TECHNICAL NOTE

Liquid Chromatography/ Mass Spectrometry

Theoretical Studies of Swirling Flow and Heating Methods on Droplet Evaporation in a Heated Coaxial APCI Ion Source

Introduction

As part of the continuous effort of improved sensitivity and ruggedness of mass spectrometric components, this discussion involves the theoretical results of using a swirling heated coaxial gas flow- as opposed to a simple heated coaxial gas flow- to rapidly evaporate droplets in an atmospheric pressure chemical ionization source. The world of the outer part of a swirling flow is already effectively used in many applications[1,3].

Although traditional APCI ion sources direct a nebulized droplet/vapor mixture down a tube with heated walls, modern APCI sources use coaxial heating and nebulizing flows that are in the same direction. This new approach of directing the mixture into a coaxial swirling super-heated gas flow is compared with the prevalent method- namely gas flows in the same direction- with respect to the desolvation dynamics and ultimately, droplet evaporation. Here is a first discussion of a theoretical study of droplet evaporation and droplet containment in a coaxial flow APCI source with hot swirling external gas.

Method

This numerical study of droplet evaporation through the various APCI ion source configurations is provided using a commercially obtained numerical computational fluid dynamics (CFD) code called FLUENT[2]. The turbulent flow is simulated by RNG modified k-epsilon model for swirl dominated flow. Calculations are done using finite-volume analysis with second order discretization. Droplets are introduced in the flow using the discrete phase model option. The qualitative analysis is performed to verify numerical results using approximate phenomenological theory of turbulent jets, including ordinary differential equations for boundary-layer-type flow.

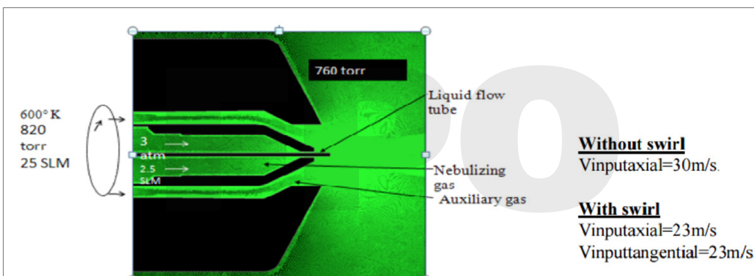

Figure 1. A physical example of a typical APCI coaxial flow ion source. The liquid flow tube, nebulizer gas region and auxiliary hot gas flow regions are identified.

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Results

Simulation Results for Heated Gas Swirl vs No Swirl in a Coaxial Flow Ion Source.

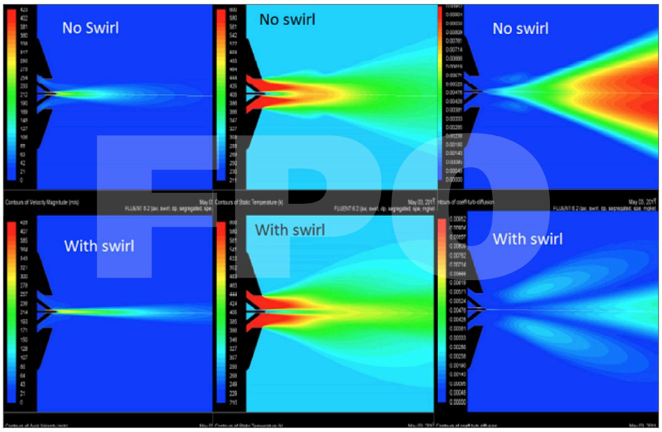

Figure 2. Flow Simulation of the ion source of Figure 1 (heated gas no swirl vs with swirl). The left, middle, and right columns are the velocity, temperature, and coefficient of turbulent diffusion vs source physical profile.

There are several points of interest for the heated gas flow with swirl as opposed to no swirl:

- A sharp velocity gradient on the jet border induces large shear stress helpful for droplet nebulization.
- The central jet containing the analyte is narrower and extends further.
- Although the center line for no swirl flow has a higher temperature in the tip vicinity, beyond that it decays much more quickly. Whereas more thermal energy is supplied to the droplets initially for no swirl flow, swirl flow provides more overall thermal energy for droplet evaporation and Figure 3 illustrates a manifestation of this phenomenon.
- Turbulent mixing is much less in the case of swirl flow, which helps to keep droplets confined, reducing radial diffusion from the hot axial flow.

Conclusion

Since the analyte is contained in the spray droplets, it is extremely important to evaporate as many droplets as possible to avoid analyte loss. The temperature profile of a swirling heated gas greatly helps to evaporate the typical-sized droplets. The direct simulation of the droplet motion shows that the turbulence damping assists to keep the droplets in the main flow in the high temperature region, providing improved droplet evaporation, especially at extended distances from the ion source.

Figure 3. A simulation of droplet diameter vs source physical profile for swirl flow and flow without swirl for an identical distribution of drop diameters. Note the droplet motion simulation confirms that the effect of turbulence. Clearly, far fewer of the droplets remain unevaporated in the swirl case (far enough from the source).

References

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2. ANSYS, Inc. 3255 Kifer Road, Santa Clara, CA 95051 USA.
3. A. A. Khalatov, Swirl Flow: Foundations and Engineering. Kiev, Ukraine. Naukova Dumka (Publishers), 1989 200p. (in Russian).

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