

DESIGN ANALYSES OF CAPILLARY BURST VALVES IN CENTRIFUGAL MICROFLUIDICS

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Abstract

This paper presents current research in analysis of passive microfluidic capillary burst valves. A capillary burst valve stops the liquid flow using a capillary pressure barrier that develops when the channel cross section expands abruptly. Valves of this type provide the capability of precise control on sample location in microfluidic device. Detailed numerical analyses of the valve behaviour is presented and compared with experimental measurements. A model for the valve is then extracted that characterizes the valve performance for various common cross sections.

Keywords: Micro fluid control, Valves, Capillary Gating, Centrifugal force, FlumeCAD

I. Introduction

There is a wide interest in micron-scale integrated chemical/biochemical analysis or synthesis systems, also referred to as lab-on-a-chip[1]. An essential ingredient in these devices is the ability to control the spatial and temporal position of the sample as it flows through the device. Conventional diaphragm valves can fulfil this task, but require both moving parts and an external actuation mechanism, often complicating the implementation and integration. Several methods of electrokinetically controlling the liquid flow have been demonstrated. These methods are however sensitive to the physicochemical properties of the components and by the presence of trapped air.

An alternative approach presented in this paper uses a passive microfluidic capillary-driven valve that exploits the surface tension force to stop flows in micro-channels. The principle of operation is based on the pressure barrier that develops when the cross section of the capillary expands abruptly. These valves have the advantage of not requiring moving parts. They are not sensitive to the properties of the buffer/samples pumped or the presence of trapped air and bubbles. They also alleviate problems associated with Joule heating that occur in electrokinetic systems that demand high field strengths. Valves of this type recently have attracted considerable attention [2-4] and present strong appeal for applications to various micro-fluidic systems.

The specific problem that we analyse in this paper is the gating of the fluid using capillary burst valves driven by centrifugal force [2]. The overall objective is to demonstrate a mechanism to design these valves. For effective implementation, the physical phenomena in the gating process needs to be understood, including the parameter space that it is sensitive to. This parameter space is difficult to explore experimentally – CAD tools, on the other hand, provide an effective mechanism, and is the focus of this paper.

We will begin by presenting a theoretical analysis of the gating process. Following that the numerical methodology is presented and validated with experiment. The CAD analysis will then be extended to analyse micro-channels with various

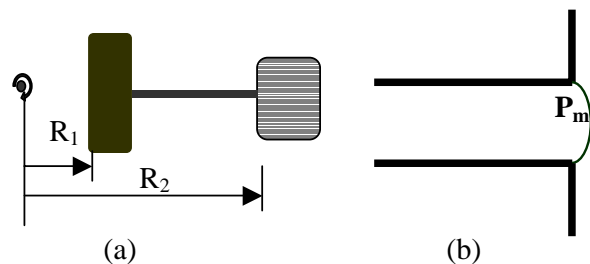


Fig. 1. Schematic of gating operation driven by centrifugal force. (a) shows top view of the rotating plate. The reservoir resides at R_1 and the abruptly-expanding open is at R_2 . The reservoir and channel are filled by liquid sample. (b) shows a close-up view of the abruptly-expanding opening. Liquid pressure at the meniscus is P_m .

cross-section and a reduced-order model will be extracted for application in the design of devices employing such valves. It should be noted that valves of this type and the analysis methodology presented here is not limited to centrifugal-driven devices but can be applied to various microfluidic devices in which precise gating is desired.

II. Theory

A schematic of the gating operation is shown in Fig. 1. A narrow channel connects two large containers, a reservoir full of sample liquid and an initially empty reaction chamber. This device is placed on a rotating plate and extends radially outwards. The centrifugal force drives the sample liquid from the reservoir to the chamber. The capillary force acting at the channel opening resists the forward motion of the liquid – the “capillary barrier”. When the liquid pressure at the meniscus overcomes the capillary barrier, the liquid bursts into the chamber. Precise control of the liquid position is accomplished by tuning the driving force. Although centrifugal force is the driving mechanism here, this principle applies to pressure, pneumatics or electrokinetic forces as well.

The maximum capillary barrier may be derived from thermodynamics in terms of interfacial free energy [4-5] and expressed as $P_{cb} = 4\gamma_{al}\sin\theta_c/D_h$, where γ_{al} surface energies per unit area of the liquid-gas interface, θ_c the equilibrium contact angle, and D_h the hydraulic diameter of the channel. This equation is derived assuming axisymmetric cross-sections.

The Navier-Stokes equations, that describe the flow of the liquid, reduce to a balance between the centrifugal force and the pressure gradient, under the assumption that the liquid velocity at the opening is small. The reservoir has much larger interfacial area and the liquid pressure at R_1 is close to ambient. The liquid pressure at the opening P_m , accordingly, may be expressed as $\rho\omega^2 r\Delta r$, where r is the average distance from the liquid element to the rotating center, Δr is the radial length that the liquid sample occupies.

To adequately gate the liquid, the pressure at the meniscus P_m should not exceed P_{cb} , assuming the ambient is zero. This yields the capillary stop condition, expressed as: $\rho\omega^2 r\Delta r < 4\gamma_{al}\sin\theta_c/D_h$. A critical point is reached when these two terms balance each other. Such $\rho\omega^2 r\Delta r$ defines the maximum sustainable pressure that can be restrained by the meniscus. In this paper we refer to this maximum as the *critical burst condition*, it is of great interest to design engineers. Designers may cause the meniscus to burst by exceeding this critical burst condition by varying the radius r , the frequency of plate rotation ω or other parameters.

III. Numerical Methodology

The Navier-Stokes equations represent the detailed fluid motion through the device. A Volume-of-Fluids (VOF) approach [6] was used to simulate the two-phase flow in the capillary burst valve. The VOF approach weights the equations with a phase fraction to adequately represent the constituent phases at each location in space. An additional equation tracks the interface as it migrates through the domain.

The simulation capability is incorporated into FlumeCAD, which is a design environment consisting of 3D design, modeling and simulation software tools that enable the creation and analysis

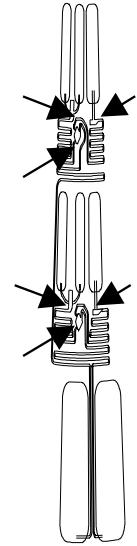
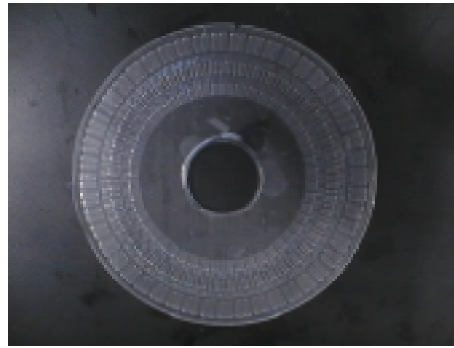


Fig 2: Centrifugal Device that uses capillary burst valves for gating [2]. The sketch at right shows one microfluidic structure positioning on the rotating plate radially. Gating components are marked by arrows.

of complex microfluidic devices. A finite-difference solver engine is used as the back-end solver for the analysis.

IV. Results and Discussion

In this section the CAD tool is first validated by comparing against experimental measurements. It is then applied in modifying the classical analytical gating behaviour of the valve by examining and accounting for the three-dimensional effects of the cross section.

A centrifugal microfluidic device, shown in Fig. 2, was fabricated and tested by Gamera Bioscience[2]. Each microfluidic structure is distributed on a rotating plate evenly along radial direction and is composed of fluid reservoirs, transport channels and reaction chambers. The capillary gating mechanism described above is applied to precise control of the fluid sample. Details of the fabrication process for making these devices and the experimental setup and measurement is reported in [2] and is not reproduced here.

The results of the simulation are presented in Fig. 3-6. Details of the meniscus located at the channel opening is shown in Fig. 3. The meniscus extends a certain distance into the channel, depending on the physical properties of the fluid and the geometry of the intersection. It is however stable. As the rotation speed (the centrifugal strength) is increased, the meniscus extends further and further out into the chamber until the capillary barrier is no longer able to sustain the applied force. The liquid then bursts into the chamber. This effect is also seen by positioning a probe at the meniscus and recording the meniscus velocity as shown in Fig. 4. When the centrifugal strength is less than the critical burst condition the meniscus oscillates but the oscillations eventually damp out and the meniscus returns to a steady state. When the centrifugal strength exceeds critical, the meniscus oscillations do not damp out but increase until the meniscus breaks and fluid spills into the chamber.

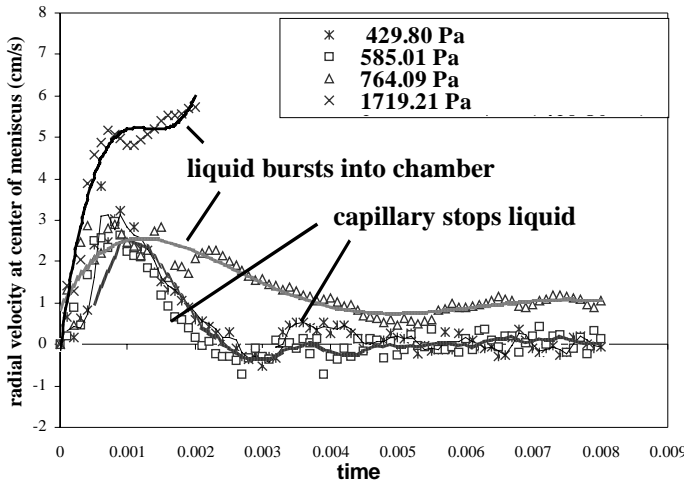


Fig. 4: Radial velocity of the meniscus verse time recorded by a probe (numerical simulations). This figure shows critical burst condition is between 585.01Pa and 764.09 Pa.

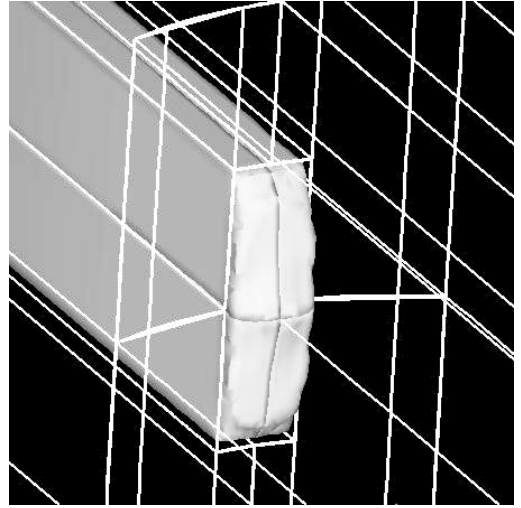


Fig. 3: A close-up view of liquid meniscus at channel opening (simulation).

Experimental validation is shown in Fig. 5. The critical burst condition $\rho\omega^2r\Delta r$ is shown for channels with different diameters, D_h . The numerical results agree quite well with the experimental measurements for the entire range of diameters studied.

The simulation results shown here were for rectangular channels. We will now turn to predictions of channels with different cross-sections to examine their effect on the gating frequency. The detailed simulations account for the fact that the meniscus contact line may be a complex 3D shape, dependent on the geometry. This relaxes the inherent assumption in the theoretical (or hydraulic diameter based) models that assume a circular contact line of diameter D_h , regardless the geometry of

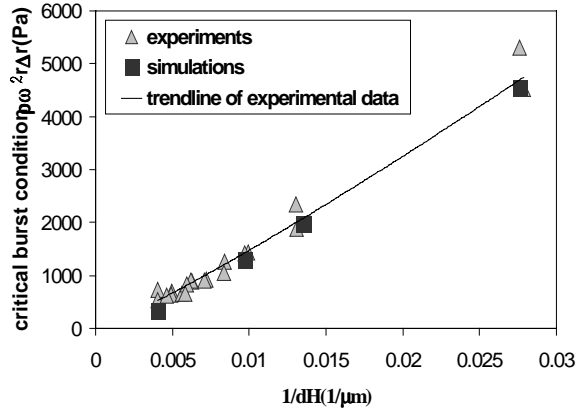


Fig 5: Critical burst frequency verse channel geometry. The channel is of rectangular cross-section (d_H varies from $36 \mu\text{m}$ to $250 \mu\text{m}$). FlumeCAD simulation results are plotted against experiments.

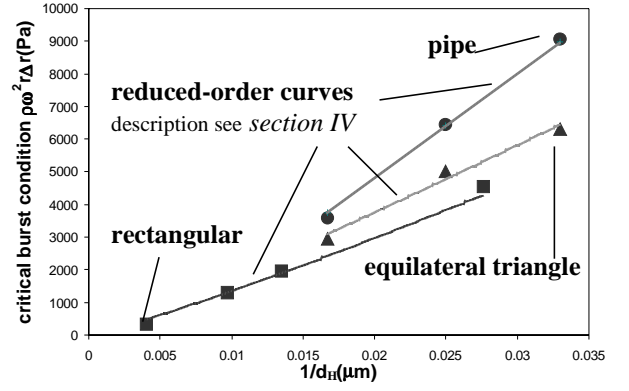


Fig. 6: Critical burst condition verse micro channels with different type of cross-sections. Reduced models are drawn from the simulation data for each type of cross-sections.

the channel. The CAD analyses presented in Fig. 6 indicate that the effect of the channel cross-section is not actually negligible but differs depending on the cross section.

To account for this variation, we will modify the theoretical critical burst condition definition as $\rho\omega^2 r \Delta r < 4\gamma_{al} \sin\theta_c (D_h)^n$, where $n=-1.08$ for duct with equilateral triangular cross-section, $n=-1.14$ for duct with rectangular cross-section. An additional term is present in the reduced-order model for pipe flow, the critical burst condition is $4\gamma_{al} \sin\theta_c / D_h + \gamma_{al} \sin\theta_c (1/D_h - 1/D_0)$, where $D_0=40\mu\text{m}$. Additional cross-sections can be computed and correlations developed using a similar methodology.

V. Conclusions

In this paper we present a microfluidic valve utilizing capillary effects and CAD applications to design/analysis of such type of microfluidic control mechanism. A CAD tool FlumeCAD is used to perform detailed simulations and characterize critical burst condition as a function of geometrical parameters. Comparison with experiments is used to validate the CAD analysis and shows good agreement. The simulations are then extended to develop a model for the effect of cross-section geometry on the capillary burst frequency. A modified model is developed that incorporates the effect of the geometry, based on the simulation results. This model can be incorporated into models for the devices that use these valves as a gating component. Similar models can be developed for other applications where capillary gating is a desirable effect.

Acknowledgments

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References

1. D. J. Harrison, A. van den Berg, Eds. *μTAS '98*.
2. D. C. Duffy et al, "Microfabricated Centrifugal Microfluidic Systems: Characterization and Multiple Enzymatic Assays", *Analytical Chemistry* 71, 20 (1999)
3. R. M. Moroney, et al, "A Passive Fluid Valve Element for a High-Density Chemical Synthesis Machine", *MSM 98*, Santa Clara, CA.
4. P. F. Man, C. H. Mastrangelo, M. A. Burns and D. T. Burke, "Microfabricated Capillary-Driven Stop Valve and Sample Injector", *MEMS '98*, pp.45-50
5. E. Kim and G. M. Whitesides, "Imbibition and Flow of Wetting Liquids in Noncircular Capillaries", *The Journal of Physical Chemistry B*, Vol. 101, No. 6, pp.855-863 (1997)
6. C. W. Hirt and B. D. Nichols, "Volume of Fluid (VOF) Method for the Dynamics of Free Boundaries", *Journal of Computational Physics*, Vol. 39, pp. 201-225 (1981)