An Engineering Application of BPH Method

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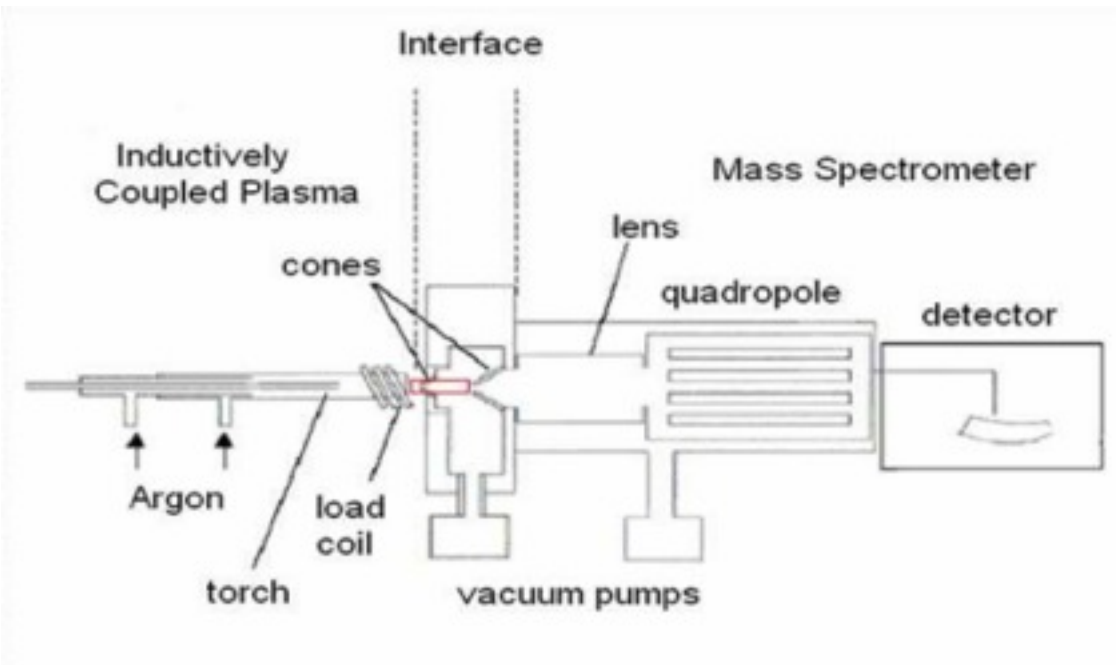
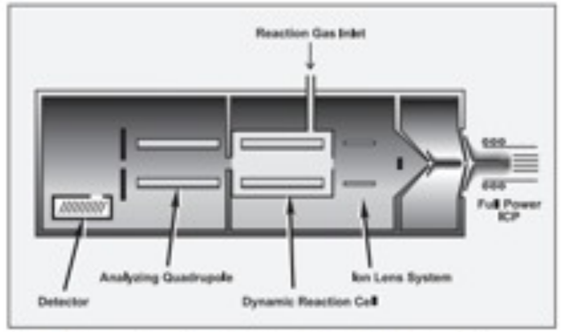
Outline

- Boltzmann Particle Hydrodynamics
  - Theory
  - Verification test
- Application to ICP-MS
  - What is ICP-MS ?
  - Flow Calculation in Extraction Interface of ICP-MS
  - Conclusion

What is ICP-MS ?

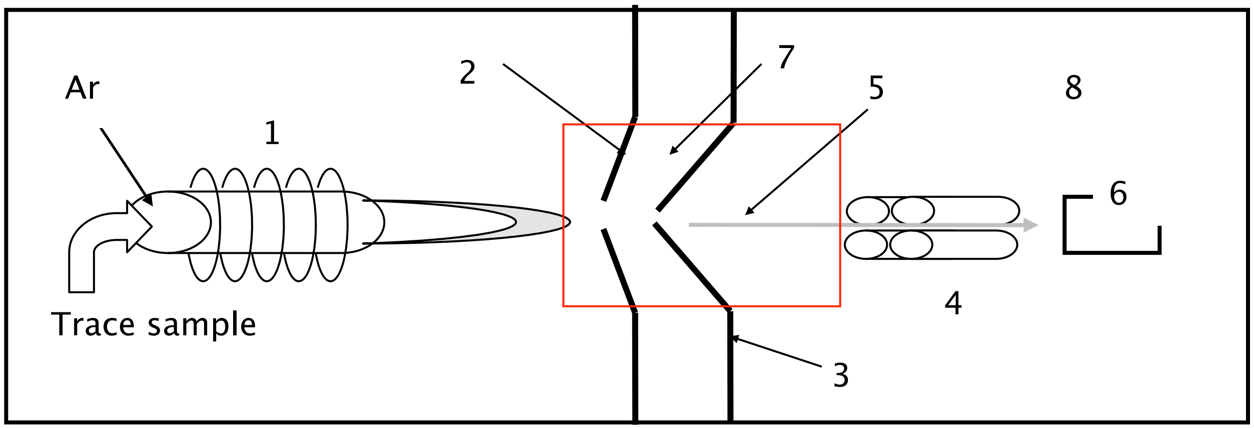
- Inductively Coupled Plasma - Mass Spectrometer
- An equipment capable of detecting and measuring trace elements such as found in concentrations as low as 1 part in a 10^{14}.





Atomic spectroscopy, vol.20, No.2, March/April, 1999, Perkin Elmer

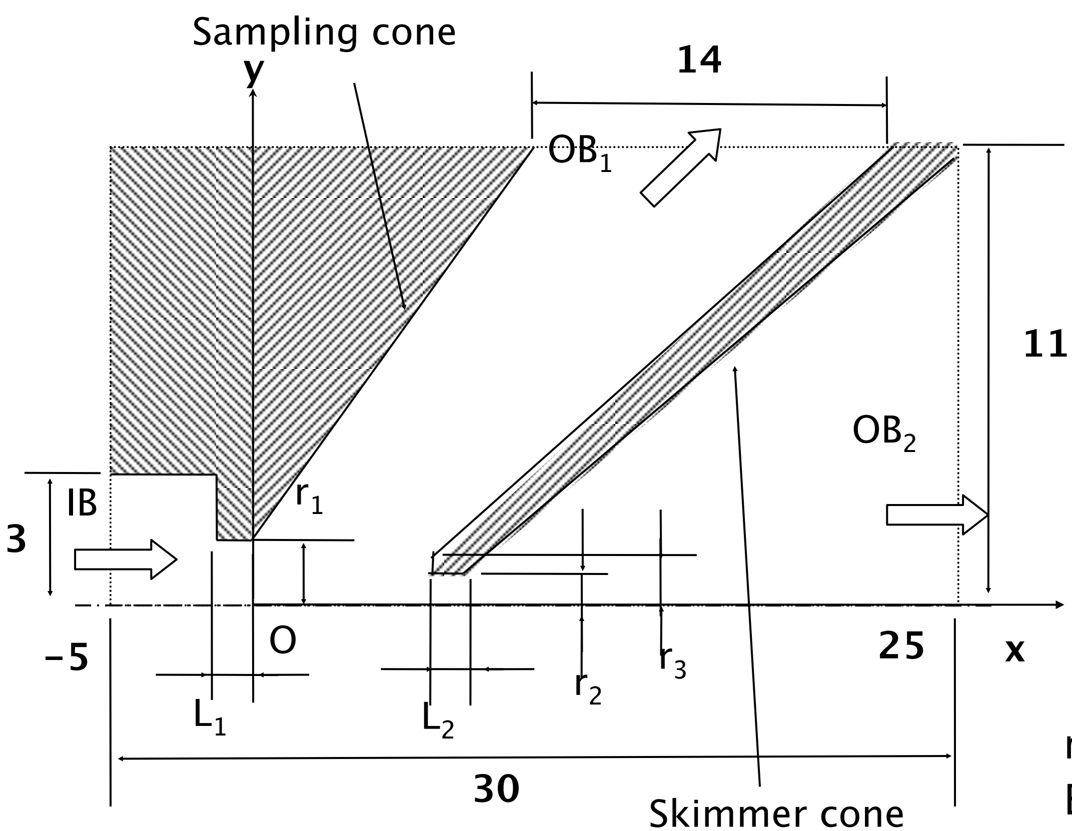
Flow calculation in Extraction Interface of ICP-MS



1: RF source
2: Sampling cone
3: Skimmer cone
4: Quadrupole
5: Ion beam
6: Detector
7: First vacuum zone
8: Vacuum chamber

Simplified diagram of an inductively coupled plasma mass spectrometer

Geometric parameters



Two dimensional flow region

Dimensions of the skimmer orifice (in mm)

case	r_2	r_3	L_2
1	0.25	0.25	0.1
2	0.50	0.50	0.1
3	0.75	0.75	0.1
4	0.25	0.30	0.1
5	0.25	0.50	0.1

mesh:600X220

Boundary condition:

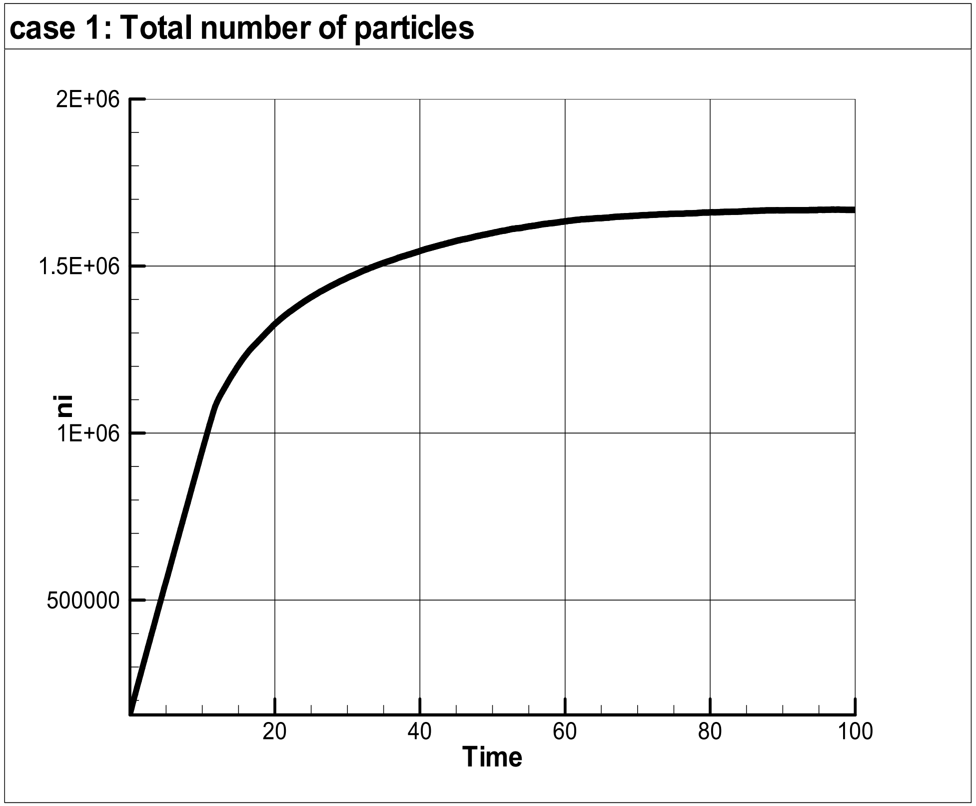
IB: 250 prtcl/step (0.1MPa,6000K)

OB1: 5 prtcl/step (100Pa, 300K)

OB2: vacuum

Time to reach steady state

- The flow becomes steady in all cases when t>80.

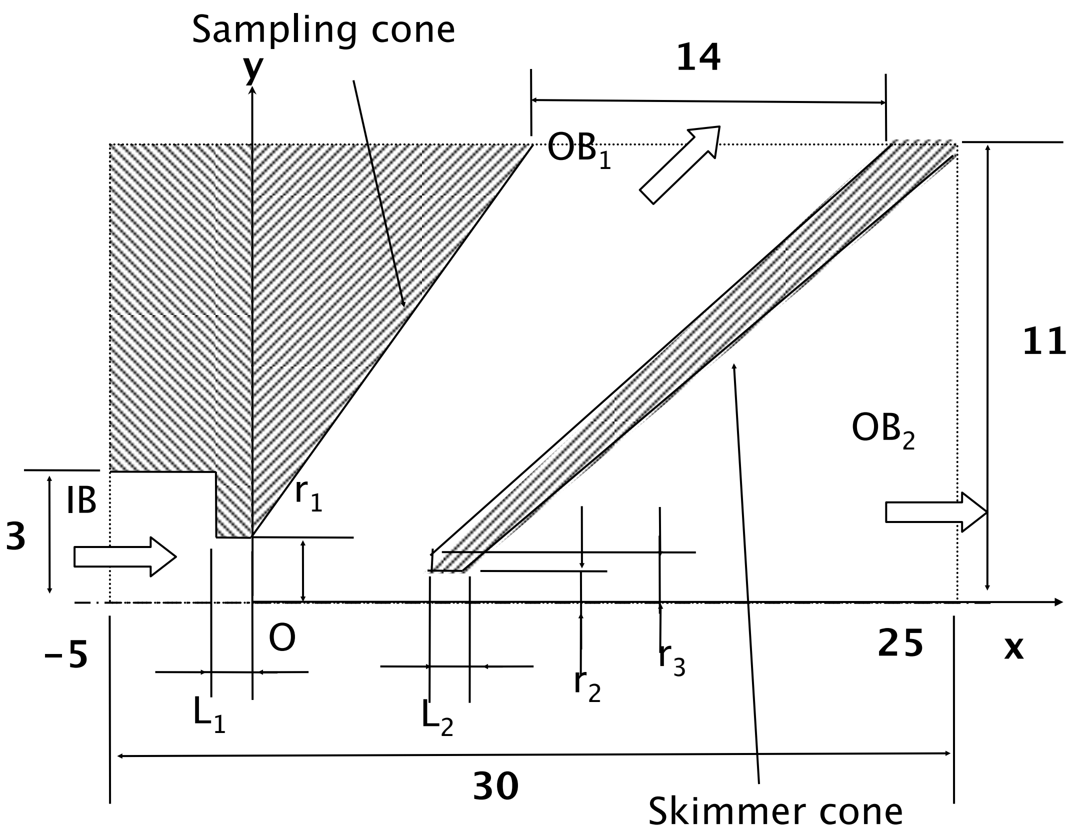


velocity: 1440m/s (sound velocity of Ar at 6000K)
time: 2e-5 s

8000 step to reach t=100
CPU time ≈7300 s

Total number of particles in the flow field (case 1).

Geometric parameters(1)



Two dimensional flow region

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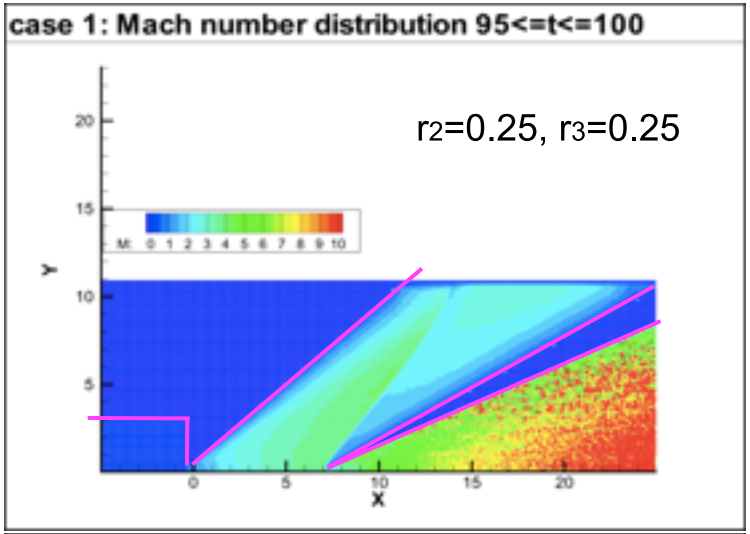
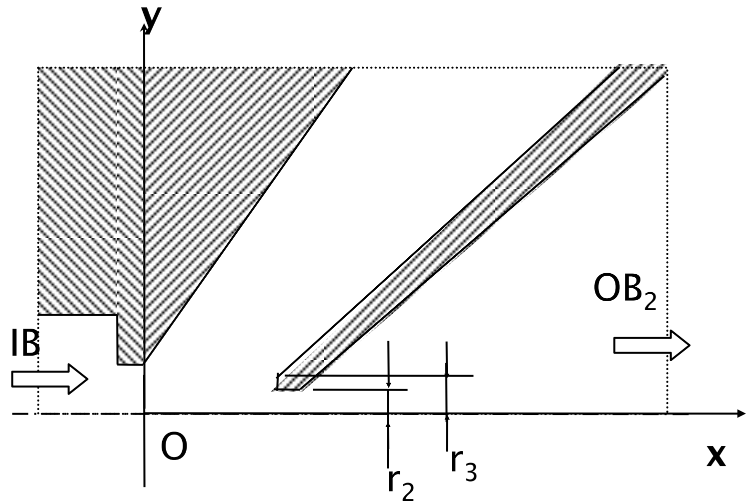
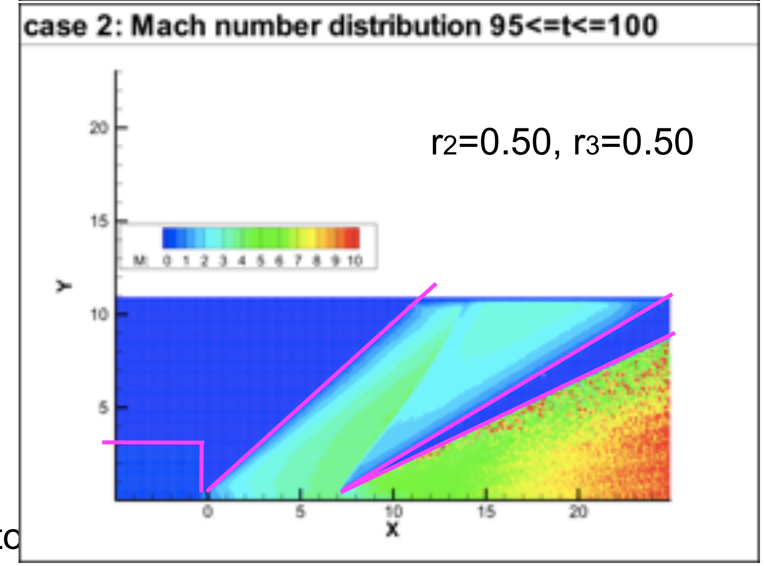
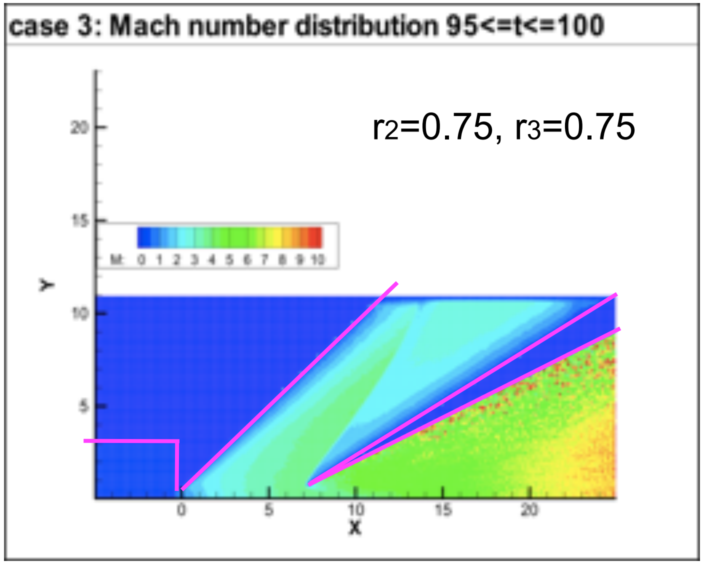
Results of case1, case 2, and case 3









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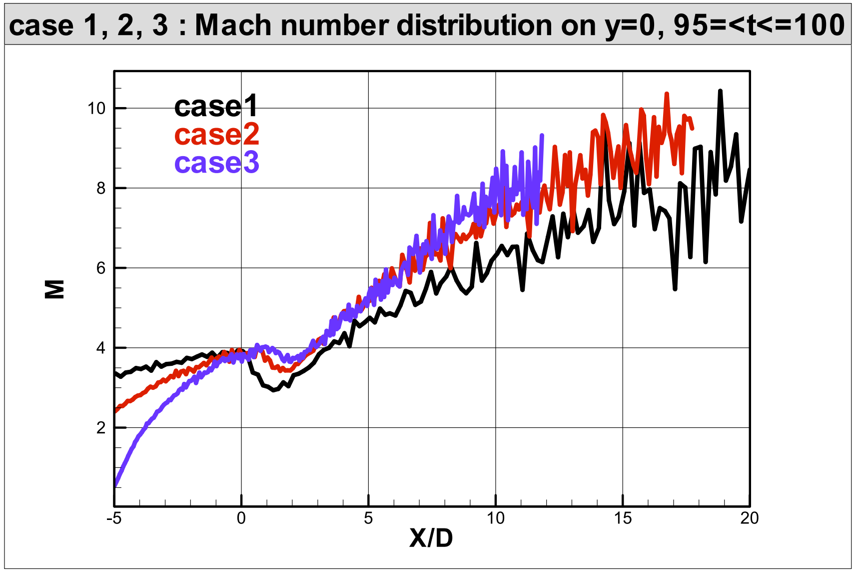
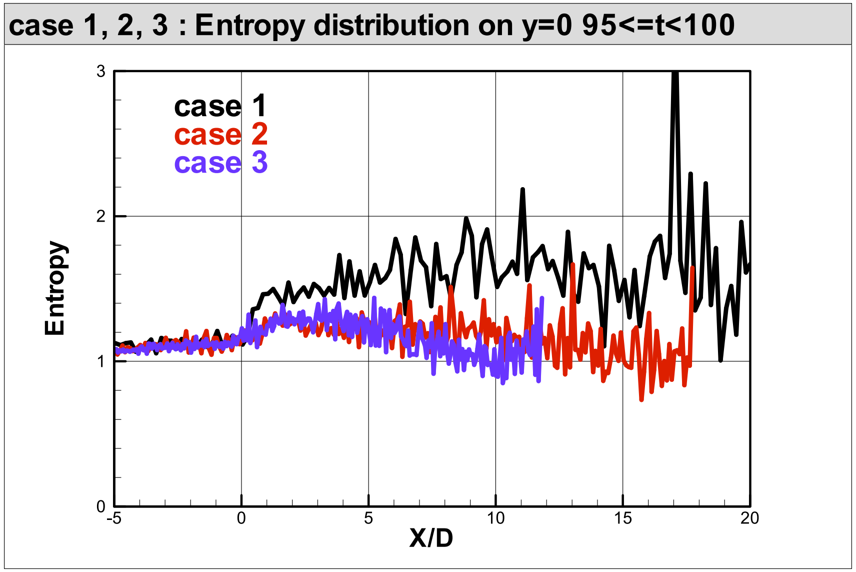
Comparison of the results (1)

- The orifice with the smallest radius causes the largest entropy generation.

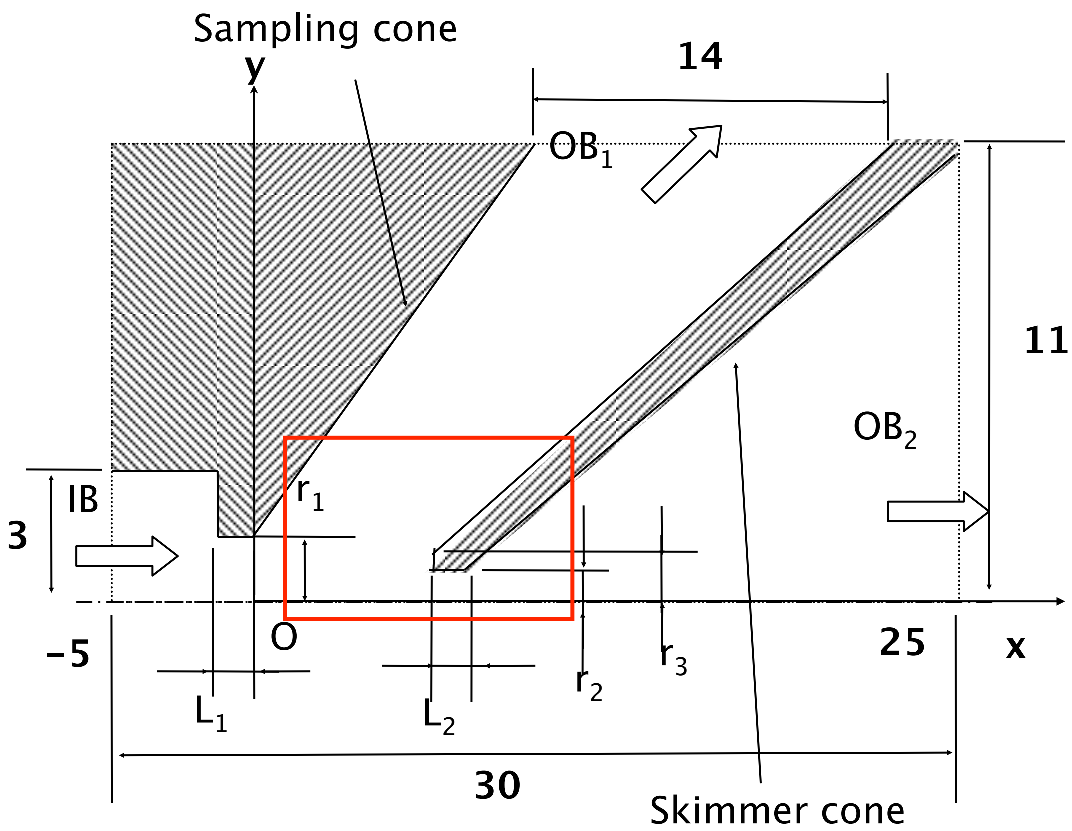


Distribution of Mach number on the center line



Distribution of entropy on the center line

Geometric parameters(2)



Dimensions of the skimmer orifice (in mm)

case	r_2	r_3	L_2
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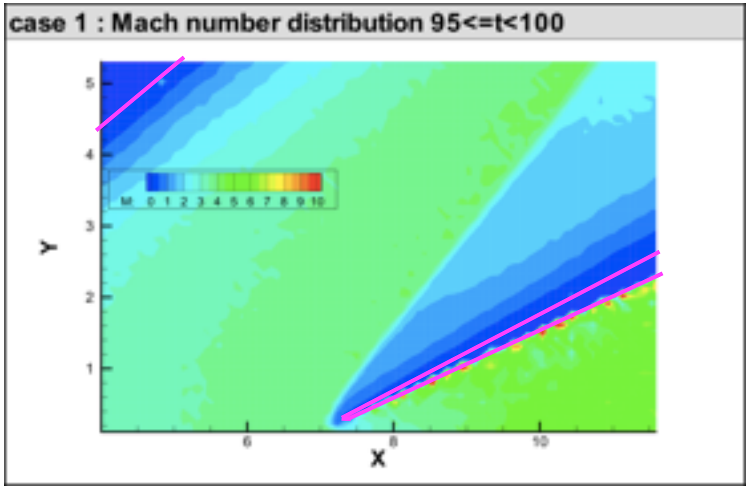
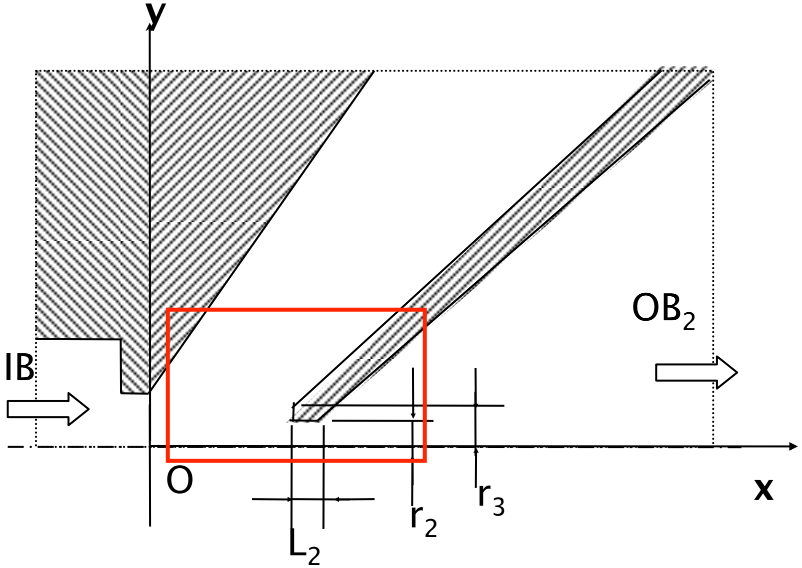
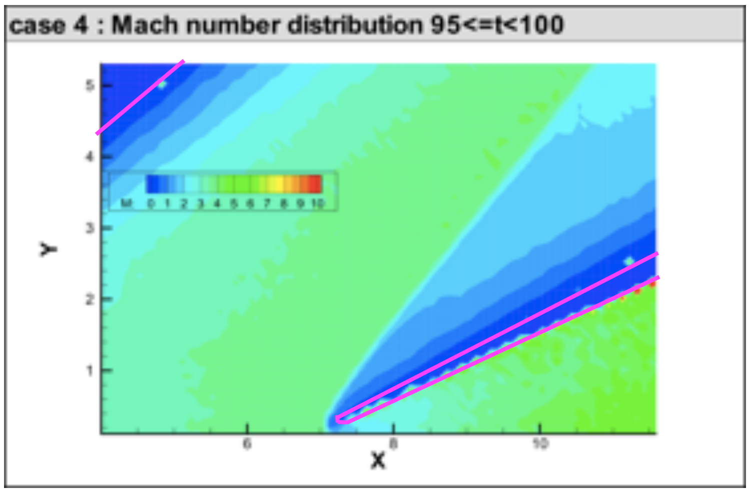
3	0.75	0.75	0.1
4	0.25	0.30	0.1
5	0.25	0.50	0.1

Results of case1, case 4, and case 5

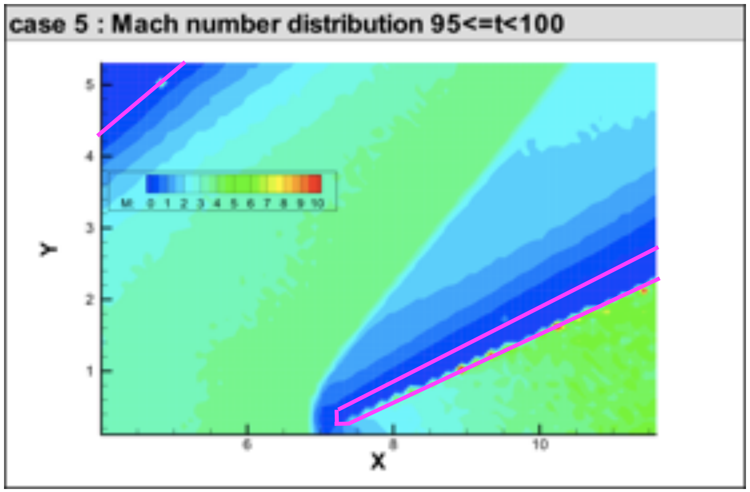


r2=0.25, r3=0.25



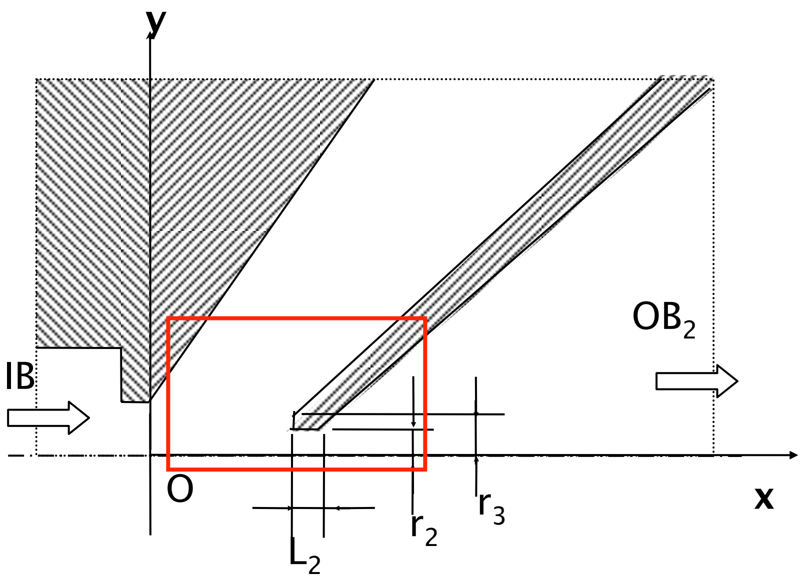


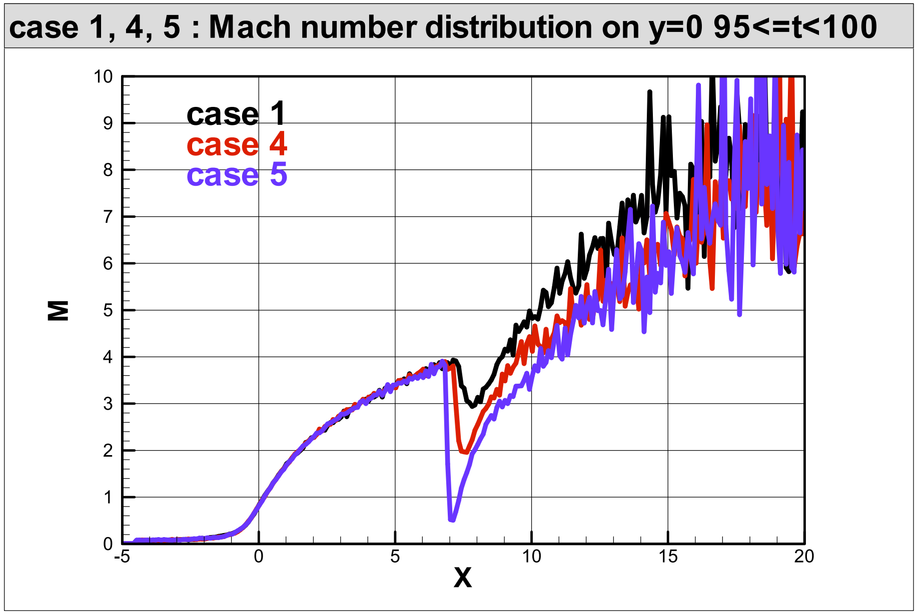
r2=0.25, r3=0.30



r2=0.25, r3=0.50

Comparison of the results (2)





- Blunt edge of the size about twice as large as the radius of the hole provokes normal shock in front of the orifice hole and leads to the subsonic through-flow.

Summary of the calculation results of ICP-MS

- Orifice with smaller radius causes larger entropy generation.
  - Optimum radius exists.

- Blunt edge of the land size twice as large as the radius of the orifice makes the through flow subsonic.
  - The orifice should be manufactured with a great care.

Conclusion

- Capability of BPH method
  - robust explicit scheme,
  - easy to treat vacuum region,
  - easy to treat Mach number of infinity, i.e., zero temperature.
- Tool for engineering problems
  - analysis tool for flows under extreme conditions such as those of the ICP-MS.