Dynamics in a Thermal Ink Jet: A Model for Identification and Simulation

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ABSTRACT

In this paper a newly developed model for identification and simulation of dynamic phenomena in a thermal ink jet is presented. As a result of the modeling the calculation of the pressure propagation in the bubble is performed by identifying the mathematical model with position measurements of the ejected liquid column. The identification of the model has been performed by minimizing the sum of quadratic deviations between simulated and measured values. Parameter studies with the identified model illuminate the behavior of the microactuator at higher overpressures.

Keywords: Thermal ink jet, microactuator, model identification, phase transition, fluid dynamics.

INTRODUCTION

The thermal microactuator used in ink jet printheads is the world's most successful microsystem, it is sold million times [1]. It offers a high potential in a large area of other applications where microdosing of different liquids is required. A detailed understanding of the dynamics of the thermal printhead is relevant for further improvement of this microactuator.

A short heating pulse drives a micro heating element and heats a thin liquid layer on the heater up to the thermodynamic limit of superheating of the liquid, the so-called spinodalian limit, within a few microseconds (see Fig. 1).

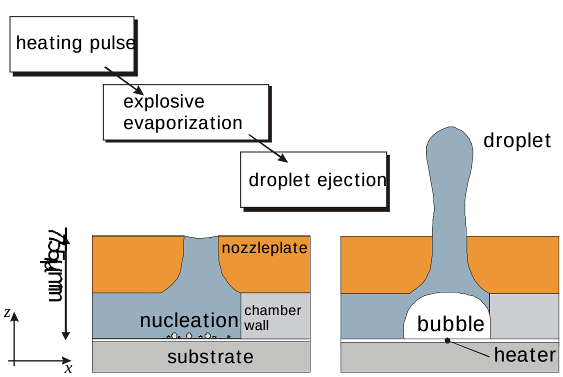

Figure 1: Schematic and principle of the thermal microactuator.

Then, the liquid evaporates explosively and the expanding bubble accelerates the liquid column above the heater and ejects a droplet through a nozzle with a diameter of approximately 60µm. The boiling can be understood as phase transition of second order [2]. In the case of water and ink the spinodalian limit is approximately 312 °C. For many other applications, e.g. the ejection of fuel in engines or the injection of drugs in minimal invasive surgery, droplet ejection against overpressures or hydrodynamic pressures is necessary. The dynamic model allows the evaluation of the potential of such thermal microactuators. For the complex dynamics in this microsystem rigorously expressed by nonlinear partial differential equations a state space representation was derived using integral methods. Despite of the model reduction the state space representation contains all important physical effects. This description is possible because all less significant influences are neglected. The input function of the model is the heating power. The thermal diffusion, the thermodynamics of the bubble, the conservation of energy, and the flow of the liquid column have been taken into account.

MEASUREMENTS

By identifying the model with measurements of the movement of the ejected liquid column realized with high speed cine photomicrography [3], [4] the calculation of the pressure propagation in the bubble was performed and is presented in this paper. The ejection was generated by a heating pulse with a length of 3µs and an amplitude of 7.5W. Investigations of the nucleation process in the ink chamber show that the nucleation starts 3.1µs after the beginning of heating. The visualization of the droplet ejection can be seen in Figure 2.

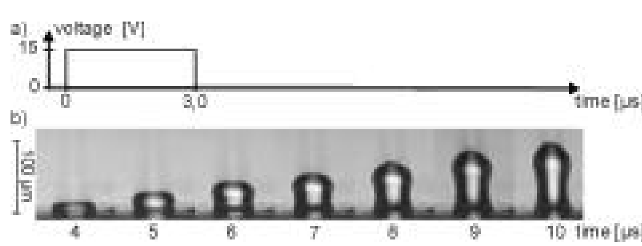

Figure 2: Input pulse (a) and visualization of droplet ejection (b).

The visualization has been performed with pseudocinematography. This method is based on the stroboscopic principle and can be applied to reproducible transient processes like the droplet ejection of an ink jet printhead in the first 10µs after beginning of heating. The top surfaces of the droplets can be connected by a straight line; consequently, the velocity v of the droplet surface is constant, v=15.3m/s. Considering that the liquid starts cutting off at 5µs it follows that there is a subpressure at this timepoint in the bubble. Consequently, the time duration of acceleration of the liquid column is between 3.1µs and 5µs. The height of the liquid column 4µs after the beginning of heating can also be extracted from the cinematographic image sequence and is 12.3µm. The measurements have been performed with a Hewlett-Packard DeskJet 500 printhead [5] and bidistilled water has been used to have adequate values for material properties available.

DERIVATION OF THE MODEL

To derive the model equations we have assumed that droplet ejection starts as a laminar flow through a tube as it is shown in Figure 3.

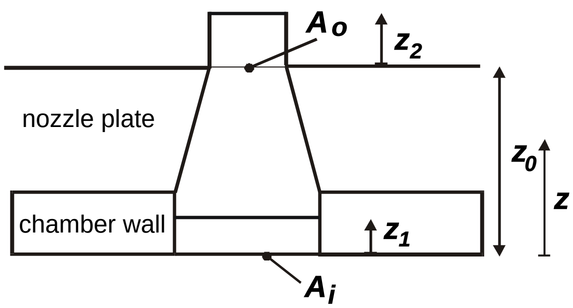

Figure 3: Dynamic model of droplet ejection.

The input plane A_i, in this model the area of the heating element, measures 3600µm^2 and the output plane A_o measures 2827µm^2. The tube length is z_0 = 75µm; $z_1 = z_1(t)$ and $z_2 = z_2(t)$ are time dependent. A cylindrical shape of the accelerated liquid column is also assumed. The assumption of laminar flow is justified by the small Reynolds number Re = 450 < 1160, the incompressibility of the liquid can be assumed due to the small Mach number Ma = 0.01<<1, and surface tensions are neglected because of the high Weber number We = 96>>1. Effects of friction are also not taken into consideration because the resistance of friction divided by the input plane corresponds with a pressure of approximately 80mbar. This is very much lower than the maximum pressure in the bubble of approximately 65bar which is calculated in this paper.

Considering that the acceleration of every element of volume $A(z)dz$ is different Newtons second law reads as

$$\int_{z_1(t)}^{z_2(t)} dz\, A(z)\rho\, \dot{v}(t,z) = \sum_i F_i \, . \qquad (1)$$

Here, ρ = 998 kg/m^3 is the density of water at a temperature of 20°C, $\dot{v}(t,z) = dv(t,z)/dt$ is the acceleration, and F_i are the forces. The tapering of the nozzle leads to a force against the force generated by the overpressure in the bubble and can be approximated by the mean value theorem of differential and integral mathematics

$$\frac{1}{A_i}\int_{z_1(t)}^{z_2(t)} dz\, p(t,z)\frac{\partial A(z)}{\partial z} \approx \frac{A_i - A_o}{2A_i z_0}\left(p(t) - p_0\right) , \qquad (2)$$

where p and p_0 = 1bar are the inner and outer pressure, respectively. Using the relation

$$A(z)v(t,z) = A_i v(t,z_1) = A_o v(t,z_3) \qquad (3)$$

and Equations (1) and (2) the dynamic equation

$$\left[\left(\frac{A_i}{A_o} - 1\right)\left(z_1(t) - z_1(t_0)\right) + z_0\right]\rho\, \ddot{z}_1(t) = \left[1 - \frac{A_i - A_o}{2A_i z_o}\right]\left(p(t) - p_o\right) \qquad (4)$$

follows. The diffusion of heat generated in the heating element to the evaporating mass in the liquid is simplified by

$$T_1 \dot{H}(t) + H(t) = K H_e(t) \ , \qquad (5)$$

where T_1 is a time constant, $H(t) = \dot{Q}(t)$ is the derivative of the heat Q of the evaporating liquid with the quantity of mass n in mol, and $H_e(t)$ is the electrical power generated in the heating element.

Neglecting dissipation the energy conservation of the evaporating mass can be expressed by first law of thermodynamics as

$$dU = -pdV + dQ \ , \qquad (6)$$

where U is the inertial energy and $pdV=pA_idz_1$ is the work performed by the bubble.

Although, the conservation of energy and impulse of the whole system is satisfied by Equations (4), (5), and (6) the propagation of $p(t)$ is not unambiguous specified. Under the assumption that the evaporating quantity of mass has equal density, temperature, and pressure over the whole volume a state function in the (pVT)-state space defined by pressure, volume, and temperature can be assigned to the evaporating mass. A good approximation of the state function for liquid water and for vaporized water is the Berthelot equation

$$\left(V - nb\right)\left(p + \frac{n^2 a}{TV^2}\right) = nRT \qquad (7)$$

with the material constants a, b and R which can calculated from the critical volume V_{cr} , pressure p_{cr} , and temperature T_{cr} of water.

The assumption that the pressure, the volume, and the temperature are connected by the Berthelot equation (7) during the phase transition is critical and can not be true for a boiling in a macroscopic glass of water. For normal boiling a part of the evaporated fluid is liquid and the other part is vapor. But for the micro dimension of the thermal pneumatic actuator the situation is completely different. The evaporating quantity of mass is heated up to the spinodalian limit [2]. Schlieren appear on the heater which corresponds to a long correlation length between the molecules. The long correlation length could lead to a phase transition where the trajectory in the (pVT)-state space moves through the forbidden area of the unstable region and the classification of the fluid into liquid and water does not make sense. However, the consideration of the conversation of energy and impulse guarantee a good approximation of the dynamics, although, no successful theory for the evaporation after reaching the spinodal exists yet and, therefore, the above assumption can be supported by the experimental findings only.

The inertial energy U can be calculated from Equation (7) and thermodynamic reflections, this leading to

$$U = nc_V T - \frac{n^2 a}{TV} \qquad (8)$$

with $c_V = 3kN$ as the heat capacity of an ideal gas with molecules with 6 degrees of freedom at constant volume, k = 1.3807 10^{-23} as the Boltzmann constant and N = 6.0225 10^{23} is the number of molecules in 1mol.

The Equations (4), (5), (6), (7), and (8) can be rewritten as nonlinear state space representation with a state space differential equation

$$\dot{\underline{x}} = \underline{f}\left(\underline{x}, u\right) \quad , \quad \underline{x} = \begin{pmatrix} x_1(t) \\ x_2(t) \\ x_3(t) \\ x_4(t) \end{pmatrix} = \begin{pmatrix} T(t) \\ V(t) \\ \dot{V}(t) \\ H(t) \end{pmatrix} \qquad (9)$$

and the measurement equation

$$\underline{y} = \underline{h}\left(\underline{x}\right) = \begin{pmatrix} y_1 \\ y_2 \\ y_3 \end{pmatrix} = \begin{pmatrix} T(t) \\ V(t)/A_o \\ \dot{V}(t)/A_o \end{pmatrix} \quad . \qquad (10)$$

The mathematical model includes furthermore that $H = 0$ when the trajectory in the (pVT)-space intersects the spinodal. This is necessary to take into account that no heat is transferred into the evaporating quantity of mass after the spinodalian limit is reached which is known as the Leidenfrost phenomenon.

IDENTIFICATION OF THE MODEL

The identification of the mathematical model has been performed by minimizing the sum of quadratic deviations between simulated and measured values. The cost function used for identification reads as

$$\begin{aligned} J(n,T) &= 1000 \cdot \left(z_2(t_1) - \hat{z}_2(t_1)\right)^2 + \left(\dot{z}_2(t_2) - \hat{\dot{z}}_2(t_2)\right)^2 \\ &+ 1000 \cdot \left(z_2(t_2) - \hat{z}_2(t_2)\right)^2 + \frac{1}{10} \cdot \left(\dot{z}_2(t_3) - \hat{\dot{z}}_2(t_3)\right)^2 \end{aligned} \qquad (11)$$

with t_1 = 3µs, t_2 = 4µs, and t_3 = 5µs. The values for the measured data are $\hat{z}_2(t_1)$ = 0µm, $\hat{z}_2(t_2)$ = 12.3µm, $\hat{\dot{z}}_2(t_2)$ = 15.3m/s, and $\hat{\dot{z}}_2(t_3)$ = 15.1m/s. The value for $\hat{\dot{z}}_2(t_3)$ was extracted from the knowledge that 5µs after beginning of heating a subpressure is in the bubble and the velocity slightly decreases. Furthermore, from the results of numerical studies of the thermal diffusion in the heating element the factor K is assumed to be K = 0.05. The costfunction was minimized by using the Nealder-Mead-algorithm implemented in the commercial software MATLAB.

The evaporated quantity of substance n and the time constant T_1 were determined by the optimization procedure and resulted in n = 4.495pmol and T_1 = 14µs.

SIMULATION OF THE DYNAMICS

By solving Equations (9) and (10) numerically with the Runge-Kutta-algorithm implemented in MATLAB the propagation of the temperature in the bubble and the movement of the liquid column have been simulated. The pressure propagation in the bubble which is shown in Figure 4 was calculated using Equation (7). Figure 4 demonstrates that the heating pulse generates a pressure pulse with an amplitude of 65bar and a width of 100ns full width half maximum. It is remarkable that this result is in good agreement with the result given in [6] derived with a completely other model for the thermodynamics in the bubble, but with a similar model for the flow through the tube. The knowledge of the propagation is important for the evaluation of the possible operational range of the thermal actuator.

Variation of the geometry or the pressure outside the actuator shows that the pressure propagation does not change very much. For example, the amplitude varies between 65bar and 69bar.

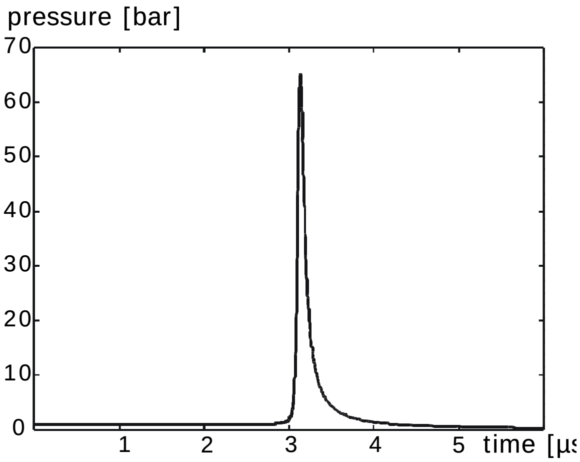

Figure 4: Pressure propagation in the thermal pneumatic microactuator.

In contrast, the movement varies dramatically. Figure 5 demonstrates the influence of a higher outerpressure on the movement of the liquid column. The broken line in Figure 5 shows the movement of the liquid column $z_2(t)$ for normal outer pressure of approximately 1bar and the solid line for an outer pressure of 5bar.

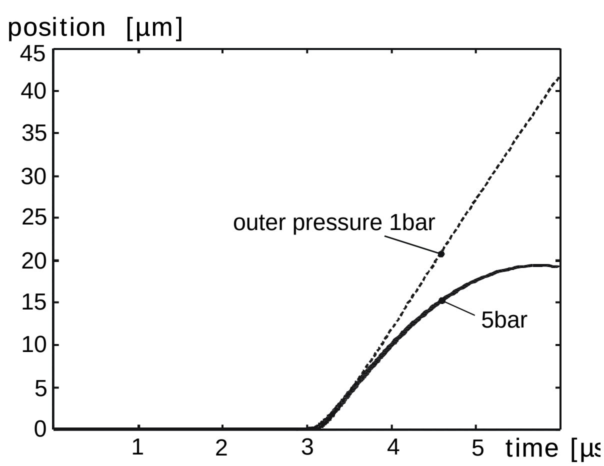

Figure 5: Movement of the liquid column $z_2(t)$ for different values of the outer pressure.

The model is not valid for t > 5µs because the droplet starts to cut off at 5µs. However, the model illustrates obvious that a droplet ejection of a thermal pneumatic actuator with a single heating pulse is not possible for outer pressures ? 5bar. Figure 6 demonstrates the simulation of the movement of the liquid column for an output plane of A_o = 1267µm^2, where all other dimensions of the actuator have been kept the same. The liquid column reaches a velocity of $\dot{z}_2(t)$ = 29m/s in course of a velocity of $\dot{z}_2(t)$ = 15.3m/s for an output plane of A_o = 2827µm^2.

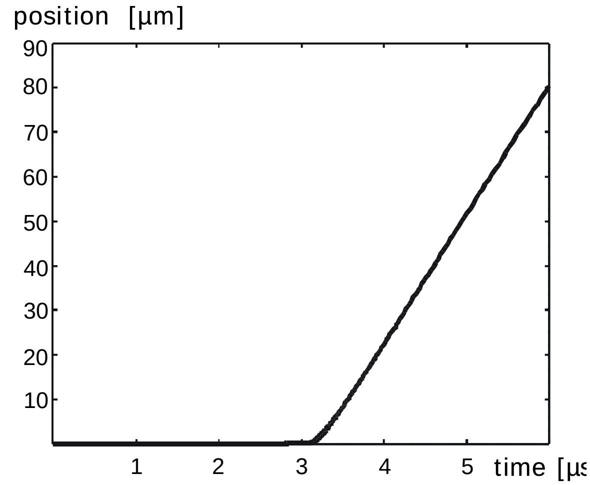

Figure 6: Movement of the liquid column $z_2(t)$ for normal outer pressure and A_o=1267µm^2.

The velocity does not change as long as the ratio of input plane and output plane remains constant. Therefore, the velocity can be adjusted by the ratio of input and output plane. An increasing of the actuator height z_0 decreases the velocity of the droplet. A variation of geometry does not essential influence the pressure propagation in the vapor bubble.

CONCLUSIONS

The identification and simulation of the dynamics in a thermal inkjet printhead with a simplified state space model has been presented in this paper. The measured data for identification have been extracted from cinematographic image sequences. The evaluation of the behavior of the device at higher outer pressures than normal pressure have been studied. The influence of a variation of the design, in particular the ratio of the area of the heating element and the area of the nozzle orifice, has been demonstrated.

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