even if precipitation does not occur, the mean fluid viscosity in the nozzle region may be too high for drop generation. In either case, the result is a printhead failure which may or may not be recoverable. This study focuses on the failure mechanism related to the viscous plug formation.

The complete analysis of the phenomena involves obtaining first the change in the species concentration distribution in the channel due to evaporation. Next the physical properties of the ink, notably the viscosity, should be described in terms of the concentration distribution. Finally this information should be integrated into a drop-ejection model to determine the impact of evaporation on the hydrodynamic behavior of the system.

## Evaporation Process

The model presented in this paper for the evaporation process of a multi-component ink from the TIJ channels shares the same basic principles as in a model previously developed by Torpey [1]. In this model the mass transport equations are solved separately inside the channels and outside in the air. It is assumed that the diffusion time scale from the nozzle into the room is much shorter than the diffusion time scale inside the channels and that solution to the steady-state evaporation process in the room can be applied as a boundary condition to the diffusion equation inside the channels. Of course, the two solutions are coupled by the constraint that what evaporates into the room must be supplied through the channel, and thus, a net bulk motion is established inside the channel from the reservoir toward the nozzle.

As we are primarily interested in the concentration distribution of different species along a channel, a unidirectional analysis is adapted here which assumes that the mass transport takes place along a centerline connecting different subsections of the channel and that the concentration profile in any plane normal to the centerline is uniform. The cross-sectional area is allowed to change with distance, *x*, along the centerline. Although this approach should be normally applied to narrow and long ducts, it is expected to give first order accuracy even when this criterion is not fully satisfied. For an *n*-component system, *n-1* solutes and a solvent, the mass conservation equations are given as

$$A\frac{\partial c_i}{\partial t}dx = -\frac{\partial}{\partial x}\left(AUc_i - AD_i\frac{\partial c_i}{\partial x}\right)dx$$
$$i = 1, 2, \ldots, n-1$$

which can also be written as

$$\frac{\partial c_i}{\partial t} + U\frac{\partial c_i}{\partial x} = \frac{D_i}{A}\frac{\partial}{\partial x}\left(A\frac{\partial c_i}{\partial x}\right)$$
$$i = 1, 2, \ldots, n-1$$

where $t$ is the time, $A$ the cross-sectional area as a function of centerline distance $x$ and $U$ the mean convective velocity, also a function of $x$ so that $UA$=*constant* inside the channel. $c_i$ and $D_i$ are the volume concentration and the main-term diffusion coefficient of the solute $i$. Here, the main-term diffusion coefficients are assumed to be constant, and the cross-term diffusion coefficients are neglected as they are normally much smaller than the main-terms.

The solvent (normally water) volume concentration, $c_0$, can be obtained from

$$c_0 = 1 - \sum_{i=1}^{n-1} c_i$$

The boundary condition at the reservoir, $x = 0$, is

$$c_i = c_{i,reservoir} \qquad i = 1,2,\ldots,n-1$$

while at the nozzle, $x = L$ , it is

$$Uc_i - D_i\frac{\partial c_i}{\partial x} = \frac{m_i}{A\rho_i} \qquad i = 1,2,\ldots,n-1$$

where $\rho_i$ is the solute liquid-phase density, and $m_i$ is the solute mass flow rate due to evaporation at the nozzle ($m_i$ = 0 for the non-volatile components).

The mean convective velocity is determined by the total evaporation rate including the solvent and it is given by

$$U(x) = \frac{\sum_{i=0}^{n-1} m_i/\rho_i}{A(x)}$$

The transport of a vapor from an orifice into the surrounding air is governed by the steady-state diffusion equation

$$\nabla^2\phi = 0$$

subject to the boundary conditions

$$\phi = \phi_L \qquad at \qquad x = L$$
$$\phi = \phi_\infty \qquad at \qquad x \to \infty$$

The solution to this equation can be shown to be

$$m = \Psi\sqrt{A_L/\pi}\; D_a\; (\phi_L - \phi_\infty)$$

here the subscript $L$ refers to the nozzle, $\phi$ is the vapor mass density, $D_a$ the diffusivity in air, $m$ the mass flow rate supplied through the channel, and $\Psi$ a non-dimensional constant that depends on the shape of the nozzle.

Using Raoult's law which states that the partial pressure due to a particular component is equal to its equilibrium vapor pressure in the pure state times its mole fraction in the liquid mixture, the mass flow rate of each volatile component $i$ through the channel can be derived as

$$m_i = \Psi\sqrt{A_L/\pi}\; D_{a,i}\; (y_i - H_\infty)\frac{P_{v,i}M_i}{TR}$$

where $H_\infty$ is equal to the relative humidity in the room if $i$ refers to water or equal to zero otherwise, $M$ is the molecular weight, $T$ the room temperature, $R$ the universal gas constant, $y$ the mole fraction at the nozzle, and $P_v$ the vapor pressure.

For a circular nozzle, the exact analytical solution can be obtained relatively easily in oblate spheroidal coordinates which shows that $\psi$ = 4.0 (see Appendix). Numerical simulations carried out using FIDAP [2], a commercial finite-element program, for different nozzle geometries with aspect ratios around unity further show that the value of $\psi$ is relatively insensitive to the nozzle geometry.

## Integrated Model and Its Application

Based on the mathematical model described above, a numerical program was written to determine the time-dependent concentration distribution in channels with arbitrary geometry. The results from this model are then used to determine the viscosity variation along the channel from experimental data. Next the drop generation is simulated with the corresponding viscosity distribution by using a modified version of FLOW-3D [3], a commercial fluid dynamics program. The modifications to this program are mostly related to the thermal bubble growth. The physical principles behind this model have been previously described and implemented [4, 5], so they will not be repeated here. The time scale for the drop generation process is normally much shorter than the diffusion time scale so that the evolution of viscosity distribution is solely controlled by convection. In the simulations this was accomplished by solving the momentum and energy equations simultaneously with a very low thermal diffusivity and by specifying the viscosity as a function of temperature.

The experiments employed a test fluid which consisted of 80% water and 20% dipropylene glycol (DPG) ($M$=134 kg/kmol). The drop ejector was a Xerox side shooter. Following a number of maintenance drops, the printing was paused for a given period of time, termed here the *waiting time*, and then started again. The velocity of the first drop after the pause was measured and tabulated in Table 1 for different values of waiting time. The change in the first drop velocity from the nominal value which has a waiting time equal to zero is a measure of the impact of evaporation losses on the performance of the drop generator. It is seen from Table 1 that the longer the waiting time the smaller the velocity, i.e., the poorer the performance.

In the first step to predict the experimental results, the evaporation model described above was applied to the same drop generator used in the measurements. The material properties except for the binary diffusion coefficient are well known for water and DPG and can be found in the literature. However, the available information on diffusion coefficients in liquids is limited. Furthermore, the concentration profiles have large variations in this application, and the diffusion coefficient should be described as a function of concentration. In the absence of empirical data, it was assumed here that the diffusion coefficient was uniform and it was calculated using the Wilke-Chang model which is written as

$$D = 7.4 \cdot 10^{-8} \; \frac{\sqrt{\aleph M}}{V_b^{-0.6}} \; \frac{T}{\mu}$$

where $D$ ($cm^2/s$) is the diffusion coefficient, $T$ (K) the temperature, $\mu$ (cp) the viscosity, $M$ the solvent molecular weight, $V_b$ the solute molar volume volume and $\aleph$ the association parameter. The Wilke-Chang equation is applicable in the limit of low solute concentration. Since the water concentration drops to low values at the nozzle exit and the drop generation process is impaired by the viscous plug formation in this region, water was chosen here to be the solute and the glycol to be the solvent. This gave a value $D$ = 6.6E-11 $m^2/s$. With this result the concentration distribution in the channel was determined at the specified waiting times in Table 1.

Using these concentration profiles the viscosity distribution along the channel at each waiting time was then obtained by the empirical viscosity equation for water-DPG mixture given by

$$\mu = e^{0.044\,X - 0.162}$$

where $X$ is the weight percent of DPG.

Finally, the viscosity distribution obtained from the above equation was integrated into the drop ejector model and the drop velocity and drop volume were determined for different waiting times. These results are presented in Table 1 where a comparison is made with measurements. The drop volume could not be obtained experimentally, but the agreement between theory and experiment for the velocity is seen to be very good throughout the range of waiting times covered. This supports the validity of the model and the underlying physical concepts.

**Table 1. Comparison Between Theory and Experiment**

| Waiting Time (s) | Drop Volume (pl) (theory) | Drop Velocity (m/s) (theory) | Drop Velocity (m/s) (experiment) |
|---|---|---|---|
| 0 | 13.4 | 14.2 | 14.6 |
| 3 | 11.8 | 12.6 | 13.0 |
| 5 | 11.3 | 12.0 | 11.8 |
| 10 | 10.2 | 10.5 | 9.8 |
| 20 | 8.7 | 8.2 | 8.0 |
| 40 | 6.8 | 5.1 | 5.7 |

## Conclusions

A comprehensive model has been developed to investigate the impact of evaporation on drop volume and velocity in TIJ printheads. The model combines the mass diffusion inside the channels with the hydrodynamics of the drop generation process through the changes in the viscosity of the ink. The validity of the concepts behind the model has been verified experimentally.

## References

1. P. A. Torpey, *Proc. IS&T Non-Impact Printing Conference* (1990).
2. FIDAP, Trademark of Fluid Dynamics International, Inc. Evanston, IL.
3. FLOW3D, Trademark of Flow Science, Inc., Los Alamos, NM.
4. P. A. Torpey, *Proc. SPSE Non-Impact Printing Conference* (1988).
5. M. P. O'Horo, N. V. Deshpande, D. J. Drake, *IS&T 10th Intn'l Congress*, New Orleans, LA (1994).

## Appendix. Diffusion from a Circular Orifice

The steady-state diffusion from an orifice into the surrounding air is governed by

$$\nabla^2 \phi = 0$$

If the orifice is circular with a radius $a$ and centered at the origin normal to the $z$-axis, the boundary conditions can be written as

$$\phi = \phi_0 \qquad \textit{for} \quad z = 0 \quad \textit{and} \quad x^2 + y^2 \le a^2$$

$$\frac{\partial \phi}{\partial z} = 0 \qquad \textit{for} \quad z = 0 \quad \textit{and} \quad x^2 + y^2 > a^2$$

$$\phi = \phi_\infty \qquad \textit{for} \quad z > 0 \quad \textit{and} \quad x^2 + y^2 + z^2 \to \infty$$

The form of the boundary conditions suggests a transformation from the rectangular coordinate system ($x,y,z$) to the oblate spheroidal coordinate system ($u,v,w$). The transformation can be carried out by setting

$$x = a \; \cosh u \; \cos v \; \cos w$$

$$y = a \; \cosh u \; \cos v \; \sin w$$

$$z = a \; \sinh u \; \sin v$$

where

$$u \ge 0$$

$$-\pi/2 \le v \le \pi/2$$

$$0 \le w \le 2\pi$$

In this coordinate system, the solution satisfying the boundary conditions are constant $u$ surfaces. Then we have

$$\frac{d}{du}\left( \cosh u \, \frac{d\phi}{du} \right) = 0$$

subject to the boundary conditions

$$\phi = \phi_0 \qquad at \qquad u = 0$$
$$\phi \rightarrow \phi_\infty \qquad at \qquad u \rightarrow \infty$$

which gives the following solution

$$\frac{\phi - \phi_\infty}{\phi_0 - \phi_\infty} = 2\left[1 - \frac{2}{\pi}\tan^{-1} e^u\right]$$

The flux through the orifice, $m$, is defined by

$$m = -D\int_A \left(\frac{\partial\phi}{\partial z}\right)_{z=0} dA = -D\int_{x=0}^{x=a} \left(\frac{\partial\phi}{\partial z}\right)_{z=0} 2\pi x\, dx$$

so that

$$m = 4Da(\phi_0 - \phi_\infty)$$

# Errata

## Impact of Ink Evaporation on Drop Volume and Velocity

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*page 20, left column, 1st equation*

$$D - 7.4 \cdot 10^{-8} \frac{\sqrt{\aleph M}}{V_b^{+0.6}} \frac{T}{\mu}$$