Multiphysics Modeling of an Ion Mobility Spectrometer

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Introduction

In Eiceman and Karpas's book *Ion Mobility Spectroscopy* (2005), they define Ion Mobility Spectroscopy (IMS) as "the principles, methods, and instrumentation for characterizing chemical substances on the basis of velocity of gas-phase ions in an electric field." This characterization of gas-phase chemical species by this technique is accomplished at atmospheric pressures. The production of the electric field and signal processing components is relatively inexpensive compared to other analytical techniques. The convenience of use and high speed of processing has made IMS a technology of choice for a number of field applications. Figure 1 shows the IMS block diagram.

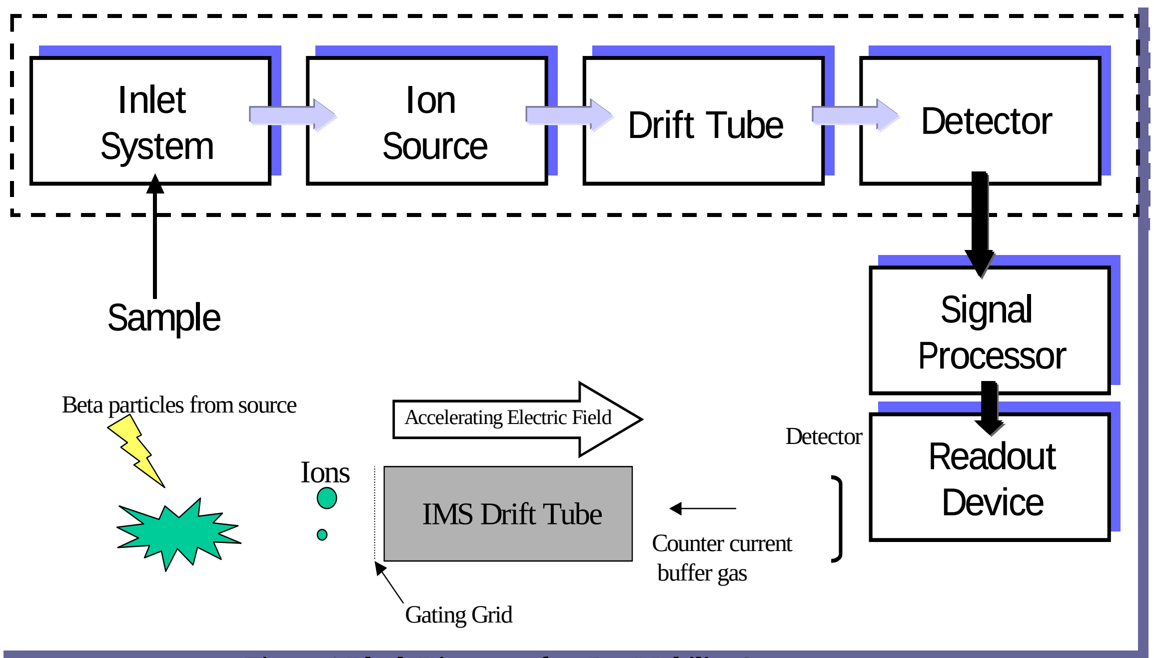

Figure 1 Block Diagram of an Ion Mobility Spectrometer

IMS systems depend on a counter flow and a driving electric field in the drift tube to provide separation between the molecules. Many aspects influence the spectra that is captured. The goal is to be able to calibrate the instrument in order to provide consistent spectra under varying environmental conditions. The use of COMSOL Multiphysics to model the system is leading to a deeper understanding of how the variables affect the performance of the system. Although the fully integrated model of an IMS system is in the future, significant understanding from both 2D and 3D models using the AC/DC, Heat Transfer, and Chemical Engineering application modes and the Reaction Engineering Laboratory. The weak form will be used to model the expected collisions. It may be necessary to use a Monte Carlo simulation for these random interactions.

Eventually, this understanding will allow an adaptive control system to be developed. Standardized spectral libraries can be developed and exchanged between ISM systems, similar to the Nation Institute of Standards and Technology's mass spectrum library.

Conclusion

The current 2D and 3D models of the electric fields match well with other models produced outside of COMSOL. In our operational systems, the temperature of the air inside of the drift tube is not measured directly. The heat transfer model has been useful in understanding how the air is heated in the drift tube. Assumptions about the drift gas have been proved to be inaccurate. The models will lead to design changes being made and tested.