Simulation of a Pressure Driven Droplet Generator

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Outline

1) Overview of microfluidics
2) Presentation of the process
3) Model
4) Results
5) Outlook
1) Overview of microfluidics

- Very studied physics
  - Potential application: 2D (microchips, MEMS, etc.), 3D (Flow focusing, manipulation of bio-ingredients)

- Dealing with a special category of microfluidics: the generation of droplets

The goal is to optimize an industrial process - the droplet generator - by computational modeling

Modeling a spray

Pictures: potomac-laser.com, upperton.com, comsol.com
2) Presentation of the process

Flow regimes & modes

<table>
<thead>
<tr>
<th>Flow regimes</th>
<th>Modes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Stationary</td>
<td>Dripping</td>
</tr>
<tr>
<td>Dynamic (SD)</td>
<td>Production at the exit orifice</td>
</tr>
<tr>
<td>Transient (T)</td>
<td>Jetting</td>
</tr>
<tr>
<td>Constant shape</td>
<td>Thread break up</td>
</tr>
<tr>
<td>over time</td>
<td></td>
</tr>
<tr>
<td>Periodic flow</td>
<td></td>
</tr>
</tbody>
</table>

Si, Li, Yin and Yin, 2009, *Modes in flow focusing and instability of coaxial liquid-gas jets*
3) Model

- Assumptions
  - Rotational symmetry → 2D-axi consideration
  - Neglecting the influence of temperature
  - No chemical reactions

- Fluids & interfacial properties:

<table>
<thead>
<tr>
<th>Property</th>
<th>Liquid (DP)</th>
<th>Gas (CP)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Density (kg/m$^3$)</td>
<td>957</td>
<td>1.225</td>
</tr>
<tr>
<td>Viscosity (Pa.s)</td>
<td>1.8e-3</td>
<td>1.8e-5</td>
</tr>
<tr>
<td>Surface tension (N/m)</td>
<td>35.6e-3</td>
<td></td>
</tr>
<tr>
<td>Contact angle (rad)</td>
<td>$\pi/2$</td>
<td></td>
</tr>
</tbody>
</table>
3) Model

- **Governing equations**

  - Liquid & gas flows governed by the Navier-Stokes equations for incompressible flows

    \[
    \nabla \cdot \mathbf{u} = 0
    \]

    \[
    \rho \frac{\partial \mathbf{u}}{\partial t} + \rho (\mathbf{u} \cdot \nabla) \mathbf{u} = \nabla \cdot [-p I + \mu (\nabla \mathbf{u} + \nabla \mathbf{u}^T)] + \rho \mathbf{g} + F_{st}
    \]

  - Interface motion of the multiphase flow: simulated with COMSOL module Two-Phase Flow, Phase Field approach.

    - Resolution of the Cahn-Hilliard equation

      \[
      \frac{\partial \phi}{\partial t} + \mathbf{u} \cdot \nabla \phi = \nabla \cdot \left( \frac{3\epsilon \sigma}{2\sqrt{2}} \chi \nabla \left[ -\nabla \cdot \epsilon^2 \nabla \phi + (\phi^2 - 1) \phi \right] \right)
      \]
3) Model

- **Numerical details**
  - Range of liquid flow rate: 1 to 10 ml/h
  - Range of gas pressure: 0.02 to 1 bar
  - Time setting: $[0, 0.01s]$ with timestep of $1e^{-4}s$
  - BDF for the time-dependent study
  - Newton-Raphson algorithm to linearize
  - PARDISO as direct solver
  - Calibration studies on mobility & phase field parameter
4) Results

Stationary Dynamic
4) Results

- Flow regimes as a function of the Weber number
  - Liquid Weber:
    \[ We_{liq} = \frac{\rho u^2 R_{in}}{\sigma} = \frac{\text{kinetic energy}}{\text{surface tension}} \]
  - Gas Weber:
    \[ We_{gas} = \frac{2P_{gas} R_{out}}{\sigma} = \frac{\text{pressure}}{\text{surface tension}} \]

- Good agreement with experimental data from Si et al.
- Experimental validation in progress
5) Outlook

- Further work:
  - Simulation of droplets modes
  - Study on the effect of geometry
  - Optimization aiming the smaller monodispersion
  - Phenomena underlying the spray: atomization, deposit, etc.
Thank you for your attention!

Any questions?

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