Monte-Carlo Optimal Inkjet Nozzle Design

JinQuan Xu, Christopher Muir; Eastman Kodak Company; Rochester, New York/USA

Abstract

A computational method for drop optimization for inkjet nozzle design using the Monte-Carlo method is demonstrated. To this end, a generic computational fluid dynamics (CFD) model of ink drop formation is developed as a platform for the Monte Carlo optimization. Important variables in the model are then parameterized so that they can be modified within a prescribed space. By applying the Monte-Carlo method, sensitivities of drop formation output parameters to various input parameters are studied in the context of the CFD model. Once sensitivities of drop formation to input variables are understood, the parameter space is then intelligently explored to determine a set of optimized parameters for the inkjet nozzle.

Introduction

With inkjet printing speeds becoming faster and printing resolutions getting finer, ink drops must be jetted faster at higher frequencies and be smaller in volume than ever [1]. One of the technical challenges for developing such printing technology is its nozzle design. Only an optimally engineered nozzle can ensure suitable drop formation for fast and high quality printing. Among many parameters that impact drop formation, some of the most important ones include the shape and dimensions of the nozzle and ink chamber, as well as nozzle operation conditions such as dynamic pressure at the ink inlet, static pressure in the ink chamber, and ink temperature in the chamber, etc. For thermal inkjet printing, dimensions and locations of the electrical resistor, as well as thermal energy input to the resistor, would also impact drop formation significantly. In addition, the impact of these parameters to drop formation are intertwined; in other words, the degrees of freedom of the inkjet nozzle are conjugated. It is extremely difficult, if not impossible to explore all combined possibilities using traditional error-and-trial methods without deep understanding of the problem at large.

Fortunately Monte-Carlo (MC) methods [2, 3] are especially developed and designed to study such problems with a large number of coupled degrees of freedom. MC methods provide approximate solutions to problems by performing statistical sampling experiments on a computer. With a MC method, a problem with a large number of degrees of freedom can be sampled in a number of random configurations, and that data can be used to describe the system as a whole. Ink drop optimization for inkjet nozzle design can be an excellent application for the MC method. In this work, an example of the MC method applied to ink drop optimization is demonstrated.

For purposes of this study, a generic computational fluid dynamic (CFD) model of ink drop formation from an inkjet nozzle is developed as a platform for the Monte Carlo optimization. Important variables in the model are then parameterized so that they can be modified within a prescribed space automatically. By applying the MC method, sensitivities of drop formation output parameters to various input parameters are studied in the context of the CFD model. Once sensitivities of drop formation input variables are understood, the parameter space is then intelligently explored to determine a set of optimized parameters for the inkjet nozzle.

Problem Formulation

Figure 1 schematically shows a cross-sectional view of a three-dimensional generic thermal inkjet nozzle assembly. For clarity of presentation, dimensions in Figure 1 are not scaled.

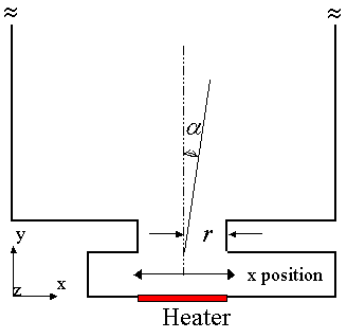

Figure 1 *Cross-sectional view of a generic thermal inkjet nozzle assembly (dimensions are not scaled)*

The generic thermal inkjet nozzle assembly shown in Figure 1 primarily consists of a cylindrical-shaped nozzle, a hexahedral ink chamber operatively connected to the nozzle, a rectangle electrical resistor lying on a wall of the ink chamber, and aqueous-based ink fluid. The cylindrical nozzle has a radius of r, a height of h, and an angle of α as defined in Figure 1. To optimize an ink drop, the x-position of the nozzle can be shifted to left and right relative to the ink chamber. For numerical modeling purpose, the ambient environment around ink droplets (not shown in Figure 1) is truncated into a bounded computational hexahedron domain filled with air of room temperature and pressure. The truncated domain should be large enough to minimize numerical boundary effects on drop formation. Initially the ink chamber and the nozzle are filled with ink fluid. To fire an ink drop, electrical current pulse is applied to the electrical resistor, creating a heat pulse on the resistor surface of a temperature as high as ~580K (higher than water saturation temperature). Ink fluid in close proximity to the hotly heated surface of the resistor film-boils instantaneously and leads to a water vapor bubble rapid expansion. The expanded

vapor bubble pushes some of ink in the ink chamber out through the nozzle, forming an ink filament. The ink filament pinches off and forms an ink drop flying away against the nozzle. Subsequent to drop ejection, the vapor bubble collapses, and the ink chamber is refilled with ink fluid through ink feeding channels via capillary force mechanism primarily.

The number of degrees of freedom of the ink drop formation processes are large. A comprehensive investigation of the impact of the all the degrees of freedom for drop formation requires long and expensive computation times and is most efficiently handled with large-scale architectures. For a simple demonstration of the Monte-Carlo optimization method, the degrees of freedom in this study are intentionally limited to three. Namely, we only explore the impact of the nozzle radius *r*, angle α, and *x*-position of the nozzle on drop formation. As a platform for the MC optimization, a generic CFD model of ink drop formation is developed.

Generic CFD Modeling

A computational fluid dynamic model for vapor bubbles induced drop ejecting from the generic nozzle assembly is developed in a three-phase (water vapor, air and ink liquid) volume of fluid (VOF) framework [4, 5]. The simulation of drop generation involves an ink liquid vaporization model that accounts for mass and energy transfer between ink and vapor due to thermal resistor heating. Parameterized scripts are developed to create geometrical variables and operational parameters for the sake of automatic implementation of the Monte-Carlo optimization. For simplicity, no ink refilling process is simulated in the model. Only drop/satellite formation is considered.

Governing Equations

Let the volume fraction of phase *i* in a computational control volume be denoted by α_i, where subscript $i = l$ represents the ink phase, $i = g$ air phase, and $i = v$ water vapor phase, where $\alpha_l + \alpha_g + \alpha_v = 1$. The continuity equation, in terms of the air phase volume fraction α_g, liquid volume fraction α_l, and vapor phase volume fraction α_v, may be respectively expressed as,

$$\begin{aligned} &\frac{\partial \alpha_g}{\partial t} + \vec{v} \cdot \nabla \alpha_g = 0, \\ &\frac{\partial \alpha_l}{\partial t} + \vec{v} \cdot \nabla \alpha_l = \frac{S_l}{\rho_l}, \text{ and} \\ &\frac{\partial \alpha_v}{\partial t} + \vec{v} \cdot \nabla \alpha_v = \frac{S_v}{\rho_v}, \end{aligned} \tag{1}$$

where S_l and S_v represent the source terms given by liquid vaporization induced by the resistor electrical heating.

The momentum equation is given by

$$\frac{\partial (\rho \vec{v})}{\partial t} + \nabla \cdot (\rho \vec{v} \vec{v}) = -\nabla p + \nabla \cdot \mu \nabla \vec{v} + \rho g + F_\sigma . \tag{2}$$

Here g is the gravitational acceleration and p is the pressure; the density ρ and the viscosity μ are defined as

$$\rho = \alpha_l \rho_l + \alpha_g \rho_g + \alpha_v \rho_v \text{ and } \mu = \alpha_l \mu_l + \alpha_g \mu_g + \alpha_v \mu_v , \tag{3}$$

and F_σ is the body force due to surface tension, which can be defined as [6]

$$F_\sigma = \sigma \frac{\kappa \rho \nabla \alpha_l}{\frac{1}{2}(\rho_l + \rho_g)}, \tag{4}$$

if the interface is between air and ink drops. Here the local curvature $\kappa = \nabla \cdot \hat{n}$, where $\hat{n} = \nabla \alpha_l / |\nabla \alpha_l|$, and σ represents the surface tension coefficient. Surface-tension force, is one of the critical mechanisms that determine the shape of a drop and its breakup/detachment [7]. For the interface between vapor and ink, we assumed the body force could be approximated by Equation (4) as well.

Similarly, a single energy equation is solved among the phases,

$$\frac{\partial}{\partial t}(\rho h) + \nabla \cdot (\rho h \vec{v}) = \nabla \cdot \left(k_{eff} \nabla T\right) + S_E , \tag{5}$$

where h is enthalpy, T represents temperature, k_{eff} is effective thermal conductivity, and S_E denotes the energy source term given by electrical energy input to the electrical resistor.

Solution Techniques

A volume of fluid (VOF) multiphase-phase fluid model, which solves the volume fraction of each phase within each control volume, along with a piece-linear interface calculation (PLIC) approach of Youngs [6, 8], is implemented to track interfaces between the vapor-liquid phases evolving in time. For numerical solution of the system, Equations (1), (2) and (5) are cast in an integral form as,

$$\frac{d}{dt}\int_V \rho \phi dV + \int_{\partial V} \rho \phi \vec{v} \cdot dA = \int_{\partial V} \Xi \nabla \phi \cdot dA + \int_V S_\phi dV , \tag{6}$$

where ϕ represents a general transport quantity. In the continuity equation, $\phi = 1$, in the momentum equation $\phi = v$, and in the energy equation $\phi = h$; Ξ is the diffusion coefficient, and S_ϕ is the source term for quantity ϕ. A is the area vector, and V represents the control volume, which is identified with each mesh element. The governing equations (6) are solved using a commercially available CFD software package Fluent (www.fluent.com) with customized source terms implemented in user defined functions (UDF).

A three-dimensional generic computational domain is automatically created using a commercially available meshing software package Gambit. A Gambit script is developed to parameterize the computational domain so that the Monte-Carlo

program can automatically modify these parameters for modeling and optimization. The computational domain is discretized with an unstructured grid initially comprising twenty thousands or so tetrahedral elements. The mesh would have been refined to render the drop shape more accurately if large-scale computational resource were available for the simulation.

For the time-dependent drop formation simulation, the governing equation is solved using an explicit time-marching scheme. A solution algorithm so-called the semi-implicit pressure-linked equation algorithm [9] is adopted for the numerical solution of the governing equations Equation (6). The interface Γ between the ink liquid and air or vapor is a material surface that follows the ink fluid motion. A linear interface is assumed between the two fluids within each computational element, *i.e.*, the interface Γ is approximated by a piecewise-linear function [8]. At each time step the location and slope of the linear interface within an element is approximated from the volume fraction of liquid hydrogen α_l, and a normal vector to the interface $\hat{n}$. The piecewise interface Γ is advanced with the normal velocity $\vec{v}_\Gamma = \vec{v} \cdot \hat{n}$ (which constitutes the PLIC approach of Youngs [7]). The mass flux of each fluid into neighboring computational elements can be determined, during time τ across the face Γ of a computational element, by $\Phi_F = \int\int \alpha_i \vec{v}_\Gamma dF dt$.

Monte Carlo Optimization

Figure 2 shows a flow diagram for the Monte Carlo simulation.

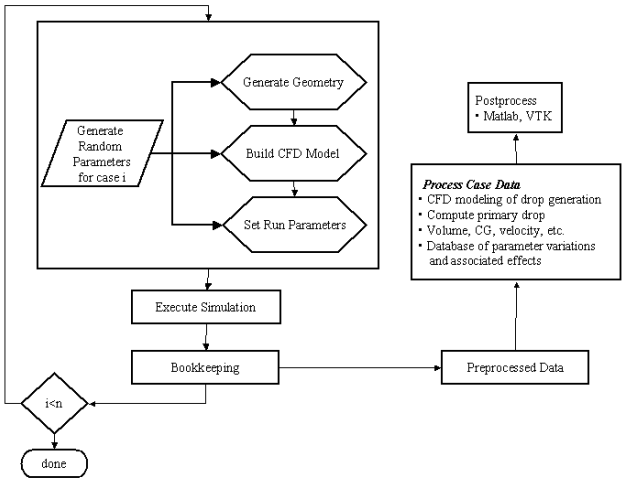

Figure 2 *Monte-Carlo optimization flow diagram*

Since this simulation must run non-interactively, scripts are employed to take advantage of the open architectures of the components. In this case, parameterized Gambit and Fluent scripts are created. The Gambit script is used to create variable geometry model, and the Fluent script is used to drive solution output data. Python, C and Cygwin/Unix utilities are used to glue the various components of the simulation together and massage the data. The scripts are created in a flexible manner to allow for the addition of new parameters as the project progresses and the solution space is broadened.

Within a prescribed dimensional space, the Monte Carlo program generates random parameters for each case. In this example, the parameters are the radius *r* and angle α of the nozzle and the *x*-position of the nozzle relative to the ink chamber. Although they can be any geometric, non-geometric, or solution related parameters, only geometric parameters are considered in the current demonstration. The Gambit script creates the appropriate computational domain, and generates meshes; the Fluent script builds the CFD model, sets up operation parameters and runs the CFD model automatically. After each computation, the result data is stored, and the mesh is efficiently swept to determine drop volume, drop center of gravity, number of satellites, and extents, etc., using custom C code developed for these purposes. The reduced data for each case is stored as to be easily retrieved and visualized. VTK and Matlab scripts are created for post processing.

As the database of information grows it is important to be able to easily go back and examine the parameters and results of a specific case. We often find that the simulation will stray outside a feasible (or desirable) region; for example, these cases can remain in the database, but can be excluded from the Postprocessing step. The excluded cases may or may not have results associated with them. This has an additional benefit: we don't need to be especially careful about the scope and interdependencies of the input parameters. A common example of this occurs when driving complex geometries where there can be significant interdependencies and the domain may fail to resolve. If this occurs the case fails, but the simulation continues with no corruption of the database and those results are excluded by default.

Typically a merit function is set to control optimization iteration. Here we are creating a database of simulations to explore the domain. We can write multiple optimization functions against that data before *or after* the simulation is complete. In this case we can run the number of simulations up to a level where we achieve the a desired statistical fit for the response surface, or use it to simply understand the response of various outputs to the input parameters, as demonstrated in Figure 6 in the "Results and Discussion" chapter.

Results and Discussion

Figure 3 shows a snapshot of a simulated ink drop with a satellite from a nozzle. An elongated drop, followed by a satellite flying away the nozzle is shown in the figure. This kind ink drop is very commonly observed in experiments.

Figure 3 *Visual representation of a drop and its satellite simulated by the CFD model.*

For MC optimization efficiency, the number of elements in the computational domain is limited to no more than 20,000 to

ensure for each case, simulation machine time is less than 10 minutes. Due to this constraint, the simulated drop shown in Figure 3 is rather coarse. But the resolution is fine enough for technical demonstration purposes that the paper is intended. Also, please notice that that the CFD model should be validated first before using the model to run any optimization. Due to time constrain, no model validation is conducted so far. But again, the work is intended for methodology demonstration purpose only at this point.

All example parameters in this study are driven with uniform random variables and the examples are for proof-of-concept application only. Figure 4 shows visual representations of six randomly selected geometric changes within a prescribed space. The change of the radius r, angle α, and x-position are randomly combined with the parameters are selected by the MC method.

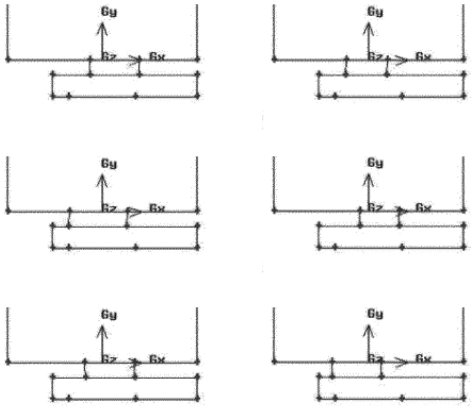

Figure 4 *Visual representations of six randomly selected geometric changes*

Figure 5 shows visual representations of nine randomly selected drops ejected from a nozzle at the same elapsed time with different geometric parameters, similar with what are shown in Figure 4. Figure 5 vividly suggests that geometric configuration of the nozzle impacts drop formation dramatically in a manner of drop pinch-off, jetting direction, satellite formation, drop shape, and size, etc.

Figure 5 *Visual representations of nine drops ejected from a nozzle at the same elapsed time with different geometric parameters*

A beauty of using Monte-Carlo optimization is to be able to statistically analysis the parametric impacts to the merit function. In other words, sensitivities of output drop formation parameters to various input parameters can be studied. For example, Figure 6 shows statistic matrix of scatter plots generated using the MC simulation data, which descriptively suggests the geometric parameters' impacts on drop formation.

To be specific, the scatter plot suggests that the x-position of the nozzle drives the centroid and possibly the total volume, while the radius clearly drives the centroid, eject length, and total volume. Figure 6 also suggests that the nozzle angle has little impact on drop characteristics, largely due to the height of the nozzle is thin in the model. In short, this type of plot visually demonstrates scope and scale of input and output correlations, and can help identify and bound the inputs of a particular problem. For example, Figure 6 shows that, to generate a drop of around 1.4 pL in size, the radius of the nozzle may be varied between 7 and 9 micrometers.

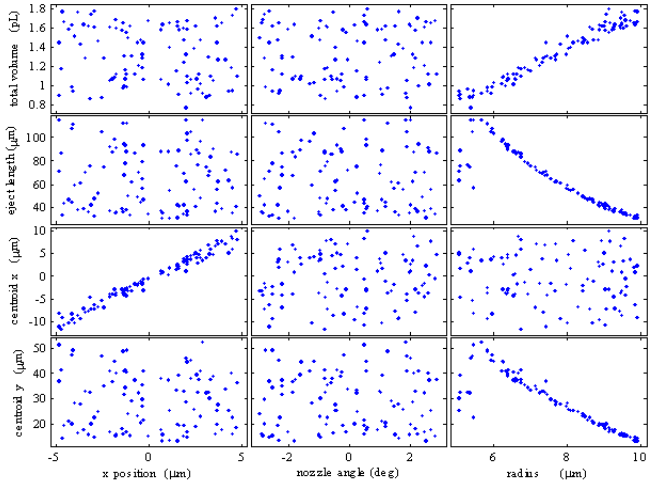

Figure 6 *Matrix of scatter plots*

Figure 7 shows a response surface for a particular merit function in 3 normalized parameters based on the data above (90% confidence bands are shown for the quadratic surface fit). These plots are particularly useful in refining the ranges of parameters to find a local optimum for a given merit function. Multiple merit functions can be considered using a Pareto-front approach [10, 11].

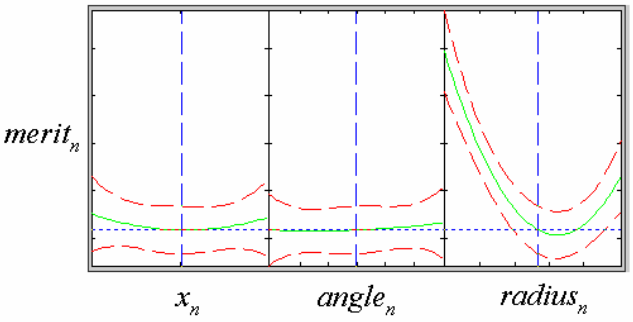

Figure 7 *Response surface for a volume based merit function using the rstool function in Matlab.*

Concluding Remarks

A computational method for drop optimization for inkjet nozzle design using the Monte-Carlo method is demonstrated. A generic computational fluid dynamics model of ink drop formation is developed as the platform for the Monte Carlo optimization.

Although they can be any geometric, non-geometric, or solution related parameters, only geometric parameters are considered in the present demonstration. Namely, the impacts of nozzle radius, angle and its *x*-position on drop formation have been studied. Results of numerical experiment suggest that geometric configuration of the nozzle impacts drop formation dramatically in a manner of drop pinch-off, jetting direction, satellite formation, drop shape, and size, etc.

This work, as a first step towards to an optimal inkjet nozzle design, sheds some light on how the Monte Carlo method can be conjugated with a CFD model to facilitate engineering design of these difficult problems. This technique can yield not only an improved set of operating parameters for a system, but will generally result in a deeper understanding of the problem at large.

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Author Biography

JinQuan Xu joined Kodak Research in 2005. Earlier, JinQuan spent four years in National High Magnetic Field Laboratory, and School of Computational Science at Florida State University as a Research Associate. JinQuan has extensive experience in multi-physics analysis such as fluid dynamics and heat transfer. JinQuan also has solid experience in applied mathematics and large-scale scientific parallel computing. JinQuan graduated from the University of Alabama with PhD in Chemical Engineering, 2001.

Christopher Muir received his PhD in Mechanical Engineering from Lehigh University in 1996 in the area of computational geometry and tolerance analysis. He has worked closely with the research and commercialization teams of many of the business units in the last 11 years at Kodak. Chris is currently part of the Corporate Engineering Division. His duties include support in the areas of Opto-Mechanical Tolerance Analysis, Image based Data Analysis, Finite Element Modeling and Mechanism Analysis, as well as associated tool research and development.