NUMERICAL STUDY OF FLUID ATOMIZATION IN A HIGH-VELOCITY SPRAY

Wei Wang1,2, Steve Bajic1, Benzi John1, David Emerson1
1Waters Corporation, Altrincham Rd, Wilmslow, Cheshire, SK9 4AX, UK
2STFC Daresbury Laboratory, Warrington, Cheshire, WA4 4AD, UK

OVERVIEW
Computational fluids dynamics (CFD) simulations were carried out to study gas flow dynamics and liquid droplet formation in two types of gas-assisted nebulizers.

- At their typical operating conditions, both nebulizers produce strong shock diamonds and a high frequency of vortex shedding.
- The volume of fluid simulation of the nebulizer atomization shows that flow-blurring occurs in both nebulizers and the droplet generation frequency is strongly correlated with gas flow vortex shedding frequency.

INTRODUCTION
Nebulizers play an important role in the ionization source of mass spectrometers. The high-velocity spray plume in nebulizers strongly influences the atomization of liquid solutions, especially the primary droplet size distribution, which is an important step in the production of gas-liquid flows for a mass spectrometer. It is desirable to predict gas flow properties of nebulizers in an ion source and understand their influence on droplet generation in a high-velocity spray. To capture the underlying physics, we carry out the present study.

METHODS
ANSYS Fluent [1] is applied to carry out simulations of high-speed nebulizer gas flow and liquid injection. Unsteady Reynolds-Averaged Navier-Stokes (URANS) equations with the k-ω SST turbulence model are applied to simulate nebulizer gas flow. The transient simulation captures vortex shedding dynamics, which will strongly affect droplet generation once the liquid injection is introduced.

RESULTS
Computational model and configuration
This study simulates flow dynamics and droplet generation in two types of Meinhard® nebulizers, which are named “TR-50-A0.5” and “HEN-90-A0.1”. Their operation parameters [2] are summarized in Table 1. The listed dimension diameters were measured in-house. A schematic of the computational domain is shown in Figure 1. A 2D axisymmetric CFD model is used to save computational cost. The simulation results agree with the above calculations.

<table>
<thead>
<tr>
<th>Nebulizer Type</th>
<th>TR-50-A0.5</th>
<th>HEN-90-A0.1</th>
</tr>
</thead>
<tbody>
<tr>
<td>Operating pressure (psi)</td>
<td>50</td>
<td>90</td>
</tr>
<tr>
<td>Gas flow rate (L/min)</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>Liquid flow rate (mL/min)</td>
<td>0.5</td>
<td>0.1</td>
</tr>
<tr>
<td>Liquid tube OD (µm)</td>
<td>200</td>
<td>35</td>
</tr>
<tr>
<td>Gas annular OD (µm)</td>
<td>340</td>
<td>170</td>
</tr>
<tr>
<td>Gas annular ID (µm)</td>
<td>280</td>
<td>95</td>
</tr>
</tbody>
</table>

The simulation results are validated against laboratory measurements. The liquid firstly transfers into a liquid channel area, which is a typical feature of the flow field. The liquid then enters the liquid tube area. The liquid tube gas entrainment is a typical feature of the flow field. The liquid tube gas entrainment is a typical feature of gas flow vortex shedding.

CONCLUSION
- Strong flow expansion occurs in both Meinhard® TR-50-A0.5 and HEN-90-A0.1 nebulizers up to 1 mm away from the gas flow orifice. The geometry of HEN-A0.1 introduces high interaction between shock diamonds.
- Droplet formation occurs at the same frequency as the gas flow vortex shedding.
- Both nebulizers show flow-blurring in droplet generation, where liquid tube gas entrainment in TR-50-A0.5 is stronger.
- The VOF model shows that the majority of droplets generated by HEN-90-A0.1 have almost half the diameter of droplets generated by TR-50-A0.5.

REFERENCES