

SHORT COMMUNICATION

Simulation of Droplet Formation, Ejection, Spread, and Preliminary Design of Nozzle for Direct Ceramic Inkjet Printing

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ABSTRACT

Recent advances in drop-on-demand (DOD)-type inkjet printing techniques have increased research activities in the area of direct ceramic inkjet printing. In an attempt to develop a ceramic inkjet printer for the manufacture of ceramic components with their sizes in micro scale, the formation of ceramic ink droplet (ethyl alcohol loaded with different volume fractions of alumina particles) and its spread from a reservoir using piezoelectric actuation are simulated. The properties of the ceramic ink are taken from the data reported in literature. The simulations were performed with computational fluid dynamics software (CFD-ACE+), CFDRC. This study gives details of the interaction among different physical phenomena that contribute to the droplet formation and ejection process. The results from this study are being used for a preliminary design of nozzle and for the preparation of ceramic inks to achieve the desired droplet characteristics.

Keywords: Drop-on-demand, direct ceramic inkjet printing, piezoelectric actuation, DCUP solid free forming, SFF, inkjet printing

NOMENCLATURE

F	Liquid volume fraction
t	Time
Δ	Standard spatial grad operator
v	Velocity vector
ϕ	Volume-averaged quantity
ϕ_1	Value of the quantity for fluid 1 (air)
ϕ_2	Value of the property for fluid 2 (ceramic ink)
ε	Induced strain
d	Induced strain in a direction per unit electric field applied in the same direction.
V	Applied electric field

V_c	Volume of the whole cell
V_{cut}	Volume of the cell truncated by the cutting plane

1. INTRODUCTION

Direct ceramic inkjet printing (DCIJP) is one of the solid free forming (SFF) techniques developing rapidly. DCIJP uses a suspension containing ceramic particles, which is deposited using a delivery system actuated by a piezoelectric device^{1,2}. Two types of inkjet printers are being deployed. In a continuous-inkjet printer, ink is pressurised to produce a jet through a nozzle. A piezoelectrically generated pressure wave is superimposed on the jet which breaks up the jet into small droplets at a preset frequency. In the modified drop-on-demand jet printer, a pressure pulse generated by a piezoelectric actuator adjacent to the nozzle forms a droplet of ink³.

Inkjet printer manufacturers develop their products in a highly competitive environment. The designs involve transient interaction between fluids and structures to eject ink droplets. This requires a significantly streamlined process for simulating fluid-structure interaction (FSI)⁴ that will allow shortening the design cycle, improvement in the print quality, and speed⁵. In this study, the formation of a drop in DCIJP is simulated using CFD-ACE+, a computational fluid dynamics software that can handle multi-physics problems. For this study, two typical nozzle geometries were used. The force was applied directly on the membrane at the top of the chamber, which imparted the required momentum for the droplet ejection⁶. Based on these results, the optimum dimensions of the nozzle were determined.

In this regard, an exhaustive literature survey was carried out to know the various approaches adopted by several researchers in studying DCIJP. A critical study revealed that attempts were made on experiments for preparation of ceramic inks and their deposition⁷⁻⁹ and nozzle design¹⁰. But it was observed that attempts on modelling and simulation of droplet formation, ejection, and spread in DCIJP were reported. Hence, the relevance of this study.

2. PRESENT WORK

The formation of droplet and its spread are important as these control the accuracy with which a solid can be formed by DCIJP. Droplet formation is controlled by the properties of ink, nozzle geometry, and the amplitude of actuation. The spread is controlled by the impinging velocity of the droplet, the rheological properties of ceramic ink, and the interfacial energy prevailing at the droplet-substrate interface. The objective of the present study was to develop a preliminary design of the nozzle for DCIJP by simulating the flow of ceramic ink in a microchannel for optimum flow characteristics and drop formation.

Details of the geometry of the nozzle used for simulation are shown in Figs 1(a), 1(b), and 1(c). The model consists of a cylindrical ink reservoir 10 mm in dia and 0.4 mm in depth. In this, the length of nozzle was 1.4 mm and the throat dia of the convergent-divergent portion was 0.038 mm at inlet and outlet [Fig. 1(b)]. The other geometry considered was with a throat dia 0.05 mm at inlet and outlet [Fig. 1(c)] keeping other dimensions constant as shown in Fig. 1(a). The chamber diameter was large when compared with modern office printers.

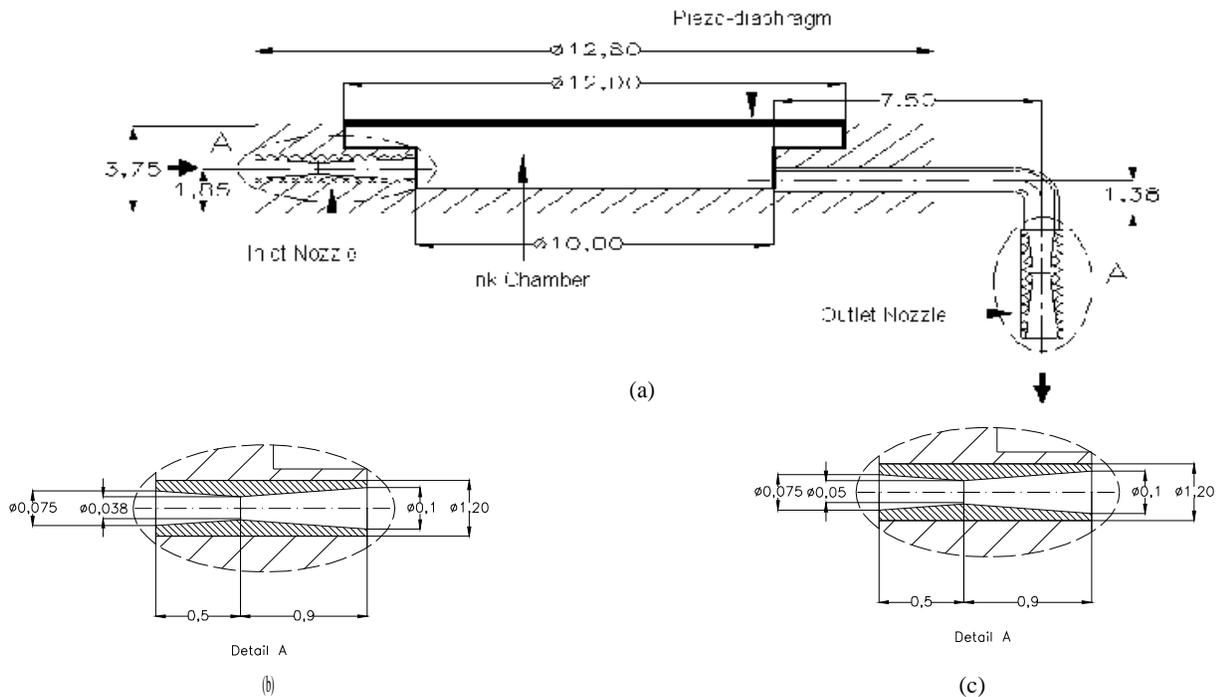


Figure 1. Details of the nozzle dimensions with varying throat dia. used for simulation: (a) geometry of the nozzle used for simulation of droplets, (b) nozzle with 0.038 mm throat dia, and (c) nozzle with 0.05 mm throat dia. (all dimensions in mm)

Piezoceramic discs with smaller dimensions were not available in India at the time of this study. At the inlet, there will be an ink reservoir (in practice) to ensure a continuous supply of ink. In the geometry, it is not represented. The model includes an air space below the nozzle where the droplets are to be ejected. The top of the chamber contains a deformable membrane that can be actuated piezoelectrically. Displacement given to this membrane imparts the necessary momentum for the droplet formation and ejection. The data on viscosity and surface tension for DCIJP were taken from the literature¹¹ available and is shown in Table 1. The flow module coupled with the VOF of CFD-ACE+ has been used to simulate the droplet formation and its spread by considering the effects of surface tension, viscosity and amplitude of actuation. This study yields a better understanding of the fundamentals affecting the droplet formation and its spread. This also helps in finding out the optimum nozzle dimensions. From the dimensions obtained, the fabrication of the nozzle was carried out.

Table 1. Properties of ceramic ink used for simulation

Volume fraction of alumina (%)	Density (kg/m ³)	Viscosity (m ² /s)	Surface tension (N/m)
5.0	947.550	2.3×10 ⁻⁵	0.025
7.5	1026.825	2.45×10 ⁻⁴	0.025

2.1 Simulation of Droplet Formation from the Piezoelectrically Actuated Chamber

The CFD-ACE+ software was used to perform the coupled fluid dynamic analysis of the formation of ceramic ink droplet and its spread on the substrate¹². CFD-ACE+ utilises a modular approach for performing coupled simulations that allow the user to invoke the necessary physical models. For this simulation, the VOF module was coupled with the flow module. First fluid was air and the second fluid was ceramic ink. Computation of scalar value F for each cell specified the fraction of the cell's volume that contains only liquid. Thus, volume fraction F of secondary fluid ranges from 0-1 according to the relative proportion of two fluids. The characteristic feature of the VOF methodology is that the distribution of the ceramic ink in the computational grid is

accounted for using a single scalar field variable, F , which specifies the fraction of the volume of each computational cell in the grid occupied by fluid 2 (ceramic ink). Thus, F takes the value 1 in cells, which contain only fluid 1 (air). A cell that contains an interface would have a value of F between 0 and 1. By definition, any value outside the range of 0-1 is physically unrealistic for a given flow field. The manner in which the volume fraction distribution F evolves is determined by solving the transport equation.

$$\partial F / \partial t + \Delta * \upsilon F = 0 \quad (1)$$

This equation must be solved together with the fundamental equations of conservation of mass and momentum to achieve computational coupling between the velocity field and the distribution of liquid.

2.2 Mixture Property

The proportion of fluid 1 and fluid 2 in the mixture determines the average density, viscosity, thermal conductivity, and specific heat capacity, etc. The average value of any volume-specific quantity Φ in a computational cell can be computed from the value of F in accordance with

$$\phi = F\phi_2 + (1 - F)\phi_1 \quad (2)$$

2.3 Surface Reconstruction and Secondary Fluid Flux Calculations

In CFD-ACE-GUI, surface reconstruction is a prerequisite for determining the flux of fluid 2 from one cell to the next and for determining surface curvatures when the surface tension model is activated¹³. Here, upwind scheme with the piecewise linear interface construction (PLIC) method is used. In the PLIC scheme, the liquid-gas interface is assumed to be planar and allowed to take any orientation within the cell and will therefore generally have the shape of an arbitrary polygonal face. The facet in a cell is defined by specifying: (i) the spatial orientation of the infinite plane that contains the facet, and (ii) the location of a point within the cell through which the infinite plane passes. The orientation is specified by specifying the outward-pointing unit normal of the infinite plane, and the sense of the normal is here arbitrarily chosen so that it points

out of the liquid phase and into the gas phase. The unit normal of the plane is determined by assuming that it is parallel to the gradient vector of F . The gradient of F is determined from the local distribution of F in a set of cells which includes the target cell and all its immediate neighbors. The location of the anchor point is determined by finding the infinite cutting plane perpendicular to the unit normal of the infinite plane that truncates the correct liquid volume from the cell, i.e., that satisfies the condition

$$V_{cut} = FV_c \quad (3)$$

In the PLIC scheme, each cell has a unique surface normal that can be used to compute the surface curvature from cell to cell. This enables the calculation and addition of surface tension forces for the free surfaces. Having computed the interface shape and orientation in an upwind cell, the flux of the secondary fluid for a given velocity can then be determined by back projection from the cell face. The back projection concept for the PLIC scheme is shown in Fig. 2.

3. RESULTS AND DISCUSSION

Several simulation studies were carried out for different dimensions of nozzle and properties of inks. Studies were focused on droplet shape, pressure distribution in the nozzle, tailing effect, and spread of droplet. In the case of the pure liquid, a nearly-symmetrical neck rapidly develops which narrows uniformly as it undergoes stretching¹⁵. This appears as a tail which finally ruptures at either end forming a single satellite drop. Immediately after rupture, the drop is nearly spherical and liquid remaining at the tip of the orifice resembles a hemispherical cap. In addition to qualitatively altering the shape of the structure at pinch-off, the particles also lead

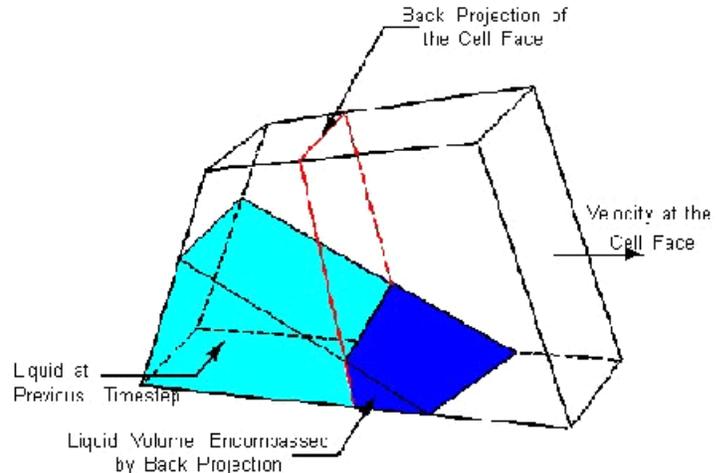


Figure 2. Back projection concept for the PLIC scheme.

to much different behaviour of the developing thread as the drop falls away from the tip of the capillary. In direct ceramic inkjet printing, it was observed that the ceramic ink droplet detached from the nozzle with an elongated portion which appeared as a tail that finally ruptured at either end forming a single satellite drop (Fig. 3). The formation of liquid droplets during the application of the displacement given to the top surface was monitored. Several plots have been obtained from this simulation to understand the droplet shape, pressure distribution, tailing effect, and spread.

3.1 Observations on the Droplet Shape

Several trials were required to obtain a good droplet shape in simulation. The behaviour of the droplet ejected from the nozzle that contains 5.0 and 7.5 volume percentages of alumina (Figs. 4-7) shows the tailing effect. The drop when formed is to have a spherical shape but when the same is sheared through the nozzle, the ink appears to be stretched. This leads to further breakup of drop.

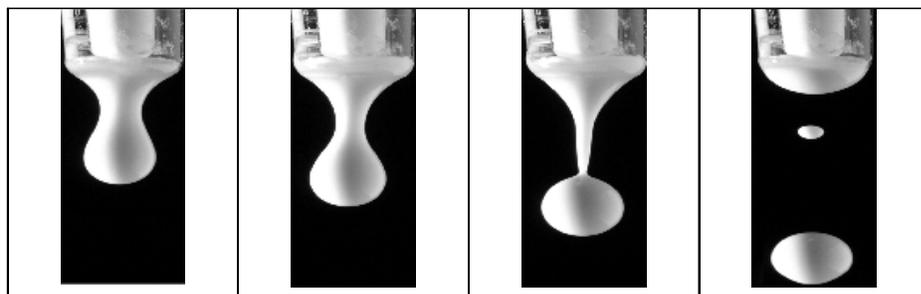


Figure 3. Tailing while droplet formation and ejection.

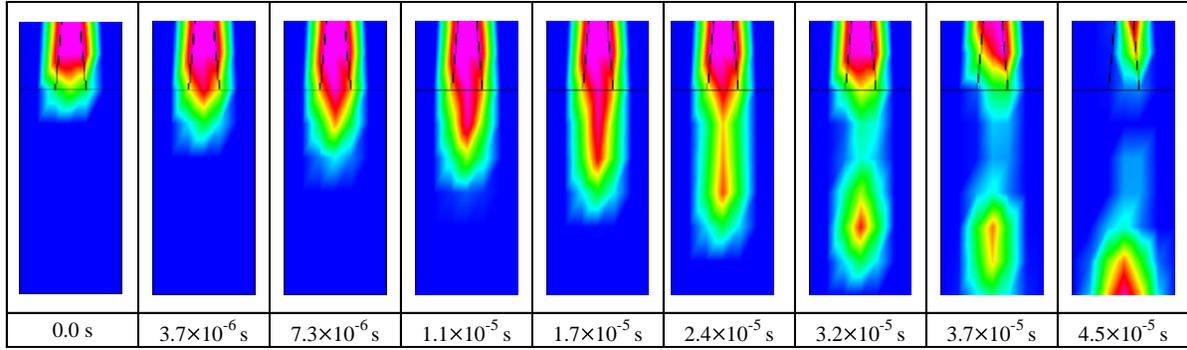


Figure 4. Tailing effect and droplet formation for fully wetting substrate (nozzle dia 38 μm and 5.0 vol % of alumina in ethanol).

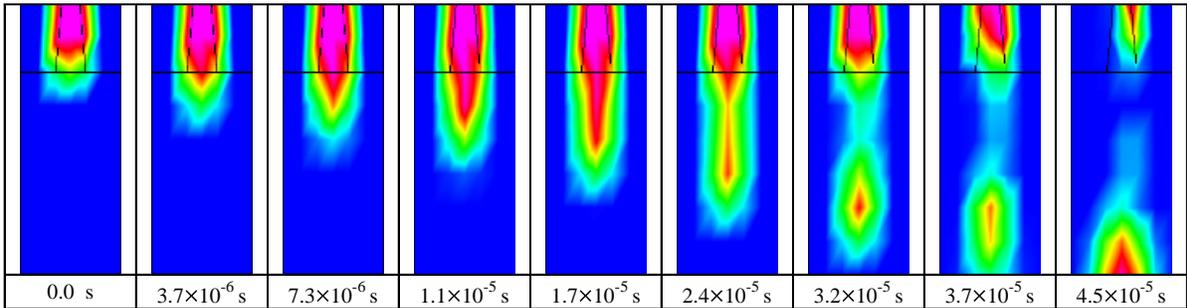


Figure 5. Tailing effect and droplet formation for fully wetting substrate (nozzle dia 38 μm and 7.5 vol % of alumina in ethanol).

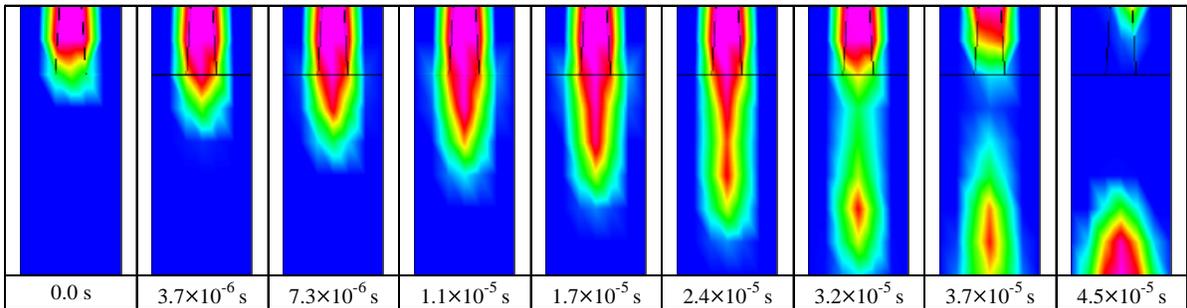


Figure 6. Tailing effect and droplet formation for fully wetting substrate (nozzle dia 50 μm and 5.0 vol % of alumina in ethanol).

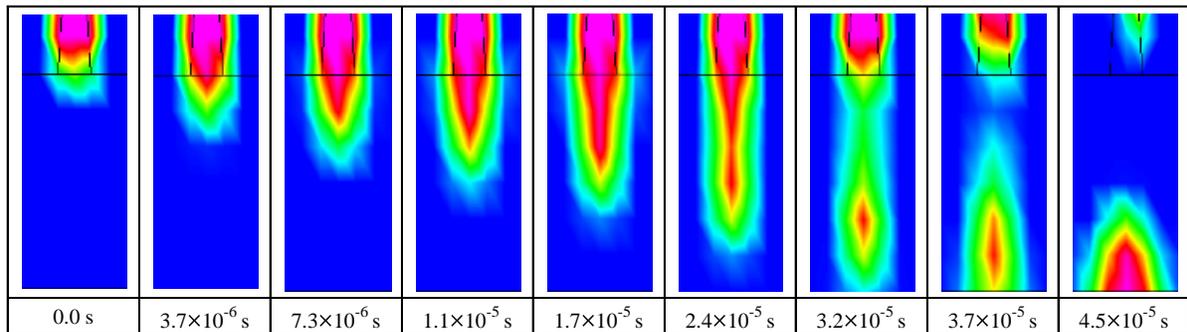


Figure 7. Tailing effect and droplet formation for fully wetting substrate (nozzle dia 50 μm and 7.5 vol % of alumina in ethanol).

Tailing effect increases as the volume fraction of alumina increases in ceramic ink because of the increased apparent viscosity and increased interparticle interactions. When the diameter of the throat is increased, tailing effect on the droplet formed for the same input conditions is also increased. The fully formed droplet for different nozzle diameters and different volume percentages of the alumina shows that the nozzle diameter is having effect on the droplet size and also on the formation of secondary

droplets due to tailing effect. (For suspensions with 5.0% and 7.5% ceramic content, values of surface tension are assumed to be the same).

3.2 Observations on the Pressure Inside the Nozzles at Inlet and Outlet

The pressure distribution inside the nozzles at the inlet and outlet is shown in Figs. 8(a) to 8(d). The pressures were plotted at the inlet plane, throat, and

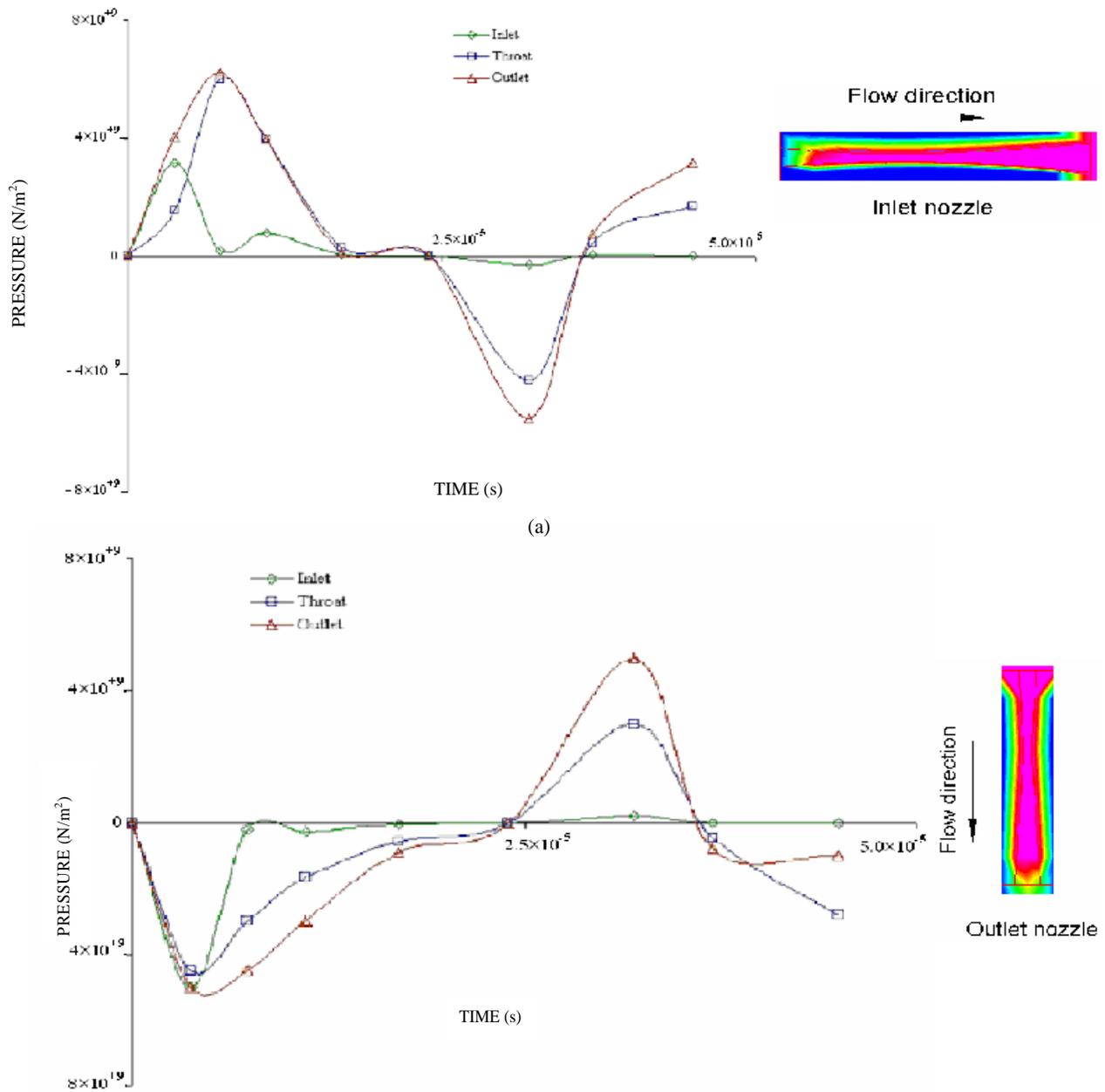


Figure 8. Pressure variation at: (a) inlet of the nozzle (throat dia 38 μm), (b) outlet of the nozzle (throat dia 38 μm).

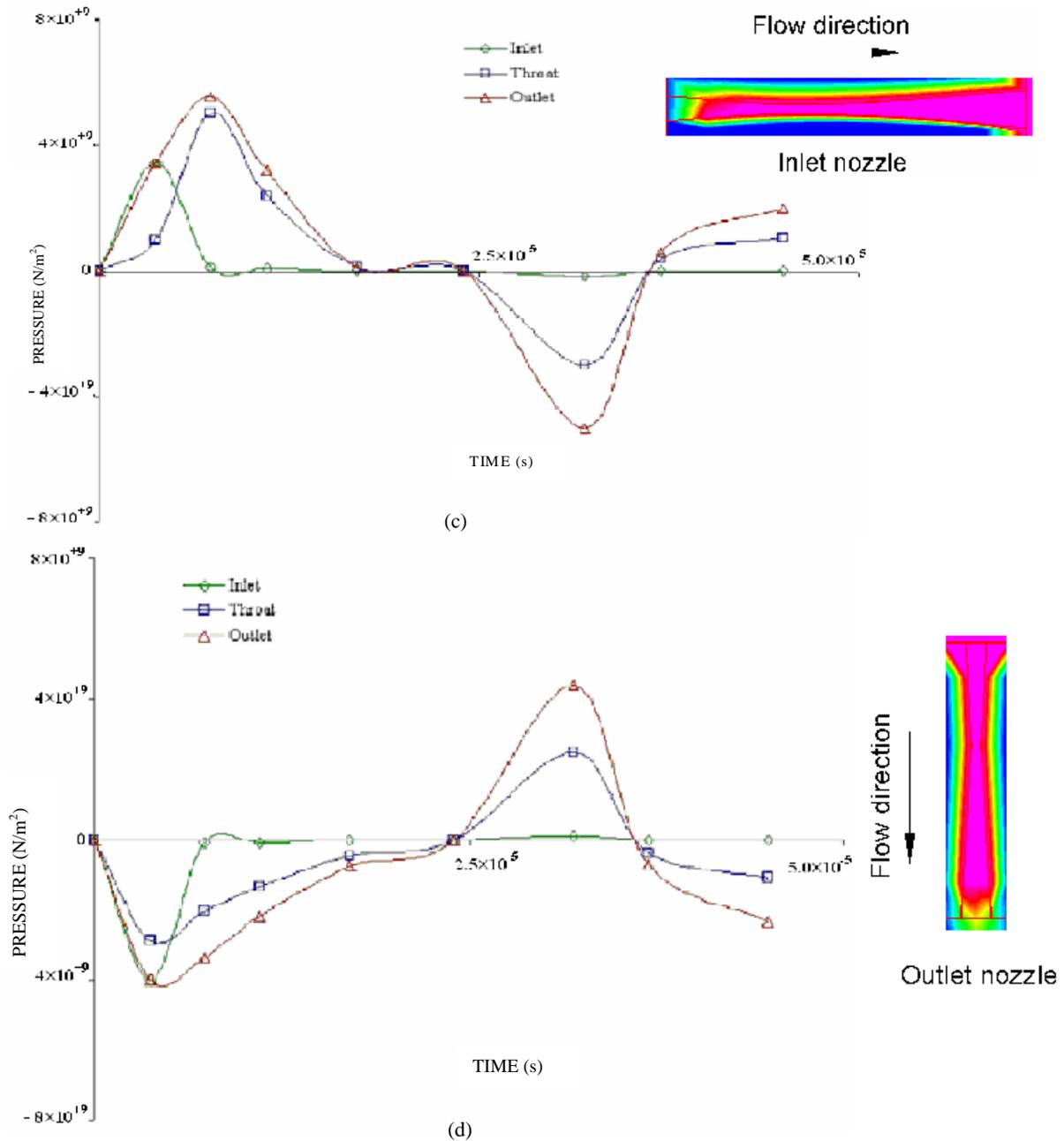


Figure 9. Pressure variation at: (c) inlet of the nozzle (throat dia 50 μm) and (d) outlet of the nozzle (throat dia 50 μm).

and outlet plane for the nozzles for one cycle of actuation. From these Figures, it can be inferred that the nozzle characteristics ensure a desirable formation and delivery of ink droplets. The cyclic variation of pressures and the simulation of drop formation and ink flow as shown in Figs. 8(a) to 8(d) confirms this. There is a variation in pressures for two nozzles. As the dimensions are not vastly different, pressures are also closer.

3.3 Observations on Spreading

Spreading of droplet on the substrate depends on the density, apparent viscosity, and surface tension of the ceramic ink, interfacial energy between the droplet and substrate, and amplitude of the displacement given to membrane. The spread is simulated for a fully wetting substrate condition. Spread of ceramic ink containing various volume

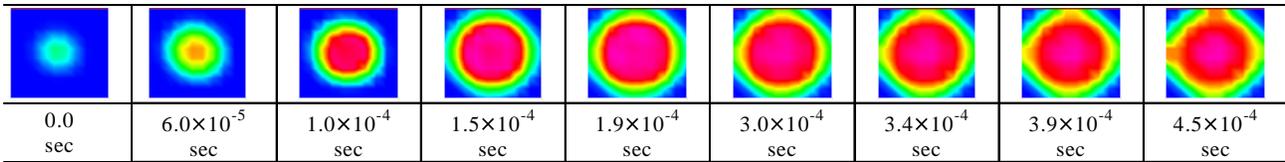


Figure 9. Spread of droplet on fully wetting substrate (nozzle dia 38 μm and 5.0 vol. per cent of alumina in ethanol).

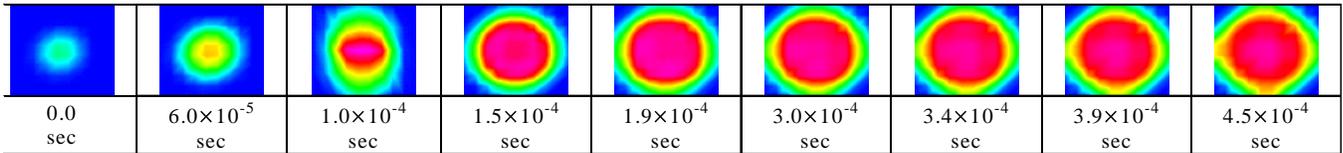


Figure 10. Spread of droplet on fully wetting substrate (nozzle dia 38 μm and 7.5 vol. per cent of alumina in ethanol).

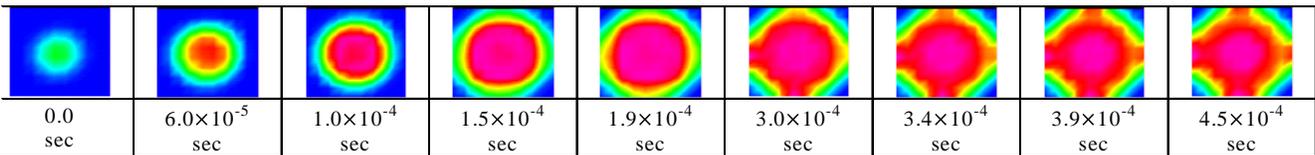


Figure 11. The spread of droplet on fully wetting substrate (nozzle dia 50 μm and 5.0 vol per cent of alumina in ethanol).

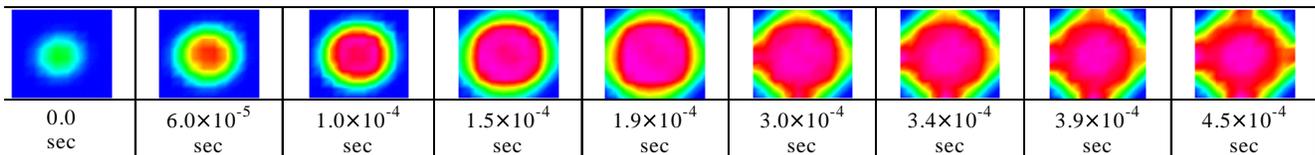


Figure 12. Spread of droplet on fully wetting substrate (nozzle dia 50 μm and 7.5 vol per cent of alumina in ethanol).

fractions of alumina shows (Figs 9 to 12) influence of density, viscosity, and surface tension of ceramic ink and the nozzle diameter on the spread over the substrate. As the viscosity of the ceramic ink increases, it offers higher resistance to spread. When the results of Figs 9 to 12 are studied at 3.9×10^{-4} s, the ink shows a good spread (Figs 9 and 10). When nozzle diameter is more, drop is not available for an increased spread i.e., much before 3.9×10^{-4} s, the spread is complete (Figs 11 and 12). Thus for a given composition of ink, there is an optimum nozzle diameter. (During trials it was observed that amplitude of actuation was to be increased when the ceramic content was increased so that the resistance to flow was overcome with increased energy of actuation). These observations can be used in the design of ink for desired droplet characteristics and also in finding the optimum dimensions of the nozzle.

3.4 Fabrication of a Prototype Nozzle

Based on the simulation studies, the dimensions of the nozzle that can be manufactured are determined as

shown in Figs 1(a) and 1(c) and a prototype was made with the specified dimensions with a CAD software as shown in Fig. 13. The dimensions were larger compared to that used in simulation. This is due to difficulties in machining. The nozzle with the specified dimensions was fabricated with wire cut EDM process with a tolerance of ± 0.0025 mm. This prototype will help researchers to pursue an improved design. The nozzle was then fixed to the ink chamber (Fig. 14). The piezoelectric actuator made of lead zirconate titanate (PZT) material was fixed with the electrodes (Fig. 15). The voltage that can be applied to the PZT disc (for different dia and thickness) to get given displacement¹⁴ is also given in Table 2 using Eqn (4).

$$\varepsilon = d * V \tag{4}$$

4. CONCLUSIONS

Following conclusions have been drawn:

- A coupled multi-physics simulation has been done for DCIJP for various volume fractions

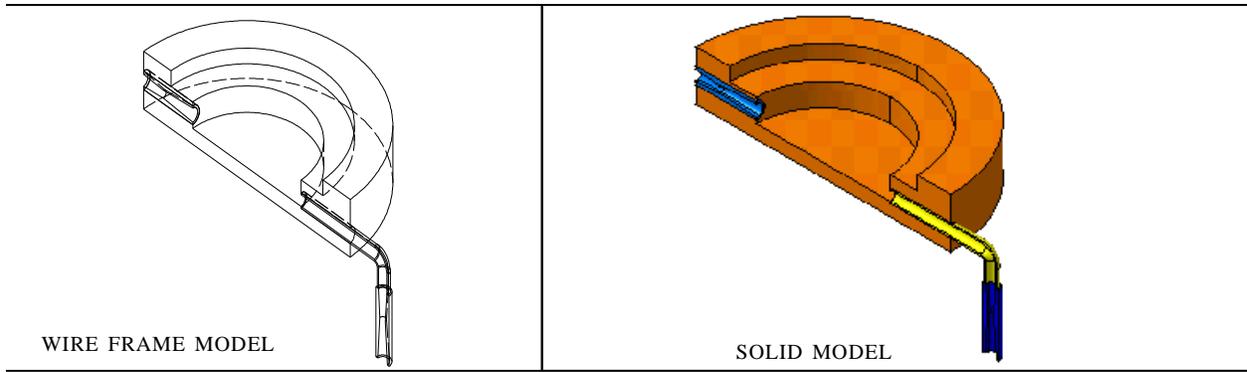


Figure 13. Chamber and nozzle assembly in CAD.



Figure 14. Nozzle assembly.

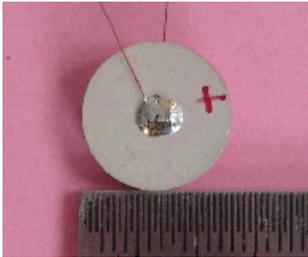


Figure 15. Piezoelectric actuator with electrodes fixed.

of alumina in ethanol for different nozzle dimensions to study the flow of ceramic inks in microchannels for desirable drop formation and deposition. From this study, the following salient points can be inferred.

- The interaction among the different physical phenomena that contribute to the droplet formation and ejection process has been found out. The apparent viscosity is known to increase as the fraction of particles in suspension increases. As volume fraction of ceramic increases, the tailing effect of the droplet also increases due to increased interaction among particles, leading to changes in interfacial energy.
- The pressure distribution at selected position of nozzles at inlet and outlet shows that flow can take place in the system without any adverse pressure gradient.
- The substrate condition and rheological properties of the ceramic ink influence the spreading of ceramic ink droplet. Amplitude of displacement given to the top membrane is also important in controlling droplet spreading when the ceramic content is increased, leading to increased apparent viscosity. Spreading of the ceramic ink droplet increases when the substrate condition is full wetting. Tailing effect increases and spread is

Table 2. Input voltage and displacement calculations for piezoelectric membrane

Diameter of piezoelectric disc, μm	Length of piezoelectric disc, L (μm)	Diameter of nozzle, D (μm)	Vertical expansion of piezo disc, $W \times 10^{-11}$ (m)	Strain (d)	Applied electric field (V/m)	Applied voltage (V)
12500	2000	100	426.700	2.133×10^{-6}	3878.780	7.760
12500	2000	50	53.300	2.665×10^{-7}	484.500	0.969
12500	2000	38	23.420	1.171×10^{-7}	213.000	0.426
12500	2000	20	3.413	1.706×10^{-8}	31.018	0.062
5000	500	20	21.330	4.266×10^{-7}	775.600	0.387
2000	500	20	133.300	2.667×10^{-6}	4848.470	2.424

reduced as there is an increased resistance to flow when the substrate is not fully wetting and ceramic content is increased, other condition remaining the same. A prototype of the nozzle is made for understanding the working of such a system. The development of nozzle with fine dimension (in μ) is under progress.

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