A kinetic approach in modeling compact Siegbahn molecular drag stages: physical and numerical aspects

64th IUVSTA Workshop on Practical Applications and Methods of Gas Dynamics for Vacuum Science and Technology

R. Arpa, H.Telib *
I.F.Cozza, L.Campagna, E.Emelli **

Leinsweiler, May 16, 2011

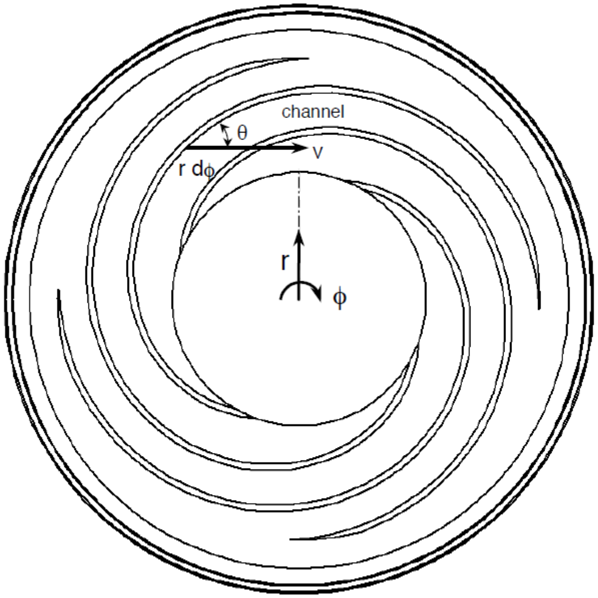
* Politecnico di Torino/Optimad Engineering s.r.l.
** Agilent Technologies, Vacuum Product Division, Torino, Italy

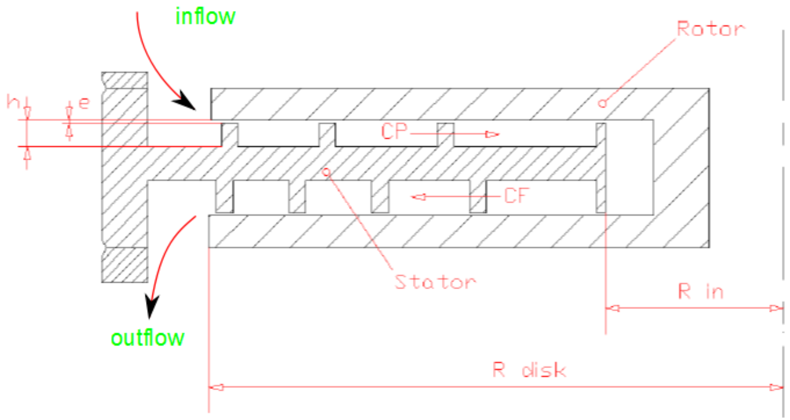
Outline

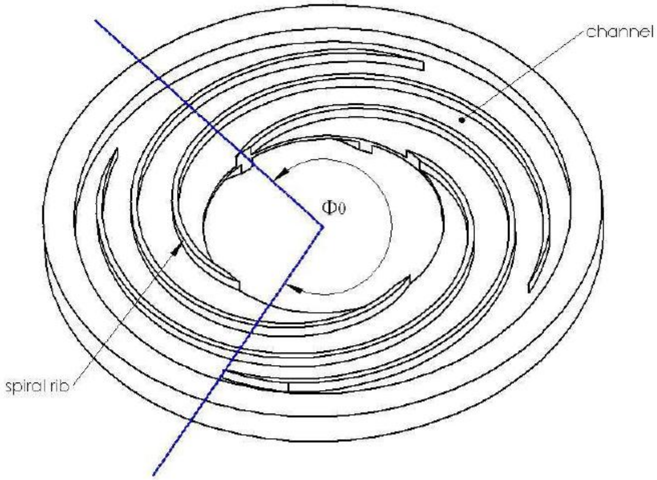
- Introduction: Statement of the problem and typical approaches
- The starting point: Sharipov's Holwek model
- Extension to Siegbhan stages
- A rough approximation:
  - Theory
  - Results
- A consistent approach:
  - Theory
- Conclusions and open questions

Statement of the problem

- Need for a computational model for Siegbahn drag pumps that takes into account:
  - Transitional rarefied flow regime
  - Curved channels (spiral grooves)
  - Clearances
- The pumping effect is due to a circumferential velocity induced by the rotor motion:
  - It develops a 3D flow along the channel
  - It imposes a pressure jump
- Presence of inertial forces:
  - Centrifugal force
  - Coriolis force







Typical approaches

The flow properties (flow rates and stresses), in the limit of its stationary solution, could be computed by means of various modeling approaches:

- Fully 3D approaches
  - **Direct Simulation Monte Carlo - DSMC** (*J.Heo, Y. Hwang, J. Vac . Sci. Technol. A 20, 2002*)
  - **Kinetic – Boltzmann equation**

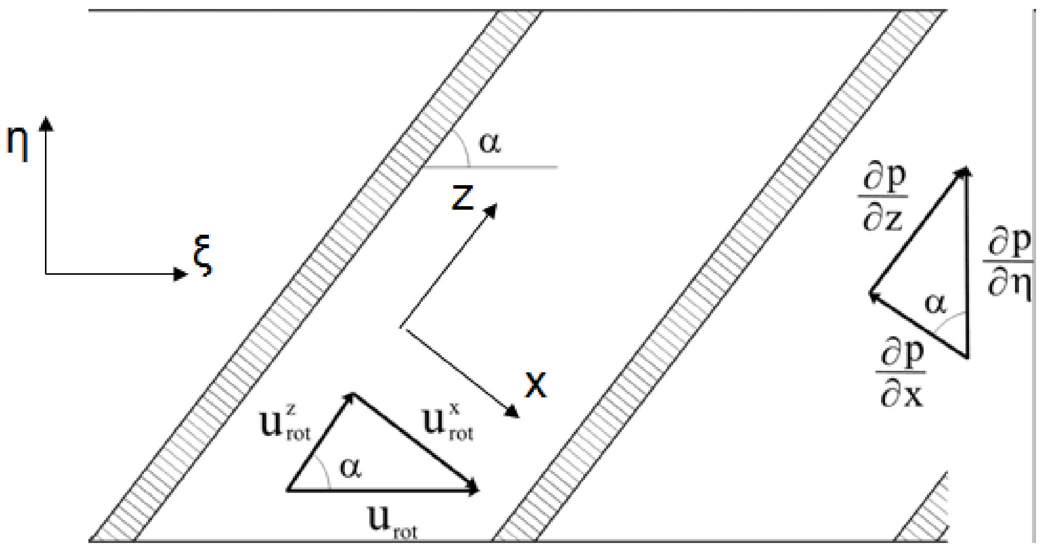
- Reduced order approaches based on the kinetic equation (**linearized 2D Boltzmann equation**)
  - **Asymptotic diffusion models – spiral channel section** (*K.Aoki, P.Degond, L. Mieussens et al., Multiscale Model. Simul. 6, 2008*)
  - **Sharipov's Holweck model – drag channel section** (*F. Sharipov, P.Fahrenbach, A.Zipp J. Vac . Sci. Technol. A 23, 2005)*

Purpose of **extending** Sharipov's approach for Holweck pumps to radial pumps in Siegbahn geometry.

Summary of Sharipov's Holweck model (I)

- Flow field is characterized by two distinct phenomena:
  I. Flow field due to the **rotation of the cylinder wall** -> **Couette**
  II. Flow field due to the **pressure gradient** -> **Poiseuille**

- Flow field decoupled in two distinct directions:
  I. The **main flow** direction **along the channel (z direction)**
  II. The **leak flow across the channel and over the groove's tip (x direction)**



- A linear approach is adopted
- The main flow is expressed as the superposition of those **elemental solutions**, while no inertial effects, no curvature of the channel and no end effects are taken into account

Summary of Sharipov's Holweck model (II)

- In the **local 2D cross section** of the channel, the following **assumptions** are made:
  - Elemental flow are calculated from the stationary Boltzmann equation linearized in the rotational velocity and pressure gradients components, according to the elemental flow in exam.

$$\mathbf{v} \cdot \boldsymbol{\nabla} f = \frac{P}{\mu} \left(f_M - f \right)$$

  - BGK closure for the collisional term (isothermal flows)
  - The **order of equation** (3D) **is reduced** assuming that derivatives along the channel direction (z-coordinate) are **locally zero** (Couette Flow) or **constant** **(**Poiseuille Flow).
  - Flow is determined in the **cross section of the channel**, and it is dependent only on the local rarefaction parameter $\delta = hP/\mu v_0$, considered as constant in the section (linearization).
  - Mass conservation is locally enforced to obtain a value of pressure gradient consistent with the applied forces and boundary conditions.

Siegbahn stages modeling concepts

- Siegbahn stages are mainly characterized by a flow
  - in the direction **tangential** to the spiral channel (**rotation of the disk**)
  - in the direction **normal** to the channel (**pressure gradients**)

- In general, the same considerations made for the Holweck pump could be applied, if an **appropriate** reference system is chosen
  - **cylindrical, non-inertial reference system**

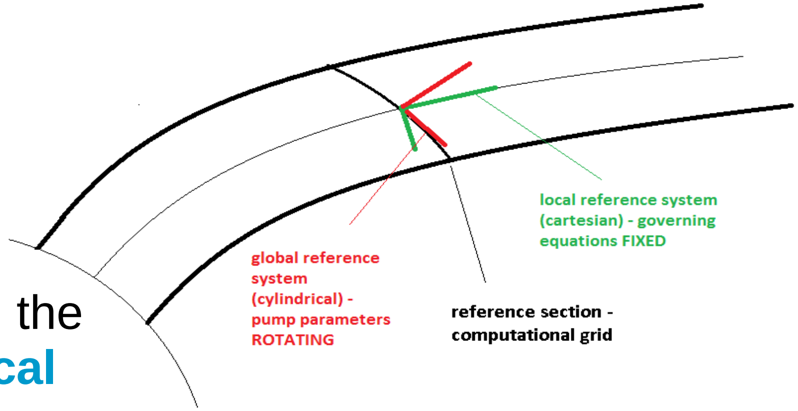
$$c_r \frac{\partial f}{\partial r} + c_\phi \frac{\partial f}{r \partial \phi} + c_y \frac{\partial f}{\partial y} + \frac{c_\phi^2}{r} \frac{\partial f}{\partial c_r} - \frac{c_r c_\phi}{r} \frac{\partial f}{\partial c_\phi} = \delta \left[M(f) - f \right]$$

- Inertial effects are **automatically** included

- Constraints in the choice of the computational channel section (**constant tangential velocity and periodicity – circumference arc**).

Siegbahn stages : a rough approximation(I)

We roughly applied the same approach of the Holweck model, with the same decomposition in 4 elemental flows provided that:



- Geometry of the channel section is expressed in the **global** reference system of the pump in **cylindrical coordinates**

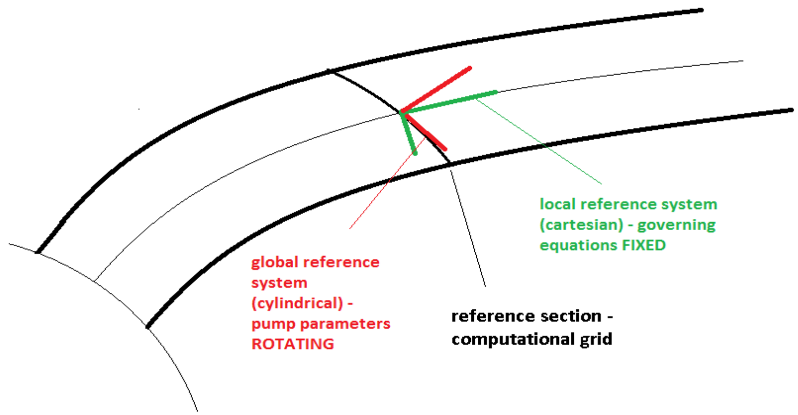
- Linearized governing equations are solved in the **local** reference system of **cartesian, fixed, coordinates** defined by the spiral geometry in the channel **centerline** (inertial forces does not appear explicitly)

- Let x,y,z be the local reference system (green) and ϕ,y,r the global reference system (red) :

$$c_x \frac{\partial f}{\partial x} + c_y \frac{\partial f}{\partial y} + \delta f = \delta f^M + g, \qquad dx = r cos(\theta) d\Phi$$

- The two system are rotated between each other of **an angle θ,** (defined by the spiral geometry, variable with the radial and tangential coordinates of the global system) . The function g is the residual of the linearization (equal to 0 in Couette flows, equal to c_x or c_z in Poiseuille flows)

Siegbahn stages : a rough approximation (II)



- Pressure evolution along the spiral channel can be still obtained enforcing local mass conservation

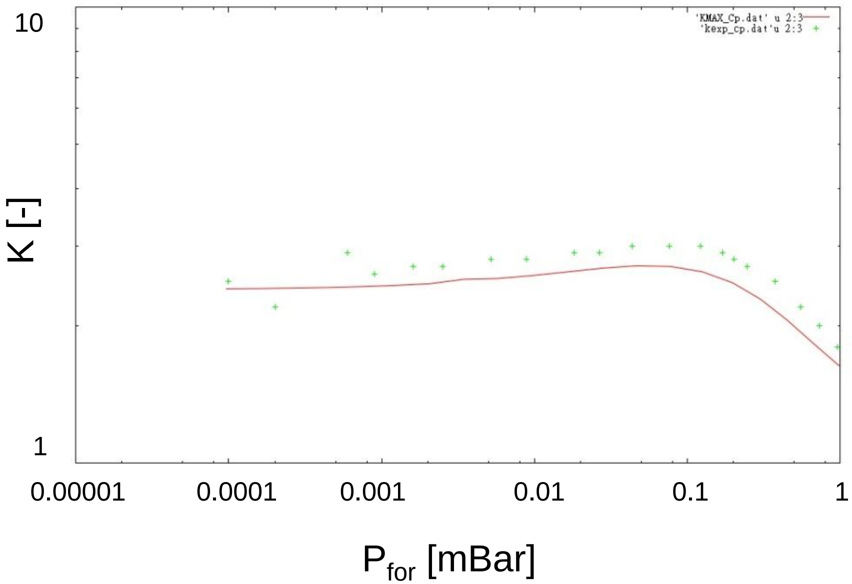
- A **variable** geometry for the section is set along the channel. Thus, a **coupled** computation of Boltzmann equation and pressure ODE is required , in order to march along the channel section by section

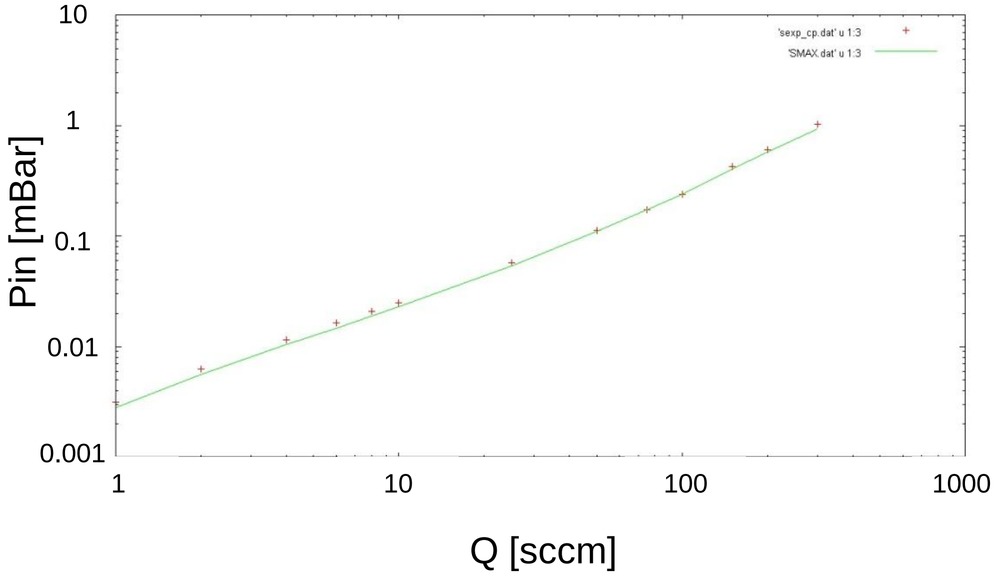
- In first approximation, we impose standard Maxwell diffuse scattering boundary conditions on walls, and zero gradient to clearances

- No wall impermeability and periodicity are provided

Siegbahn stages : Results (I)

Hydrogen



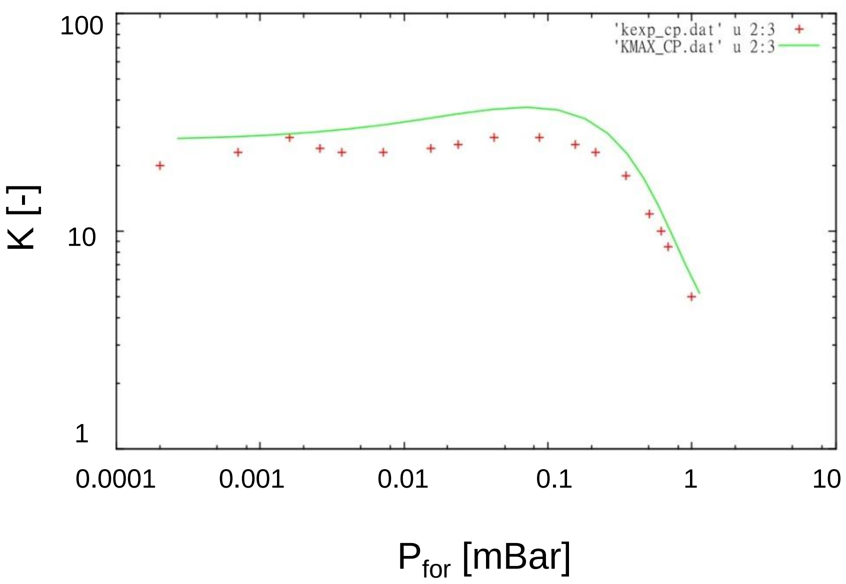


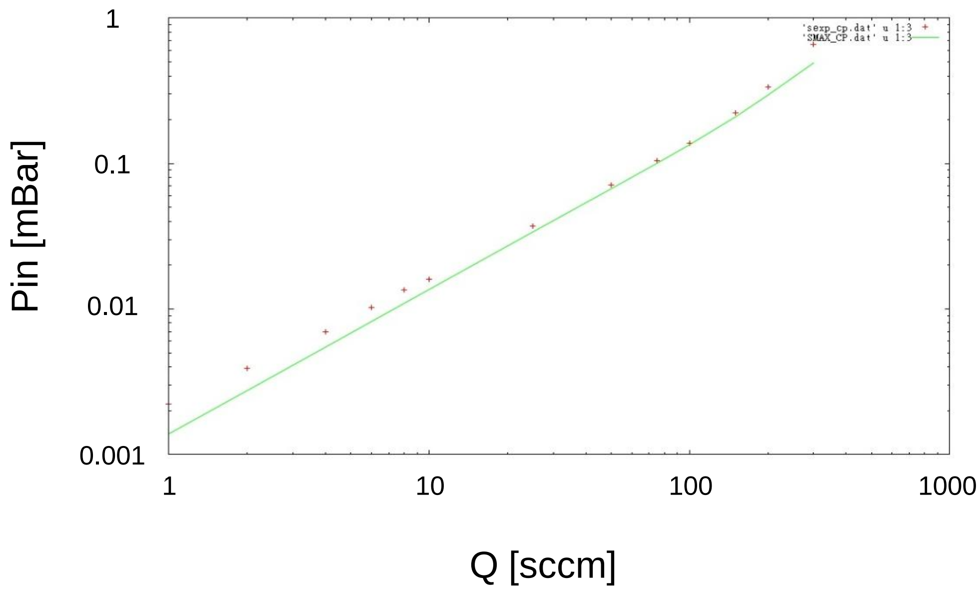
- Max error on K_{max} < 10%
- Max error on P_{in} < 10%

Φ_0 [°deg]	R_{in} [mm]	R_{disk} [mm]	h [mm]	e [mm]	N [mm]	ω [mm]	Flow Dir.
90	23	51.5	3	0.3	12	963	CP

Siegbahn stages : Results (II)

Nitrogen





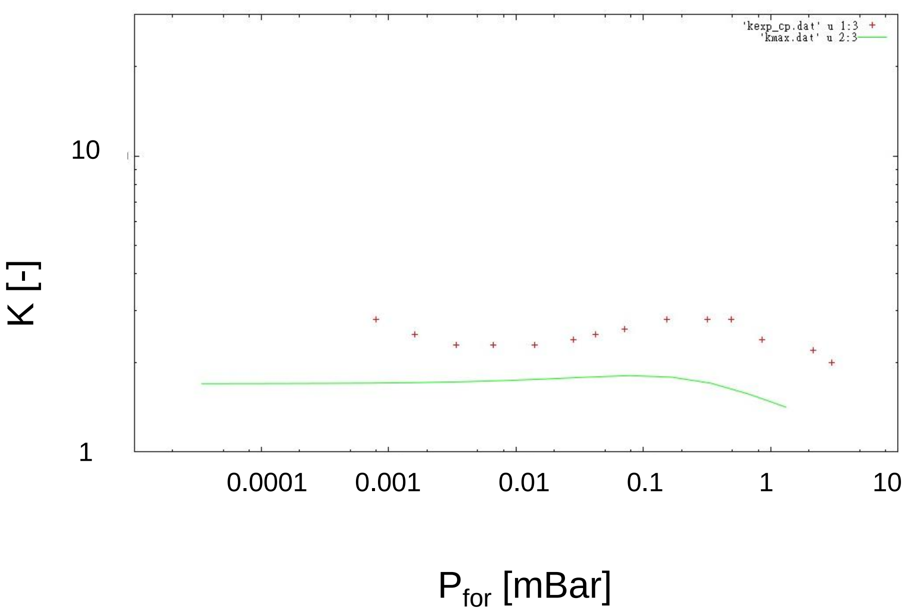
- Max error on K_{max} ≈ 50%
- Max error on P_{in} ≈ 35%

Φ_0 [°deg]	R_{in} [mm]	R_{disk} [mm]	h [mm]	e [mm]	N [mm]	ω [mm]	Flow Dir.
90	23	51.5	3	0.3	12	963	CP

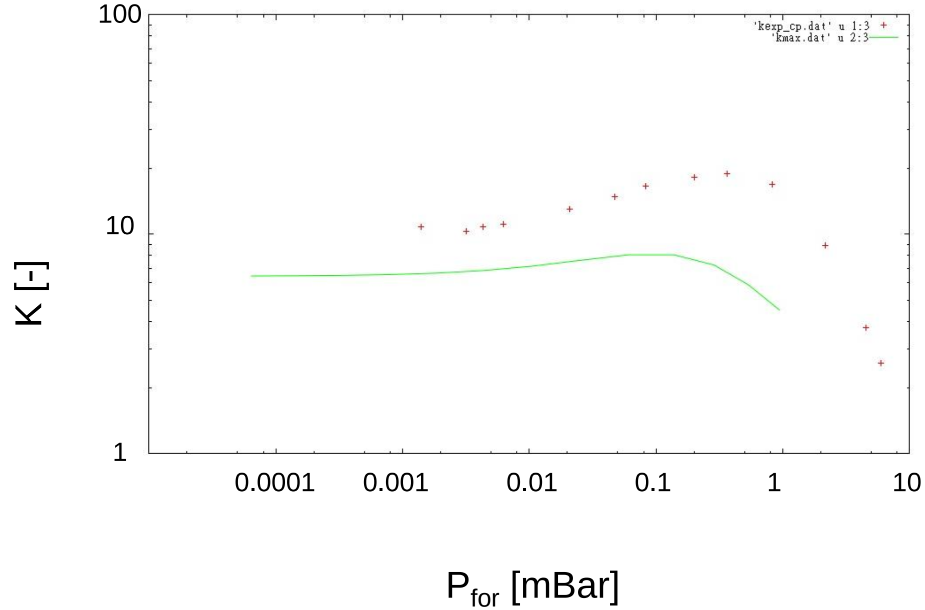
Agilent Technologies

Siegbahn stages : Results (III)

Hydrogen



Nitrogen



- H2, max error on K ≈ 50%
- N2, max error on K ≈ 30%
- Unable to predict the forline tolerance

Φ_0 [°deg]	R_{in} [mm]	R_{disk} [mm]	h [mm]	e [mm]	N [mm]	ω [mm]	Flow Dir.
360	23	51.5	1.5	0.3	4	963	CP

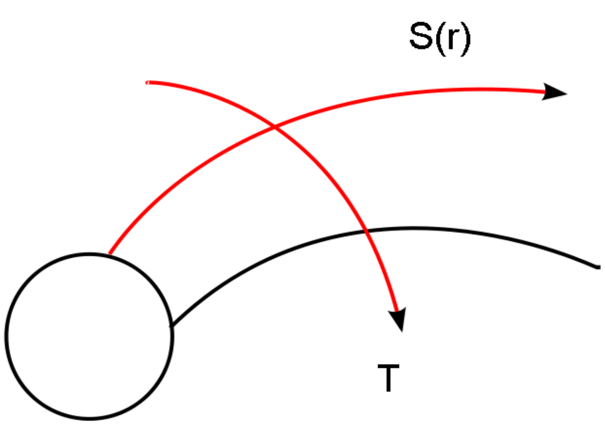
Siegbahn stages : a consistent approach

- The former method is not accurate when
  - Curvature of the spiral channel is high
  - Heavy gases are considered (not negligible inertial effects and linear approximation questionable)

- A more consistent approach will be to solve the governing equation in cylindrical

$$c_r \frac{\partial f}{\partial r} + c_\phi \frac{\partial f}{r \partial \phi} + c_y \frac{\partial f}{\partial y} + \frac{c_\phi^2}{r} \frac{\partial f}{\partial c_r} - \frac{c_r c_\phi}{r} \frac{\partial f}{\partial c_\phi} = \delta \left[M(f) - f \right]$$

- In particular, the scalar product $\mathbf{c} \cdot \nabla f$ is expressed in a general curvilinear, non orthogonal, system of coordinates (S,T,y) as described in figure:



$$c_r \frac{\partial f}{\partial r} + c_\phi \frac{\partial f}{r \partial \phi} + c_y \frac{\partial f}{\partial y} = c^S \frac{\partial f}{\partial S} + c^T \frac{\partial f}{\partial T} + c^y \frac{\partial f}{\partial y}$$

- In this new configuration, impermeability on walls and periodicity on clearances are easily recovered.

- Holweck-like approximations are imposed on the S-derivative.

Conclusions

- The prediction of the flow field in a radial drag pump with Siegbhan geometry hs been investigated
- An extension of the Sharipov's Holwek model has been proposed
- In a first approximation, a straigthforward application of the linearized 2D Boltzmann Eq. in cartesian coordinates has been employed
- The results are promising, but not sufficiently accurate, possibly due to non consistent boundary conditions
- A more accurate model, with consistent boundary conditions, is under development

Open questions

- Is there any possibility to correct the results for heavier gases, which are more sensitive to the linearization?

- What are the limits of the 2D approach?
  What are the benefits of a 3D approach?
  How much does a 3D approach increase the computational cost?

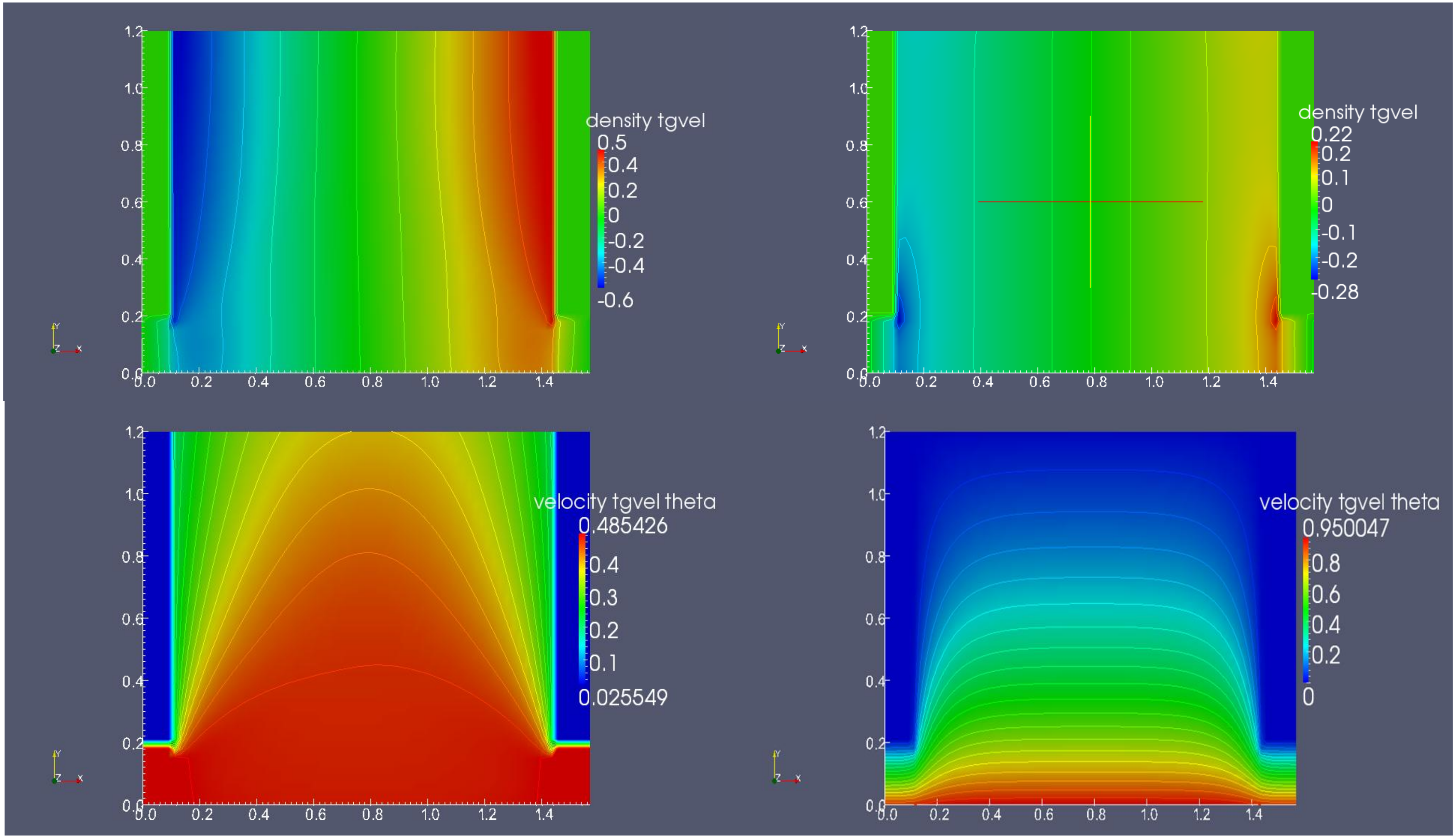
A possible approach?

1) Use the 3D non-linear equation
2) Approximate the derivative of the distribution function in the main direction by the derivative of the equilibrium
3) Use one-sided derivatives (maybe unstable) for the discretization of this derivative
4) Space marching “section-by-section” from inlet to outlet

Flow results: Couette Flow

HIGH RAREFACTION
δ = 0.003

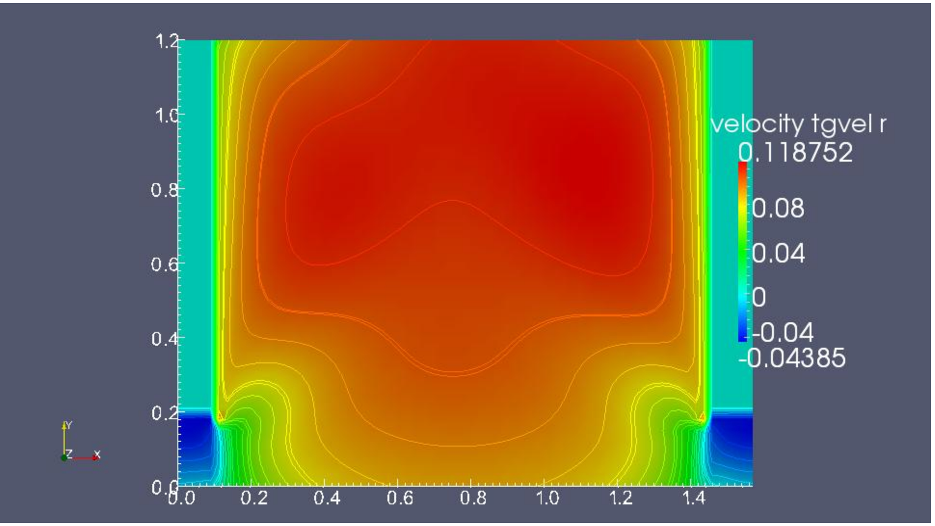
LOW RAREFACTION
δ = 25



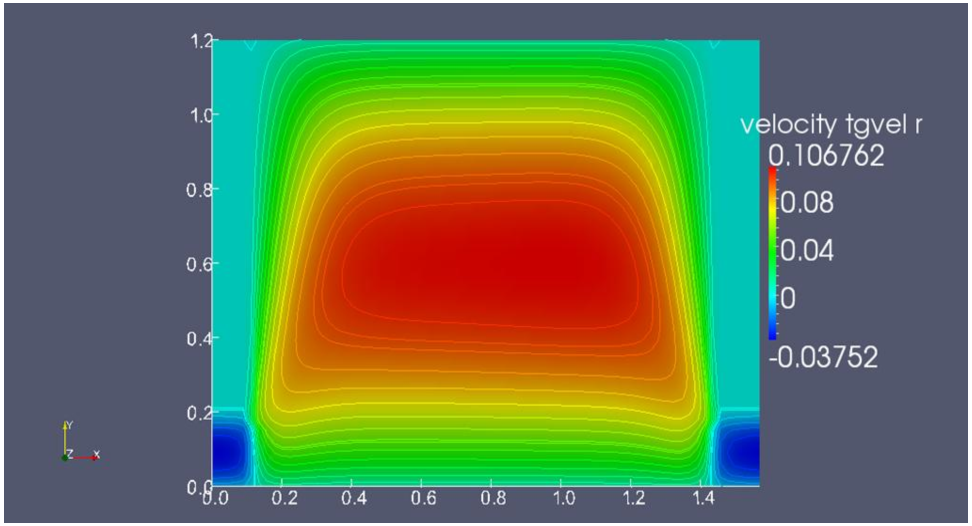
All results obtained for a hydrogen gas

Flow results: Couette Flow

HIGH RAREFACTION
$\delta = 0.003$



LOW RAREFACTION
$\delta = 25$

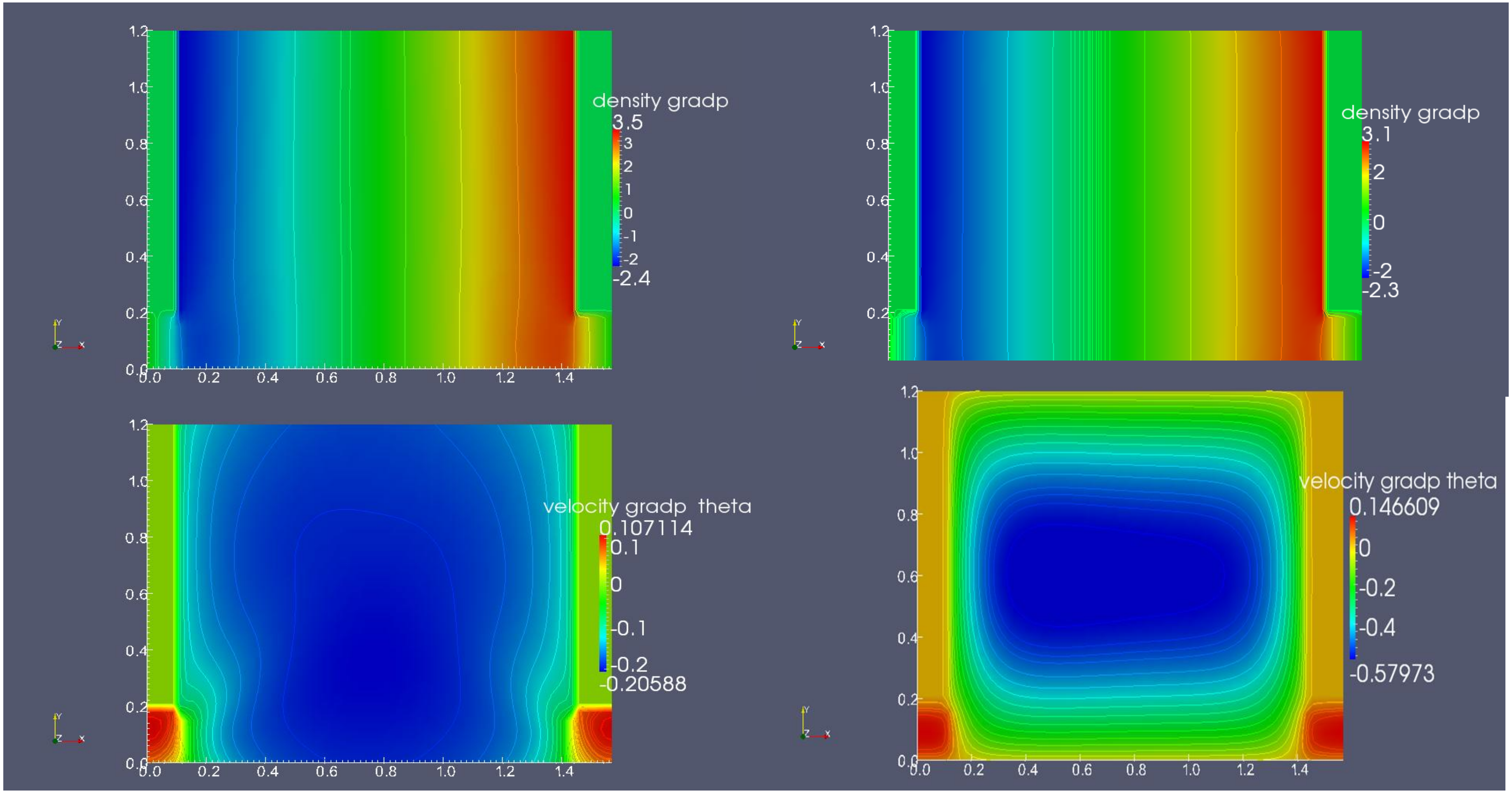


All results obtained for a hydrogen gas

Flow results: Poiseuille Flow

HIGH RAREFACTION
δ = 0.003

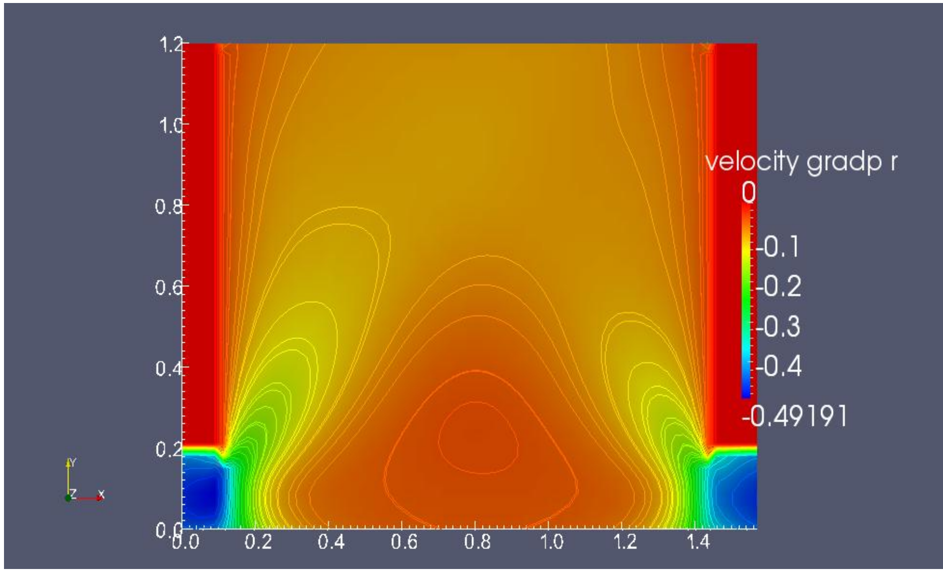
LOW RAREFACTION
δ = 25



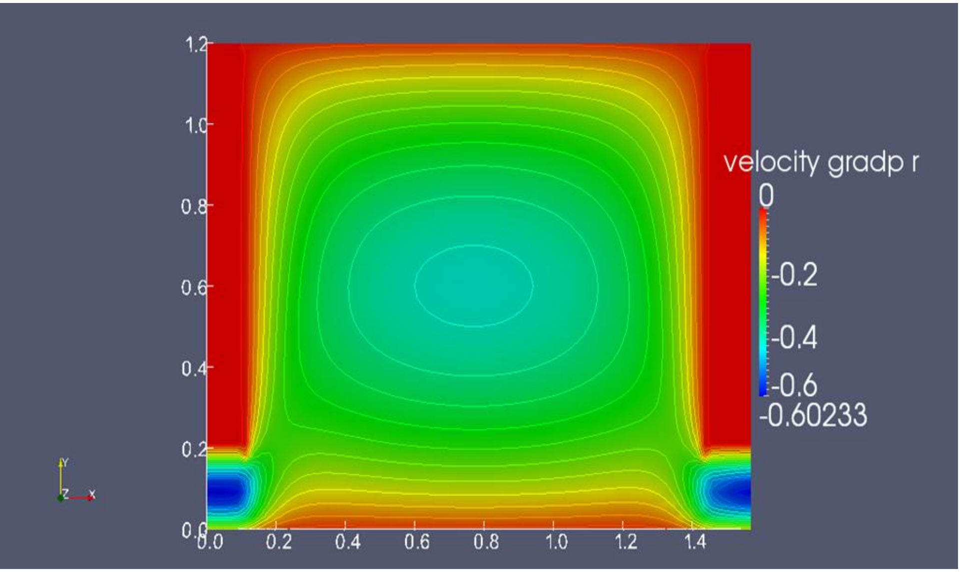
All results obtained for a hydrogen gas

Flow results: Poiseuille Flow

HIGH RAREFACTION
δ = 0.003



LOW RAREFACTION
δ = 25



All results obtained for a hydrogen gas

Details on numerical scheme (newest approach)

- A Discrete Velocity Method, with a finite difference scheme (upwind) is used to integrate the linearized Boltzmann equations
- Derivatives in the velocity space are treated with a modified upwind scheme (T-UNCE), as suggested by Mieussens (*J.Comp Phys 2000*)
- The three-dimensional velocity space (cr,cθ,cy) is rearranged in cylindrical coordinates (cm,Ψ,cy), with a typical dimension of 16x40x16 degrees of freedom.
- Integrals for macroscopic quantities are evaluated using a Gauss-Hermite (cy-velocities) and Gauss Legendre (cm-velocities) quadrature formulas.
- Stationary solutions are captured through a pseudo-transient technique (relaxation of the time-dependent linearized BGK-Boltzmann equation up to its stationary solution)
- An explicit time-marching scheme is employed. The solver is designed to work on MPI architectures to speed up calculations.