Modelling of the gas dynamics of a windowless gaseous tritium source

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KATRIN
Karlsruhe Tritium Neutrino Experiment

KATRIN experiment

WGTS (Windowless Gaseous Tritium Source)

- √ Determination of input parameters (injection pressure of Tritium gas to maintain a stable Tritium column density)
- √ Description of the behavior of Tritium flow due to the variations in temperature, acoustical waves, isotopic composition, presence of Krypton, etc.
- √ Problems associated with the pumping system.

Separation phenomenon in the tritium source

Gas mixture subjected to gradients of pressure, temperature or concentration $\rightarrow$ species tend to separate leading to a non-uniform concentration along the source.

KATRIN experiment:

- √ Tritium purity: 95% to 98%
  Isotopes: Hydrogen, Deuterium, etc.

- √ Krypton mode
  A small concentration of Krypton (10^{-5} to 10^{-4}) is added to the tritium in order to calibrate the mass spectrometer.

$\rightarrow$ In the experiment is necessary to maintain a stable Tritium column density.
$\rightarrow$ In the Krypton mode it is important to know the distribution of Krypton along the source.

Separation phenomenon in the tritium source

Binary gas mixtures:

- √ Hydrogen-Tritium (T=30K)
- √ Krypton-Tritium (T=120K)

The density and concentration distribution along the source is determined by using the methods of Rarefied Gas Dynamics.

$$\text{Methods of RGD} \begin{cases} \text{Boltzmann equation} \\ \text{DSMS (Direct Simulation Monte Carlo method).} \end{cases}$$

All my work is based on the solution of the Boltzmann equation!

Boltzmann equation and its models

- √ Integro-differential equation which describes the evolution of the distribution function of molecular velocities.
- √ All macrocharacteristics of the gas flow (pressure, bulk velocity, temperature, etc) are determined via distribution function.
- √ Even with a great computational infra-structure, to solve the Boltzmann equation is a very hard task!
- √ For practical calculations mathematical models are used to simplify the collisional term of the Boltzmann equation and reduce the computational effort significantly!!

Main parameter of RGD

Knudsen number (Kn) which characterizes the degree of gas rarefaction.

$$\boxed{\mathsf{Kn} = \frac{\lambda}{a} = \frac{\text{mean free path of gas molecules}}{\text{characteristic length of gas flow}}}$$

Rarefaction parameter (δ) which is given in terms of measurable quantities.

$$\boxed{\delta = \frac{a}{\ell} \sim \frac{1}{\mathsf{Kn}}, \quad \ell = \frac{\mu v_0}{P}, \quad v_0 = \sqrt{\frac{2kT}{m}}}$$

$$\text{Measuble quantities} \begin{cases} P : \text{pressure of the gas} \\ \mu : \text{viscosity of the gas} \\ v_0 : \text{most probable molecular velocity} \end{cases}$$

Regimes to the gas flow

- √ $\boxed{\text{Hydrodynamic regime } (\mathsf{Kn} \ll 1)}$

  All the equations of continuum mechanics are valid to describe the gas flow.

- √ $\boxed{\text{Free molecular regime } (\mathsf{Kn} \gg 1)}$

  The mean free path of gas particles is so large in comparison with the characteristic scale of gas flow so that the intermolecular collisions can be neglected.

- √ $\boxed{\text{Transitional regime } (\mathsf{Kn} \sim 1)}$

  The medium cannot be considered as a continuous medium
  The intermolecular collisions cannot be neglected.

  Boltzmann equation or DSMC (Direct Simulation Monte Carlo) method.

Gas rarefaction at WGTS

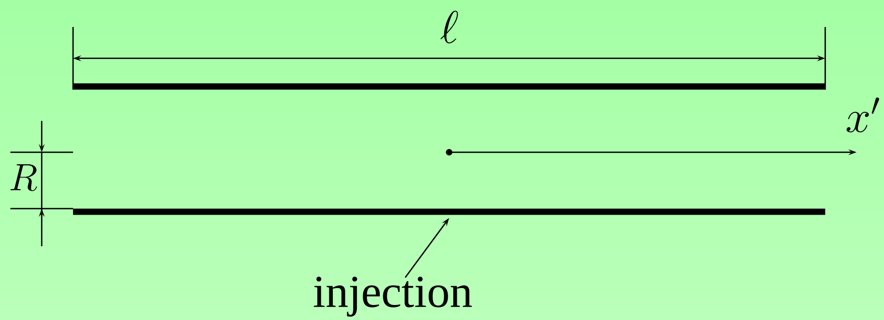
Along the WGTS the gas rarefaction changes from:

Hydrodynamic regime $\rightarrow$ transitional $\rightarrow$ free molecular regime

It is impossible to describe the gas flow by using the well known Navier-Stokes equations.

Therefore, the Boltzmann equation is used to describe the gas flow since it is valid for arbitrary degree of gas rarefaction!!

Scheme of the problem and input parameters



- √ Very long tube: $\ell \gg R$ ($\ell = 10$ m, $R = 4.5$ cm)
- √ Injection Pressure P_{in}

  $H_2 + T_2$ at 30K $\rightarrow P_{in} = 3.35\mu$bar

  Kr $+ T_2$ at 120K $\rightarrow P_{in} = 13.8\mu$bar
- √ At the tube exit the pressure is very low ($\approx 0.04 P_{in}$)
- √ Molar concentration of the mixture at the injection point

  Hydrogen-Tritium $\rightarrow C_{in} = 0.05$ (5% of Hydrogen)

  Krypton-Tritium $\rightarrow C_{in} \ll 1$ (10^{-5} to 10^{-4})

Scheme of the problem and input parameters

- √ Rarefaction parameter at the injection point

$$\delta_{in} = \frac{P_{in}R}{\mu}\sqrt{\frac{m}{2kT}}$$

Along the source the rarefaction parameter decreases (the rarefaction of gas mixture varies from hydrodynamic regime to free molecular regime)

We are interested in determining:

- √ The density distibution of species in the mixture
- √ The column density and concentration

$$N_\alpha = \int_{-\ell/2}^{\ell/2} n_\alpha(x)\,\mathrm{d}x, \quad C_{col} = \frac{N_1}{N_1 + N_2}, \quad \alpha = 1, 2$$

Main idea

Phenomenological relation:

$$\boxed{J_i = \sum_j \Lambda'_{ij} X_j}$$

J_i: thermodynamic fluxes (mass flow rate, heat flux, diffusion flux, etc)

X_j: thermodynamics forces (gradients of pressure, temperature, concentration, etc)

$\Lambda_{ij}(\delta, C)$: kinetic coefficients which depend on the rarefaction parameter δ and concentration C of the mixture

Definition of thermodynamic forces: (concentration gradients)

$$X_1 = \frac{R}{n_1}\frac{\mathrm{d}n_1}{\mathrm{d}x'}, \quad X_2 = \frac{R}{n_2}\frac{\mathrm{d}n_2}{\mathrm{d}x'}$$

Main idea

System of differential equations:

$$J_1 = \frac{n}{n_{in}}\sqrt{\frac{m(C_{in})}{m(C)}}\left[\Lambda_{11}\frac{R}{n_1}\frac{\mathrm{d}n_1}{\mathrm{d}x} + \Lambda_{12}\frac{\mathrm{d}n_2}{\mathrm{d}x}\right]$$

$$J_2 = \frac{n}{n_{in}}\sqrt{\frac{m(C_{in})}{m(C)}}\left[\Lambda_{21}\frac{R}{n_1}\frac{\mathrm{d}n_1}{\mathrm{d}x} + \Lambda_{22}\frac{\mathrm{d}n_2}{\mathrm{d}x}\right]$$

where Λ_{ij} depends on the rarefaction parameter δ and concentration C of the mixture.

To determine the density profiles $n_1(x)$ and $n_2(x)$ you just need to solve the system of differential equations!!!

The first step is to calculate the kinetic coefficients Λ_{11}, Λ_{12}, Λ_{21}, Λ_{22}.

Main idea

I. Calculation of the kinetic coefficients $\Lambda_{ij}(\delta, C)$

- $\surd$ It was based on the McCormack model to the Boltzmann equation.
- $\surd$ Assumptions:
  - $\star$ Diffuse scattering of gas species on the surface.
  - $\star$ Intermolecular interaction model of rigid-spheres.
- $\surd$ This step takes a long CPU time
  Hydrogen-Tritium mixture $\rightarrow$ 432 combinations (δ, C)
  Krypton-Tritium mixture $\rightarrow$ 336 combinations of (δ, C)

Main idea

II. Solution of the system of equations

Boundary conditions:

- √ Injection point ($x = 0$):

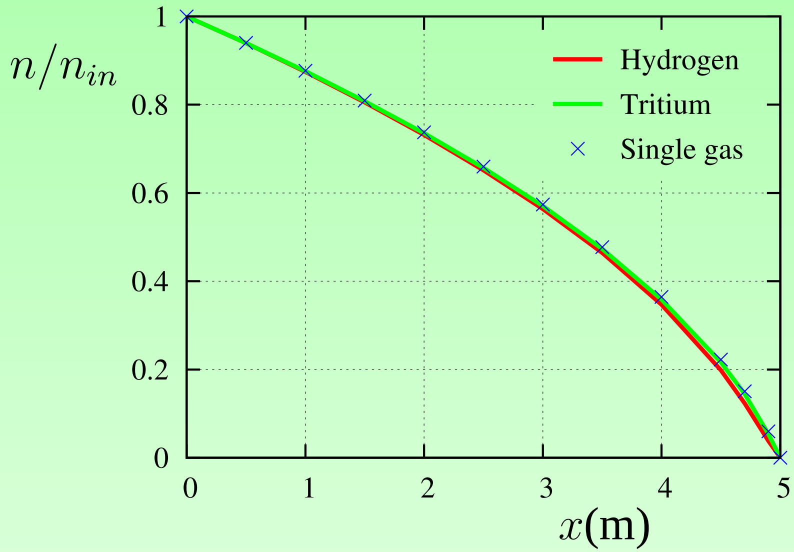
$$\boxed{n_1 = C_{in} n_{in} \quad \text{and} \quad n_2 = (1 - C_{in}) n_{in}}$$

- √ Tube exit ($x = \ell/2$)

$$\boxed{n_1 = 0 \quad \text{and} \quad n_2 = 0}$$

Results for the mixture $H_2 + T_2$ at 30K

Density distribution of H_2 and T_2



Column density of the mixture $\boxed{N = 4.97 \times 10^{17}/\text{cm}^2}$

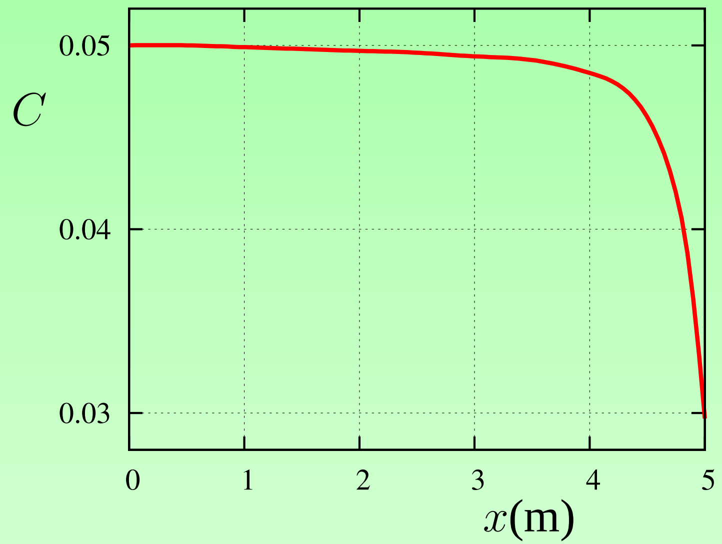
Colum density of H_2 $\boxed{N_1 = 0.24 \times 10^{17}/\text{cm}^2}$

Colum density of T_2 $\boxed{N_2 = 4.73 \times 10^{17}/\text{cm}^2}$

The column density of T_2 is 5.4% lower than that for a pure tritium.

Results for the mixture $H_2 + T_2$ at 30K

Local concentration of Hydrogen



Column concentration of the mixture $\boxed{C_{col} = 0.049}$

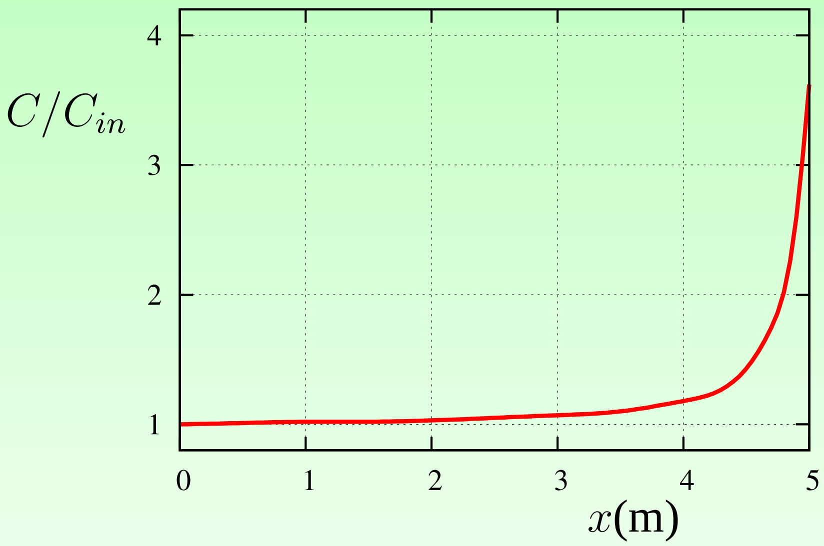
- ✓ The separation phenomenon is negligible for the mixture H_2-T_2.
- ✓ H_2 is the lightest isotope of T_2 so that for the other isotopes the separation phenomenon will be weaker than in the mixture H_2-T_2.

Results for the mixture Kr $+ T_2$ at 120K

The concentration of Kr at the injection point is very small

Since $C_{in} \ll 1 \rightarrow$ simplifications were made so that the results are valid for arbitrary injection concentration.

Relative concentration of Krypton



The column concentration $\boxed{C_{col} = 1.06 \times C_{in}}$.

The column concentration of Kr is 6% higher than its value in the injection point.

For the mixture Kr-T_2 the separation phenomenon cannot be neglected!!

Conclusions

- √ By considering 5% of H_2 in the Tritium gas the column density of Tritium is affected (5.4% lower than in a situation of pure Tritium).
- √ In the Krypton mode, since the concentration of Kr at the injection point is very low, there is no influence in the Tritium column density.
- √ The separation effect is negligible for the mixture H_2-T_2 but it cannot be neglected for the mixture Kr-T_2.
- √ Since the separation phenomenon is stronger for a mixture with larger ratio of molecular masses, the influence of such a phenomenon will be weaker for the other isotopes of T_2.

Current research

$\boxed{\text{Ternary gas mixture: Hydrogen-Krypton-Tritium at 120K.}}$

I hope to have some results soon!