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CFD SIMULATIONS OF A CAPILLARY FORCE DRIVEN TWO-PHASE FLOW IN THE ANODE FLOW-FIELD OF PASSIVE-FEED μDMFC.

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Abstract

The computational fluid dynamics (CFD) simulation results of a capillary-driven flow in a 100 μm serpentine flow-field are presented. A two-dimensional (2D) numerical model based on a conservative level set method (LSM) was developed and solved using a commercial software program called COMSOL Multiphysics. During reinitialisation of the level set function, a good conservation of the liquid phase area was achieved. Both the respective back and the front interfaces in the 300 μm reservoir and in the microchannel were monitored. Fluctuations were initial evident in the reservoir interface which later subsided. The front interface in the serpentine microchannel assumed an almost constant velocity.

Keywords: capillary, conservative, flow-field, serpentine, two-phase flow, level set method

1. Introduction

Miniaturised fuel cells or micro fuel cells have received a lot of attention over the past 10 years as potential sources of power for portable electronic devices and military applications [1],[2]. direct methanol micro fuel cells (μDMFCs) are in particular popular because of easier handling and safer storage compared to hydrogen . Methanol fuel is oxidised in the presence of a catalyst at the anode to carbon dioxide and hydrogen ions and electrons are released to create electric current. Hydrogen ions and electrones combine with oxygen at the cathode to form water. The accumulation of carbon dioxide produced during oxidation of methanol at the anode prevents further oxidation at the active surface and reduce the performance of the μDMFC with time [3]. The supply of the liquid methanol fuel to the fuel cell is still a problem whereby pumping means are required to pump the fuel in to the anode side of the fuel cell and to remove, together with the methanol fuel, the carbon dioxide gas bubbles produced during the oxidation reaction. Micropumps that are used for this purpose require some form energy to function and often use the electricity produced from the fuel cell in a parasitic manner. The of the phenomenon of a capillary rise received considerable attention and its exploitation as pumping means has been extended to studies of microchannels [4-6] and micro fuel cells [7-10].

The capillary-driven flow was was evaluated in a serpentine flow field using CFD. Although the idea of using capillary forces to induce flow in microfluidic systems is not a novel one, CFD was used as proof on concept for methanol flow in serpentine microchannels. A commercial CFD program called COMSOL Multiphysics was used [9].

2. Conservative level set method

The level set method (LSM) is a interface tracking method which is used for computing multiphase flow problems. The method used in this study was obtained from the Level Set Two-Phase Flow application mode available in the Chemical Engineering module in COMSOL Multiphysics program [11]. This is a conservative LSM based on the method proposed by Olsson and Kreiss [9,10]. More reading on the LSM for multiphase flows and the conservative LSM can be done on references [10-13].

The interface between fluids (gas and liquid) is represented by the 0.5 contour of the level set function, ϕ. A smeared out Heavisides function is used to dictate ϕ as $0 \leqslant \phi \leqslant 0.5$ on one phase and as $0.5 \leqslant \phi \leqslant 1$ in the other and the transition is varied smoothly across the interface. The level set equation (LSE) describes the convection of ϕ in the computational domain, Ω. and is expressed as:

$$\frac{\partial \phi}{\partial t} + \vec{u} \cdot \nabla \phi = \gamma \nabla \cdot \left(-\phi (1-\phi) \frac{\nabla \phi}{|\nabla \phi|} + \epsilon \nabla \phi \right) \tag{1}$$

where γ is the reinitialisation parameter and ϵ is the parameter that controls the interface thickness and $\vec{u}$ is the velocity vector with which the interface moves is obtained by the Navier-Stokes (NS) equations. The momentum equation:

$$\rho(\frac{\partial\vec{u}}{\partial t}+\vec{u}\cdot\nabla\vec{u})-\nabla\cdot[\mu\,(\nabla\vec{u}+\nabla\vec{u}^{T})]+\nabla P=\sigma\kappa\hat{n}\delta+\rho\vec{g} \tag{2}$$

and the continuity equation:

$$\nabla\cdot\vec{u}=0 \tag{3}$$

are the NS equations, where ρ is the density, μ is the viscosity, P is pressure, σ is the surface tension, κ is the interface curvature, $\hat{n}$ is the interface normal, δ is the Dirac delta function and $\vec{g}$ is the gravitational force. δ smoothens the surface tension which is concentrated at the interface between fluids and is approximated according to $\delta=6|\nabla\phi||\phi(1-\phi)|$. The interface normal and the interface curvature are determined by:

$\hat{n}=\frac{\nabla\phi}{|\nabla\phi|}$ and $\kappa=-\nabla\cdot\left(\frac{\nabla\phi}{|\nabla\phi|}\right)$, respectively.

The density and viscosity are calculated from

$$\rho=\rho_l+(\rho_g-\rho_l)\cdot\phi \tag{4}$$

$$\mu=\mu_l+(\mu_g-\mu_l)\cdot\phi \tag{5}$$

where ρ_l , ρ_g and μ_l , μ_g are densities and viscosities of the liquid and the gas, respectively.

3. Model definition and initial boundary conditions

The flowfield has a 100 µm serpentine microchannel a. The methanol hight in the 300 µm wide reservoir is 280 µm. The model geometry is illustrated in Figure 1 showing the initial conditions of the two phases. The following physical parameters were used: $\rho_g=1.293\ kg/m^3$, $\rho_l=850\ kg/m^3$ $\mu_l=5.9\,x\,10^{-5}\ Pa\cdot s$, $\mu_g=1.71\,x\,10^{-6}\,Pa\cdot s$ and $\sigma=22.7\,x\,10^{-3}\,N/m$

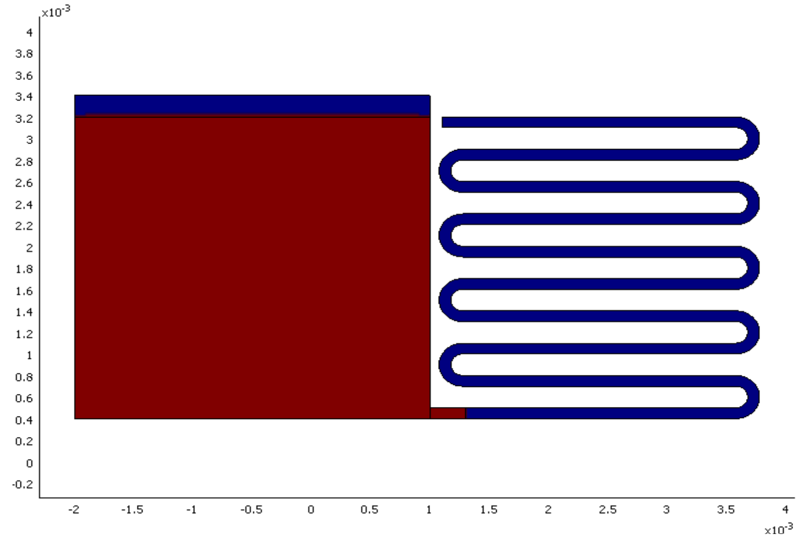


Figure 1: Diagram showing two phases. The area in red represents the liquid phase and the blue area , the gas phase.

Both sides of the air phase were open to the atmosphere. The walls were made a slip boundary condition and the contact angle of 67° was imposed at the fluid-wall interface. The flow was regarded as isothermal and turbulent conditions were not catered for in the model because the flow conditions were considered to be laminar.

4. Reinitialisation and conservation of ϕ

The conservative LSM requires the solution (level set function) to be reinitialised from the initial boundary conditions. Earlier LSM's had a shortcomings of leakages and failing to conserve. The conservation of the average cross-sectional area of the liquid phase by integrating over the computational domain but restricting to the area the isocontour of 0.5 and the following equation was used:

$$A = \int_{\phi \geqslant 0.5} d\Omega . \tag{6}$$

The solution was reinitialised for 50 ms and Figure 2 shows the graph of the liquid phase area over the reinitialisation period. Good conservation was obtained as the trend is a straight line, which indicates that the area did not change and hence the accuracy of the model [14].

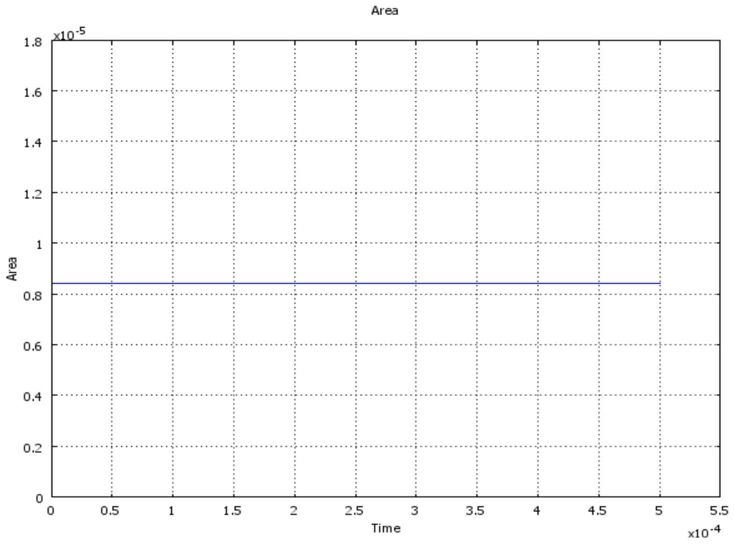
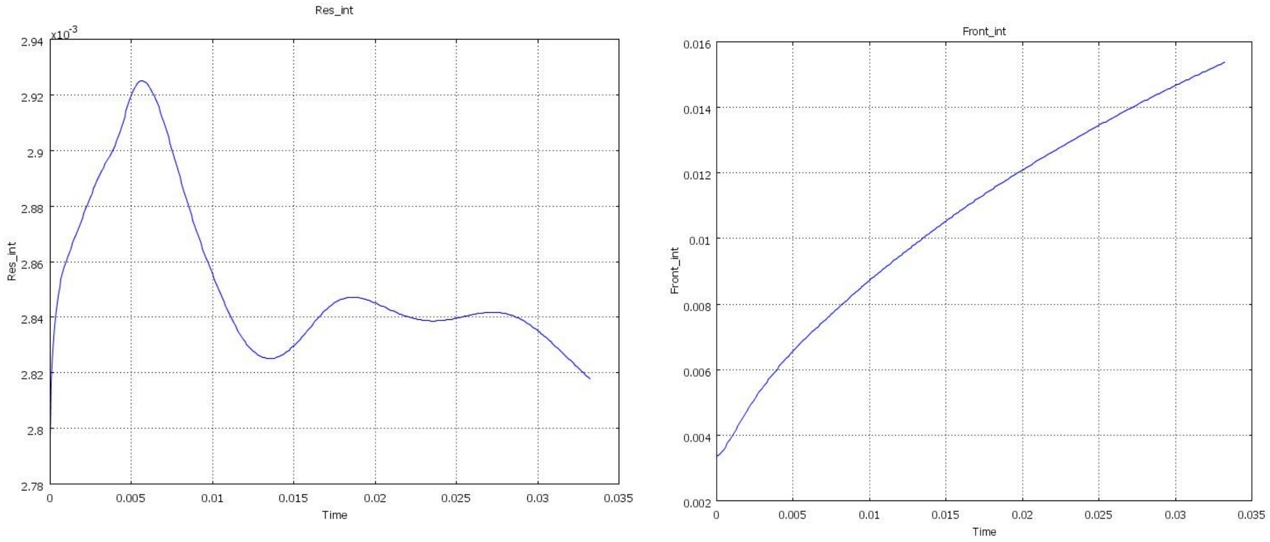


Figure 2: Cross-sectional area of the liquid phase over the reinitialisation period of 50 ms.

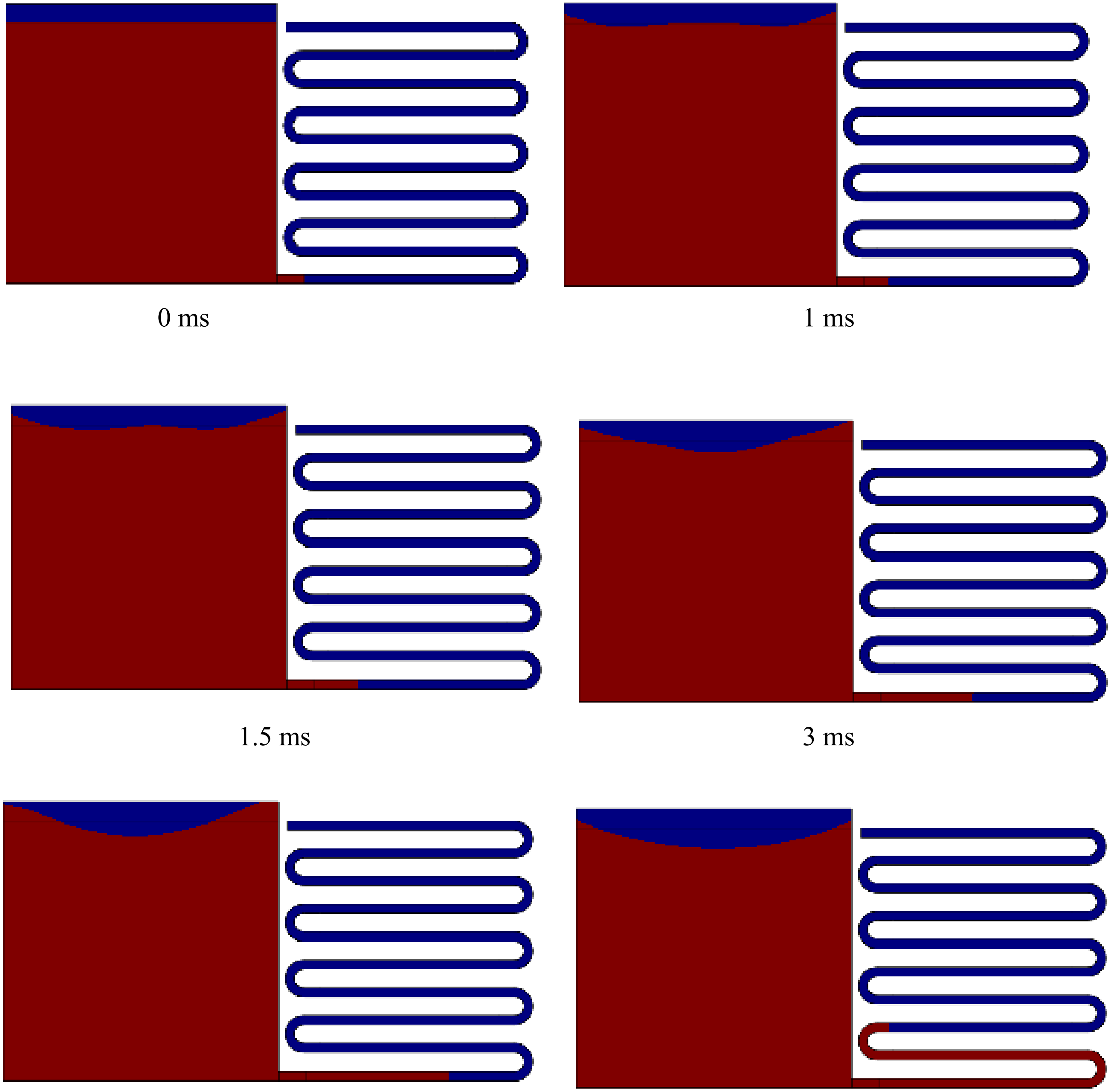
5. Interface motion

Figures 3 shows the movement of both the back interface (in thereservior0 and the front interface of the capillary flow. Initial the reservoir interface shows erratic movement which peaks sharply in the first 5 ms. On the other hand the front interface moved in almost constant velocity over 30 ms.



(a) (b)

Figure 3: Interface movement monitored at the walls of the (a) methanol reservoir and (b) the microchannel. The units are in metres.



0 ms

1 ms

1.5 ms

3 ms

5 ms

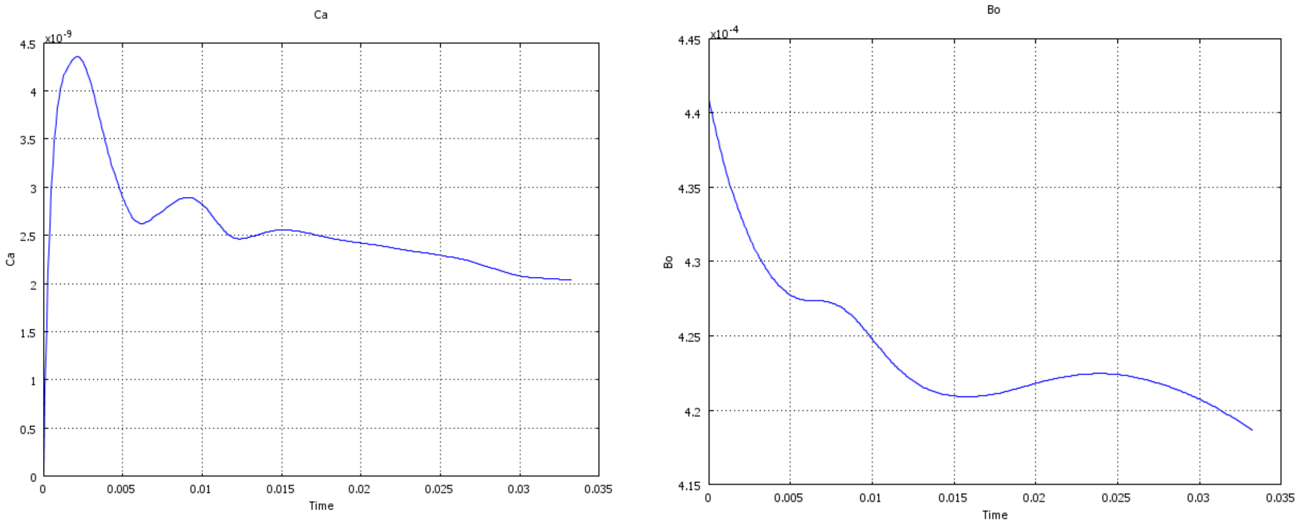
30 ms

Figure 4: Snapshots of the simulation of the capillary flow in the flowfield.

After 3 ms, the reservoir interface movement settles and a meniscus is formed which shows the contact angle at the reservoir wall.

6. Dimensionless numbers

The flow was characterised by evaluating dimensionless numbers, namely: Reynolds number: $Re = \frac{\rho v d}{\mu}$, capillary number $Ca = \frac{\mu v}{\sigma}$ and the bond number $Bo = \frac{\rho g d z_0}{\sigma}$. Re signifies the effect of the viscosity on the flow and was $0 < Re < 4.16$, which confirmed the assumption that the flow was laminar was plausible. The flow velocity was $0\ ms^{-1} < v < 0.142\ ms^{-1}$. $Ca \ll 1$ signifies the dominance of the surface effects over the viscous effects in the flow and $Bo \ll 1$ indicates the dominance of surface effects over gravity. Figure 5 shows the changes in *Ca* and *Bo* in the capillary flow over a period of 30 ms. The *Ca* values were in the order of 10^{-9} and *Bo* values were in the order of 10^{-4} meaning that pressure losses in the microchannel due to gravitational force were much comparison to loses due to surface tension.



(a) (b)

Figure 5: Plots of dimensionless numbers against time: (a) capillary number(Ca) and (b) Bond number (Bo)

7. Conclusion

The capillary -driven flow was evaluated for serpentine channel using an LSM-based CFD model. The study needs to be extended to different size channels and reservoir. A suitable validation method is required and experiments are currently being considered.

Acknowledgments

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