NUMERICAL STUDY OF FLUID ATOMIZATION IN A HIGH-VELOCITY SPRAY

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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 sample solutions, especially the primary droplet size distribution, which is an important step in the production of gas-phase ions 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. However, these tasks are challenging to achieve with laboratory experiments due to limited measurement techniques. In this study, a CFD simulation of the nebulizer gas flow fields was carried out. After achieving a fully developed nebulizer gas flow field, liquid injection through the capillary was modelled to study the droplet generation dynamics.

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.

When the liquid flow is introduced, a volume of fluid (VOF) method is applied to model the interaction of two-phase flow of the injected liquid water and the nitrogen nebulizer gas. To capture the transient topology of the liquid-gas interface, a geometric reconstruction interpolation scheme is applied to deal with the volume fraction formulation. The continuum surface force method is applied to treat surface tension modelling. Local adaptive mesh refinement is enabled to ensure improved grid resolution at the gas-liquid interface.

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 dimensions 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. At the inlets of both the gas and liquid, mass flow rates and pressure are provided. The outer edges of the domain are given a boundary condition of atmospheric pressure and room temperature. A basic mesh of approximately 500k mesh cells was generated to capture flow dynamics near the micro-scale nebulizer orifice.

Table 1. Nebulizer parameters

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

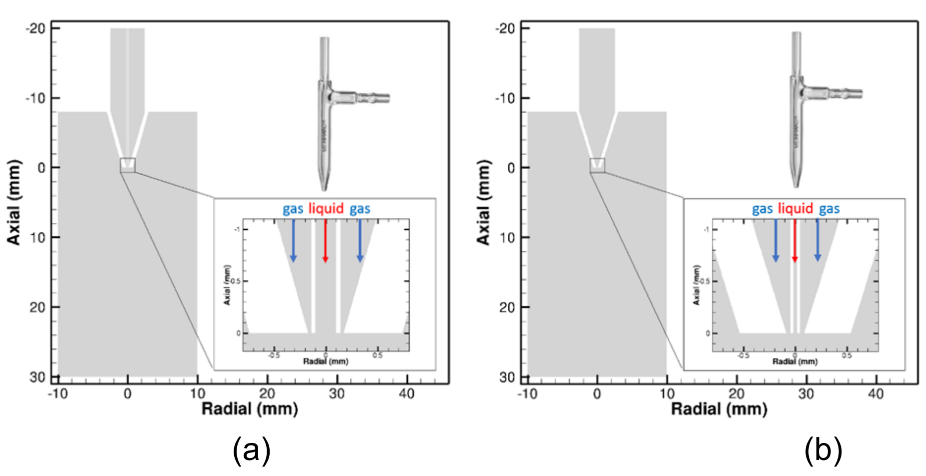

Figure 1. The computational domain of two nebulizers with an axisymmetric configuration. (a) TR-50-A0.5, (b) HEN-90-A0.1

Gas flow field

The gas flow field with high-pressure gas and no liquid flow was modelled first. Due to the high pressure of the nebulizer gas, flow expansion and shock diamonds are formed in the wake of the annular nozzle flow with a Mach number up to 2. For a circular nozzle, the distance from the nozzle to the first shock diamond is commonly approximated by $x = 0.67\,D\sqrt{P_0/P_1}$. For the current annular nozzle, if the diameter term D in the above equation is replaced by the annular gap width, the calculated distance x for TR-50-A0.5 is 42 µm, while the calculated distance x for HEN-90-A0.1 is 134 µm. The simulation results agree with the above calculations.

Figure 2 displays the velocity field for these two nebulizers. Nebulizer TR-50-A0.5 generates distinct shock diamonds in the wake flow up to 0.4 mm from the gas exit. Since the annular radius gap for gas flow in HEN-90-A0.1 is only slighter smaller than the gas tube inner radius, the shock waves from the annular orifice strongly interact with each other and gradually merge in the downstream wake flow up to a distance of 1.6 mm. HEN-90-A0.1 produces a much higher gas velocity than TR-50-A0.5.

Figure 3 plots gauge pressure contours. A lower pressure is formed near the liquid orifice exit in TR-50-A0.5 which introduces a flow recirculation. Again, because of the smaller liquid orifice diameter, the lower pressure in the shock diamonds has difficulty in penetrating into the liquid tube area.

Figure 4 plots temperature contours. Both nebulizes decrease gas temperature in the nebulizer jets. The stronger flow expansion in HEN-90-A0.1 produces a lower temperature in the nebulizer wake flow, which is a disadvantage from the point of view of droplet evaporation in an electrospray MS ion source.

The Unsteady RANS simulation captures the vortex shedding frequency of turbulent flow from the annular orifice, which is approximately 12.5 kHz (a time cycle of 80 µs) for TR-50-A0.5 and 100 kHz (a time cycle of 10 µs) for HEN-90-A0.1. This frequency determines gas entrainment frequency for a flow-blurring nebulizer during the process of droplet generation.

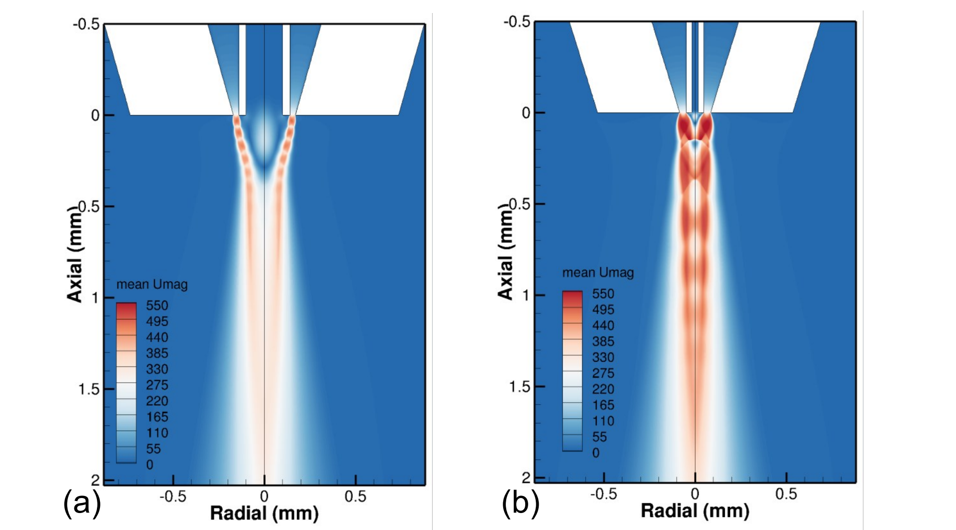

Figure 2. Gas flow velocity field. (a)TR-50-A0.5, (b)HEN-90-A0.1

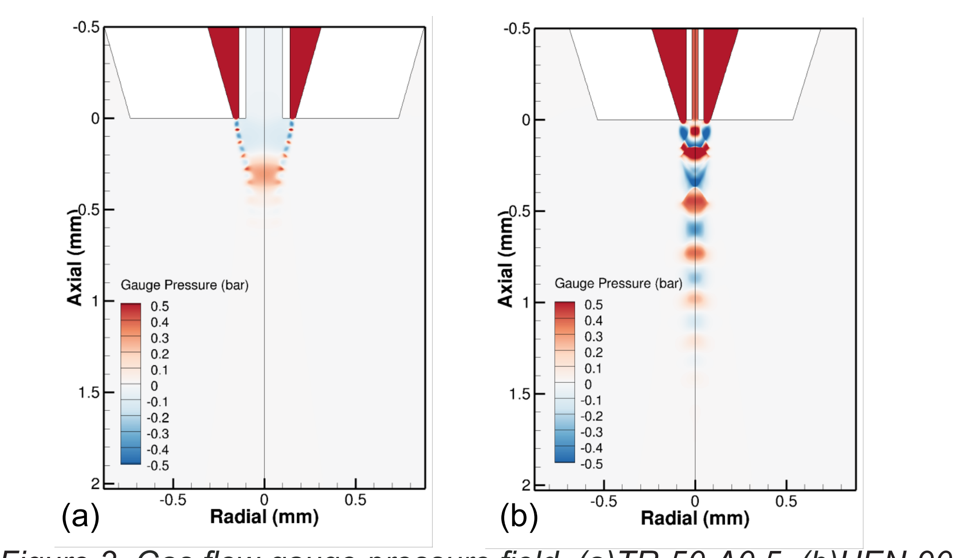

Figure 3. Gas flow gauge pressure field. (a)TR-50-A0.5, (b)HEN-90-A0.1

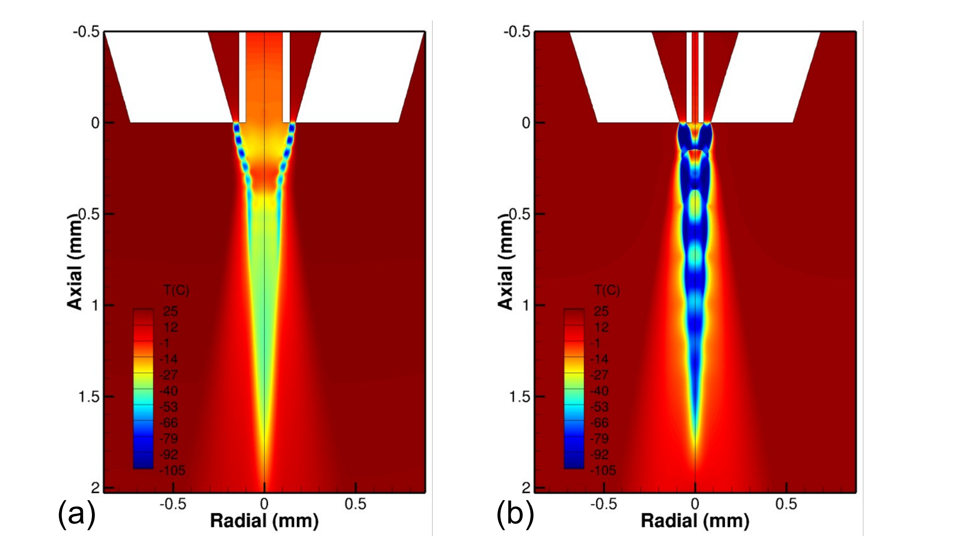

Figure 4. Gas flow temperature field. (a)TR-50-A0.5, (b)HEN-90-A0.1

Dynamics of droplet generation

High-speed coaxial gas flow results in a dynamic change in the local liquid surface topology. The liquid firstly transfers into a liquid sheet, and then breaks up into ligament and droplets due to Kelvin-Helmholtz instability in the axial direction and Rayleigh-Taylor instability in the azimuthal direction [3].

Figure 5 illustrates a droplet production cycle for (a) TR-50-A0.5 and (b) HEN-90-A0.1. The cycle time is the same as the flow vortex shedding period, which can also be seen from the shown streamlines. Gas flow recirculation near the liquid exit introduces gas entrainment into the liquid tube which is a typical feature of flow blurring nebulizers [4]. This feature is clearly observed in TR-50-A0.5, but HEN-90-A0.1 only has very mild and shallow gas entrainment.

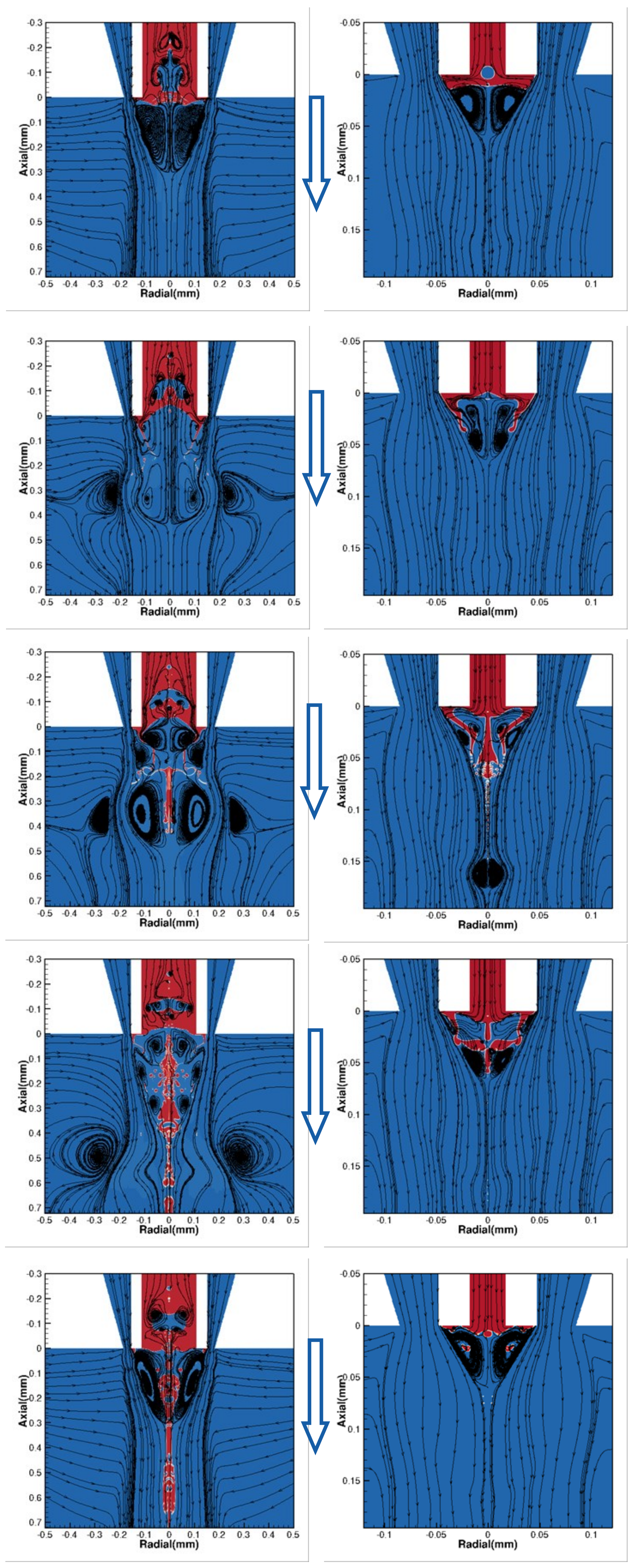

Figure 5. Snapshot of a typical droplet generation cycle for (a) TR-50-A0.5 and (b) HEN-90-A0.1. Red color for liquid and blue for gas. Streamlines with directions are also shown.

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-90-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

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