Turbulence affinity of a pipe flow

Turbulence affinity of a pipe flow with strong pressure gradient in the atmospheric pressure interface of mass spectrometry devices

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In Short

- Global project dealing with the simulation of parts of a mass spectrometry device and the understanding of the underlying physical process involved
- Specific study of the behavior of the ions in the atmospheric pressure interface, including the ion losses and the influencing parameters
- In this context and for the present project, investigation of the gas flow taking place in the capillary and its laminar or turbulent nature

The determination of the laminar or turbulent nature of the flow in a capillary is part of a broader project dealing with the simulation of the atmospheric pressure interface of mass spectrometry devices. In the considered design, it consists of a long and narrow tube called capillary through which air flows, transporting ions that are further transported inside the device, typically to be analyzed.
The objectives of the project are to understand the conditions of the ion transport, especially the fluid dynamics occurring there, and to simulate the trajectory of the ions, including the forces due to the electric charge. The objective is to understand and thus try to reduce the losses occurring when the ions hit the walls of the capillary.
Between both ends of the capillary, a strong pressure gradient is imposed, from atmospheric pressure where the ions are created to about 1 mbar. As a consequence a chocked flow is found in the capillary, as described in [2]. This chocking limits the pressure gradient that is found in the capillary itself, which still remains significant, as well as the gas flow acceleration that even reaches values slightly higher than the speed of sound (see figure 1, for Ma > 1).

This creates specific conditions making the estimations regarding the nature of the flow quite complex. Further one expects higher ions losses with a turbulent flow that with a laminar one, making this parameter important for the design of the device. Especially, elementary considerations and empirical models presented in [1] show that one can expect some modifications in the nature of the flow depending on the considered configuration, which

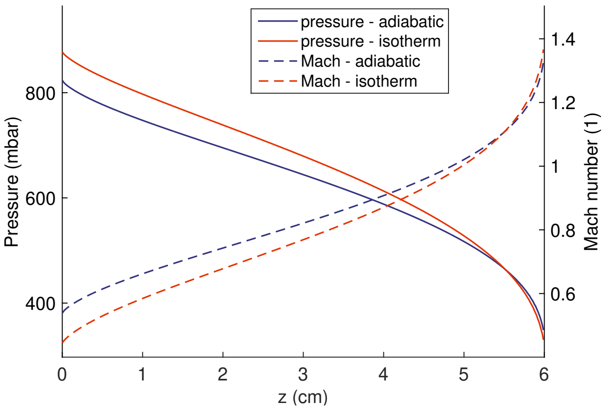

Figure 1: *Pressure and Mach number profile along the capillary and at the center line in the laminar flow as computed in [2]*

could in return explain some experimental results.

The submitted project aims to look closer at this hypothesis and determine whether turbulence can be expected in such a flow. Therefore, the same laminar flow as found in [2] should be simulated while imposing specially computed turbulent inlet conditions and consider the evolution of the perturbation along the capillary, in order to determine the affinity of such flow for turbulence.
Two cases are considered, the first one with adiabatic wall boundary conditions and the second one with isothermal wall boundary conditions, to reproduce the two cases identified in [1] as being possibly turbulent or laminar, respectively. This would let us not only have the possibility to study the affinity of the presented kind of flow for turbulent perturbations but also figure out whether the different boundary conditions have an influence regarding this aspect.

WWW

https://www.vm.tu-berlin.de/institut_fuer_stroemungsmechanik_und_technische_akustik_ista/numerische_fluiddynamik/

More Information

[1] L. Bernier, H. Pinfold, M. Pauly, S. Rauschenbach, J. Reiss; Gas Flow and Ion Transfer in Heated ESI Capillary Interfaces, *Journal of The American Society for Mass Spectrometry* **29**, 761-773 (2018). doi:10.1007/s13361-018-1895-0

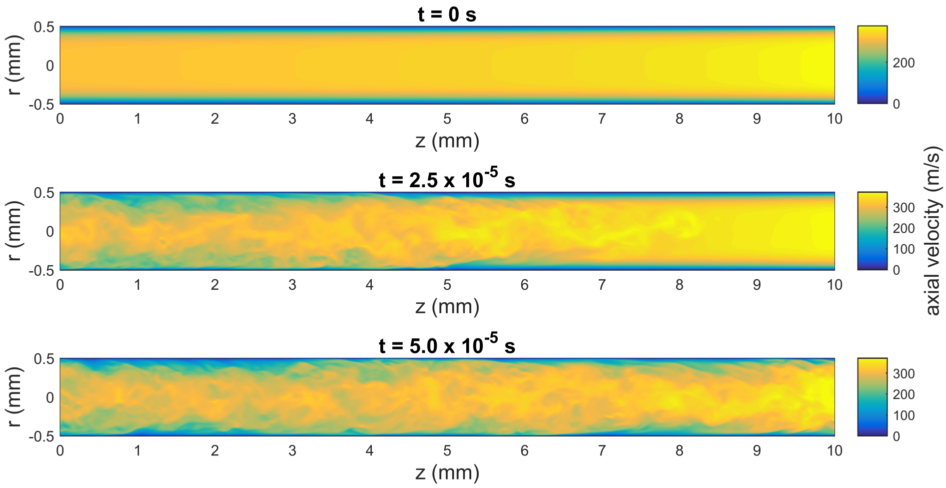

Figure 2: *Test simulation similar to the proposed one but for a shorter pipe with adiabatic wall boundary conditions. Snapshots of the axial velocity at different times are presented*

[2] L. Bernier, M. Taesch, S. Rauschenbach, J. Reiss; Transfer conditions and transmission bias in capillaries of vacuum interfaces, *International Journal of Mass Spectrometry*, accepted, to be published.

Project Partners

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