

Multiple Pass Thermal Dye Diffusion Modeling Profiles

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Abstract

A numerical model has been developed to simulate the dye transfer thermal printing process. The simulation incorporates the multiple layers of the head/media interface and uses finite difference techniques to calculate the temperature and mass distributions. Surface boundary conditions have been determined from experimental print head temperature data. This enables us to use different pulse modulation heating schemes. Also, the concentration dependence of diffusivity is taken into account which leads to a non-linear governing equation. The amount of dye transferred and its distribution in the receiving material can be predicted.

The model has been extended to incorporate multiple pass printing. Depth profile predictions are made for a variety of input parameters. Various printing line times, pulse modulation schemes, partition coefficients, donor and receiver glass transition temperatures, and receiving layer thickness are used to calculate the dye concentration profile of the receiver. The surface layer concentration and the depth of dye penetration are of particular importance. These predictions are compared to experimental cross-sectional measurements of dye transfer in receiver material.

Introduction

An application of a numerical model developed to simulate the dye transfer thermal printing process will be described. The simulation incorporates the multiple layers of the head/media interface and uses finite differences to calculate the temperature and mass distributions. Surface boundary conditions have been determined from experimental print head temperature data. This enables us to use different pulse modulation heating schemes. The concentration dependence of diffusivity is taken into account which leads to a non-linear governing equation. The amount of dye transferred and its distribution in the receiving material can be predicted.

This model has been used as a tool for identifying those factors which are most important in achieving a robust design. In particular, the effects of the donor and receiver glass transition temperatures, dye diffusion partition coefficients, line printing times, pulse enable width schemes, and receiver dimensions were studied. These factors were incorporated into a pseudo design of experiments. Responses included the amount of dye transferred from the donor to the receiver and the distribution profile of the dye in the receiving material. The responses were calculated using the simulation model previously described.

Over the past 15 years a new printing technology known as "resistive head thermal printing" has emerged. Thermal printers are used for a variety of printing needs, ranging from inexpensive monotone fax printers, to near photographic quality continuous tone color images. The highest quality output is produced by the dye diffusion thermal printer. The thermal printing operation is driven by a thermal print head that consists of a number of resistive heating elements closely arranged along the axis of the head. Between 200 and 600 heating elements are aligned per inch. During the dye diffusion printing process, the thermal printhead is brought into contact with a dye coated donor ribbon (see *Figure 1)*. A chemically coated receiver sheet sits beneath the donor ribbon. The donor/receiver surfaces are compressed between the printhead bead and an elastomeric drum creating a very small but highly pressured nip contact region. The high pressure creates the intimate contact between the layers that is necessary for efficient thermal transfer. During printing, each resistive element on the head is pulsed with current in order to create heat. This heat then drives the diffusion process. By manipulating the thermal resistor pulsing scheme one can control the temperature history, and subsequently the amount of diffusion taking place beneath each resistor. In the color dye diffusion process three printing passes are used to overlay yellow, magenta, and cyan dye. The result is a high quality, continuous tone color image.

In order to simulate the dye transfer process taking place within this heated and pressured nip contact region we have created a finite difference model that simultaneously solves the heat and dye diffusion equations. This model will allow us to optimize the system parameters that most influence the transfer process. In the past a number of studies have focused on the heat transfer aspects of the problem. Setani et al[1] created a 3D finite element code to study the thermal effects due to adjacently heated pixels. Connolly[2,3] created a 1D finite element model to study the effects of the thermal characteristics of the material within the printhead itself. In 1991 Kaneko[4,5] created a simulation using finite differences to model the heat and dye transfer process. In his simulation he enforced surface temperatures based on experimental data in order to determine media interface temperatures. He later used a finite element technique in which he accounted for 'back diffusion', meaning diffusion from the receiving layer to the dye layer on the 2nd or 3rd pass. Still others have done work in thermal and diffusion modeling and the reader is directed to the published literature for further information.

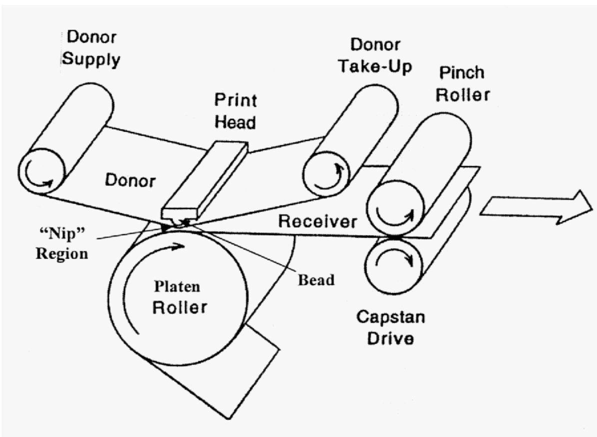


Figure 1. Thermal Printer

One of the keys to our modeling approach was to use a constant flux boundary condition at the surface of the print head resistor rather than a constant temperature. In the present model, it is not our goal to predict the thermal behavior within the head itself, but rather to determine the temperature and diffusion behavior between the donor and receiver. Therefore, our approach will be to replace the actual thermal resistor with a flux boundary condition, and to replace the heat sink of the head with a single heat loss term. Using experimental thermal head temperature data we will describe a method for finding this boundary condition. In such an approach we account for the fact that the experimental head temperatures measured in air are higher than the head temperatures we expect to find when the media is brought into contact with the head. In the model we will also account for the concentration dependence of the diffusivities that leads to a nonlinear diffusion equation. Finally, we will run a number of test cases that illustrate the capabilities of the model.

Model Development

The purpose of our heat and dye diffusion model is to simulate the transient thermal behavior within the donor and receiver layers and the subsequent dye transfer between the two surfaces.

The two equations we solve simultaneously are very similar. The simplified one-dimensional heat equation can be written as:

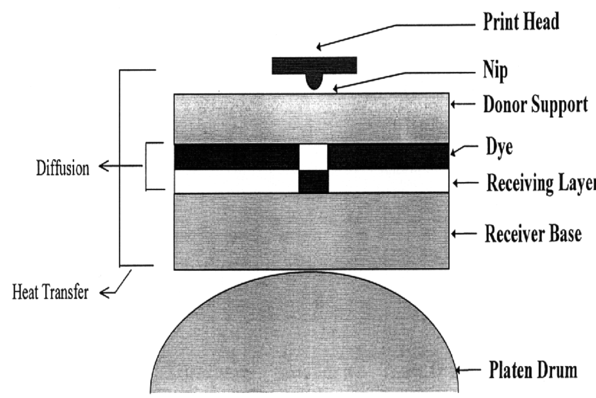
$$\partial T/\partial t = (K/C_p)(\partial^2 T/\partial x^2) \quad (1)$$

where K = thermal conductivity (W/mK), C_p = heat capacity (J/m^3K), T = Temperature (K), and t = time(sec). A description of the discretization can be found in LaFleche.[6,7]

The diffusion equation shown below cannot be solved as simply because some dyes used in the thermal printer industry have a concentration dependent diffusivity leading to the non-linear governing equation

$$\partial c/\partial t = \partial/\partial x[D(c(x))\bullet\partial c/\partial x] = D\,\partial^2 c/\partial x^2 + dD/dc[\partial c/\partial x]^2 \quad (2)$$

where D(c) = diffusivity (m^2/sec), x = position (m), t = time (sec), and c = concentration (non-dimensional). In order to account for the concentration dependent diffusivity we have linearized the diffusion equation. Details of this linearization and the finite difference solution techniques for both the heat and dye diffusion can be found in LaFleche.[7]



Cross-section of the printing system

Surface Boundary Condition

Experimental temperature profiles on the surface of a thermal printhead were measured using infrared microscopy. These experiments were performed on a 300dpi TDK thermal print head, using an EDO Corporation Radiometric infrared microscope with a 36 micron aperture. We use this experimental data to find the surface boundary condition to be used in our temperature model.. A sampling of the head temperature data can be found in *Figure 2*. The data are fitted to the relationship

$$q\alpha = -K[\partial T/\partial x] + h(T - T_\infty) \quad (3)$$

where,

q = flux (W/m^2)
α = efficiency (0-1)
h = loss term (W/m^2K)
T = head temperature
T_∞ = room temperature

Constants for a particular system are chosen by matching experimental data for the temperatures measured at the surface of the head. The constants q, h, α, and T_∞ are adjusted accordingly. During the pulsing algorithm, when the heater is on, the flux term q is included. Otherwise, this term is set equal to zero. Through the use of the loss term h, heat is constantly being removed from the system.

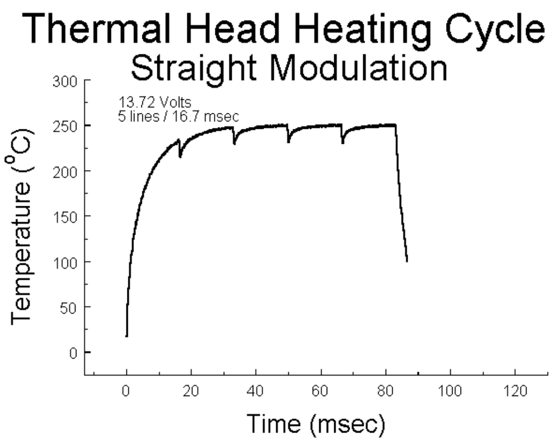
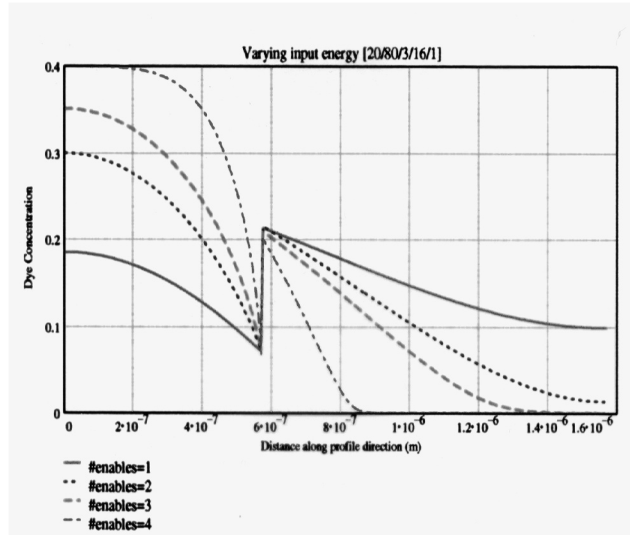


Figure 2. Experimental Head Temperature

Applications of the Model

The numerical simulation allows us to study the relationship between many different parameters that affect the transfer process. In terms of heat transfer, we can make modifications to heat capacity and thermal conductivity. We can examine the efficiency of the print head as a function of media type, thickness, number of layers, and the properties of those layers. Modifications to the pulsing algorithm can be made. Adjustment of these parameters lead to changes in temperature history, subsequent diffusivity, and the overall volume and position of the transferred dye. In terms of the diffusion equation, we can examine the effects of dye thickness and dye concentration and make changes to the diffusion laws. These laws account for glass transitions of the coatings and the chemistry of the individual dyes.

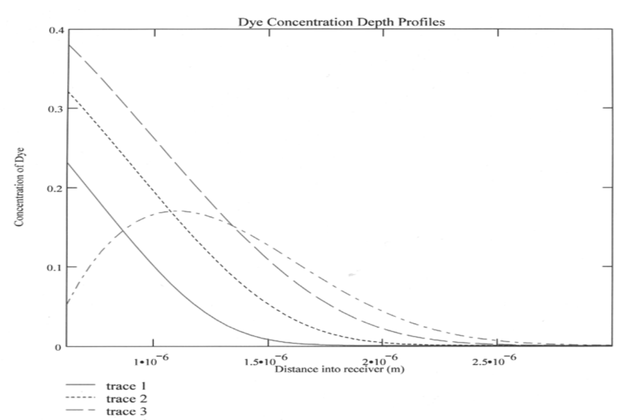
The calculations performed used 3 layers for the temperature computations. These layers represented the ceramic cover, the donor material, and the receiver. Two layers were used for the diffusion computations - the dye layer and the receiving layer. The mesh structure of the numerical calculation and the type of solution have been defined to optimize the speed of calculation, maintain convergence, and provide consistency and agreement with known closed form results.[8,9] A sample output plot is shown below:



Dye concentration profiles are shown at 4 different energy level inputs. The transition region represents the donor:receiver interface. A partitioning coefficient establishes a solubility difference between the two layers.

Multiple Pass Printing

The effect of multiple pass printing was investigated using this model. The printing process consists of 3 dye transfer passes followed by a laminate pass. Each of the dye transfer calculations assumes an initial dye concentration in the donor material. There is no initial concentration in the receiver. Dye concentration profiles in the receiver after a given pass become the starting point for the next pass. The laminate pass considers no additional dye transfer – only the effect of the heat pulse. Typical concentration profiles are shown in the graph below:



One can see the progressive accumulation of dye, especially at the surface. After applying the lamination patch, one notices the additional depth of dye penetration in the receiver as well as the diminishing of the surface dye. Back diffusion effects are also predicted in the donor material.

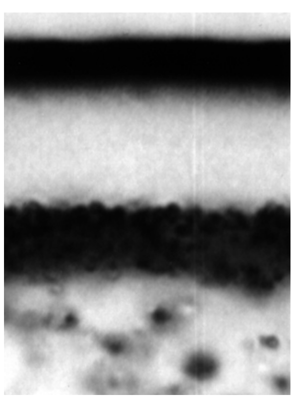
Predictive Model

One of the utilities of this type of model is to aid in the design of new coatings. In particular, to determine the receiver coating thickness boundaries. One would like to save money by not incurring extra cost by using more material than is necessary. It is critical to know the maximum depth of dye penetration in order to be able to specify the receiving layer thickness.

We looked at the extent of dye penetration for line times of 4, 9, and 16 ms at full power. Receiver thickness of 2.5 and 5.0 microns, and partition coefficients of 1 and 3 were used in the analysis. All other parameters had typical values for the materials being analyzed. Calculation times were dictated by the line time of the heat pulse. The table shown below summarizes the penetration distances. The penetration distances in microns are shown for 12 cases: Three line times (4,9,16ms), two partition coefficients (PC), and two receiver layer thickness (2.5,5.0)

Table 1.

	2.5 microns		5.0- microns	
	PC=1	PC=3	PC=1	PC=3
16ms	>3	>3	4.3	4.4
9ms	3	>3	2.8	2.9
4ms	1.6	1.6	1.5	1.5



Cross-section of dye in receiver

It is apparent that for a coating thickness of 2.5 microns one cannot use 9ms or 16ms line times without experiencing degradation to the printed image. On the other hand, 5.0 microns of thickness can accommodate all of the line times. An actual cross-section of the dye in the receiver following four printing passes is shown below. The extent of the dye's penetration is approximately 4.2 microns.

As printing speeds become faster, the need for thick coatings becomes less. The ability to predict the dye profile becomes more important. Also, it's interesting to note that the increase in partition coefficient resulted in more dye being transferred into the receiver with little to no increase in the maximum penetration depth.

Conclusion

The mathematics of the heat transfer / dye diffusion process has been represented using a finite difference modeling technique. The approach has successfully described the profile of the dye in the receiver layer. The ability to apply a heat flux boundary condition for the print head has provided a better representation for the thermal input. Its ability to do multiple pass calculations, to incorporate non-linear diffusivity behavior, and to accommodate differences in solubility by using a partition coefficient has provided the user with a valuable design tool.

References

1. Setani, K., Sasaki, E., Takeda, Y., SPIE-Hard Copy and Printing Technologies, 1252,144 (1990).
2. Connolly, D., Journal of Imaging Science, 38, 371 (1994).
3. Connolly, D., Journal of Imaging Science, 38, 365 (1994).
4. Kaneko, A., Journal of Imaging Science, 35, 49 (1991).
5. Kaneko, A., Journal of Imaging Science, 35, 263 (1991).
6. LaFleche, J.E., Deformation, Temperature, and Mass Diffusion Modeling of Thin Films with Application to Digital Thermal Printing, University of Rochester Ph.D. Thesis, (1996).
7. LaFleche, J.E., Benson, R.C., Stack, K.S., Burns, S.J., International Symposium on Information Storage and Processing Systems – ASME, 2, 21 (1996).
8. Carslaw, H.S., Jaeger, J.C., Conduction of Heat in Solids, Oxford Press, 1959.
9. Crank, J., The Mathematics of Diffusion, ClarendonPress,1975.

Biography

Edward Ozimek is a research scientist with the Eastman Kodak Company. He received the Ph.D. in experimental solid state physics from Colorado State University in 1977. He was affiliated with the Allied Chemical Corporation, the University of Arizona, and the IBM Corporation prior to joining Kodak in 1984. His work experience has included studies in ultrasonics, heat transfer, magnetic recording, image sensor packaging, and digital printing. He has received 13 US patents and is a member of the IS&T.