Simulation of Residual Gas Particles in an Ultrahigh Vacuum System

Theory behind the Analytical Solution Approach

Ida Aichinger

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Outline

1. Introduction
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   - What will change for the FCC?
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Introduction - Simulation program

- **Aim: Fulfil FCC-hh vacuum requirement: Ultra high vacuum for FCC** $\Leftrightarrow n < 2 \cdot 10^{14} \frac{\textbf{particles}}{\textbf{m}^3}$
- **Simulation of residual gas particles in the beampipe**
- **Correlation between pressure and particle density via ideal gas equation:** $P \cdot V = N \cdot k \cdot T$
- **Molecular flow regime**
- **Multi-gas-model with four dominating gas species:** H_2, CH_4, CO, CO_2
- **Simulations are characterized by:**
  - pipe geometry
  - beam induced effects
  - material outgassing
  - pumping mechanism

Model Description - Balance equation

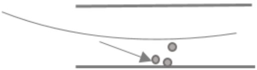
The evolution of the particle density n is described with a diffusion equation:

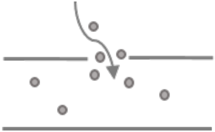
$$V \frac{dn(x,t)}{dt} = c_{spec}(x,t) \cdot \frac{d^2 n(x,t)}{dx^2} + \underbrace{Q(x,t)}_{\text{Flow into system}} - \underbrace{S(x,t) \cdot n(x,t)}_{\text{Flow out of system}}$$

System of four coupled differential equations due to four gas species.

Flow into system (Q)

Particles that are added to the system:



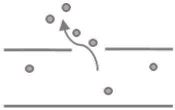


$$Q(x,t) = \underbrace{\eta_{ph} \cdot \dot{\Gamma}_{ph}}_{\text{photon-stimulated desorption}} + \underbrace{\eta_i \cdot \dot{I}_\mathrm{i}}_{\text{ion-induced desorption}} + \underbrace{\eta_e \cdot \dot{N}_e}_{\text{electron-induced desorption}} + \underbrace{q}_{\text{thermal outgassing}}$$

Local sources (e.g. due to gauges) are described in the boundary conditions.

Flow out of system (S)

Particles that are removed from the system:



$$S(x,t) = \underbrace{\alpha \cdot \frac{A \cdot v_{\text{gas}}}{4}}_{\text{wall distributed pumping}}$$

with:

α ... sticking probability

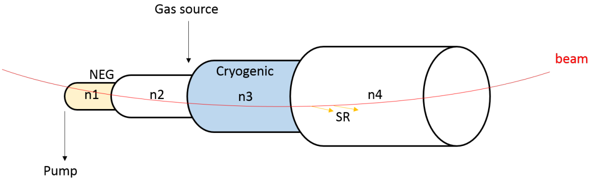
A ... lateral surface of beam pipe

v ... speed of particles

Local pumps are described in the boundary conditions.

Division of domain into finite elements

Split the domain into a finite number of segments and define for each segment a solution function n_k under steady state conditions. (with two arbitrary constants per segment)



Density and flux continuity between segments for each gas species:

$$\begin{aligned} n_{k-1}(x_k) &= n_k(x_k) \\ -a_{k-1}n'_{k-1}(x_k) + a_k n'_k(x_k) &= S_k n_k(x_k) - g_k \end{aligned}$$

Boundary conditions

Flux of molecules must equal the amount of molecules pumped or generated by a local source. (Mirror conditions)

$$
\begin{aligned}
a_1 n_1'(x_1) &= \frac{S_1}{2} n_1(x_1) - \frac{g_1}{2} \\
-a_N n_N'(x_{N+1}) &= \frac{S_{N+1}}{2} n_N(x_{N+1}) - \frac{g_{N+1}}{2}
\end{aligned}
$$

System of 1^{st}-order differential equation:

Change of variables: $y = \begin{pmatrix} n \\ n' \end{pmatrix} \in \mathbb{R}^8, \qquad M \in \mathbb{R}^{8\times 8}, b \in \mathbb{R}^8$

$$y'(x) = My(x) + b \tag{1}$$

Boundary conditions:

$N \in \mathbb{N}, \quad k \in \{2, \ldots, N\}, \quad H, S \in \mathbb{R}^{8\times 8}, \quad F_1, F_N \in \mathbb{R}^{4\times 8}, G \in \mathbb{R}^8, g \in \mathbb{R}^4$

$$H_{k-1}y_{k-1}(L) - (H_k + S_k)y_k(0) = G_k \tag{2}$$
$$F_1 y_1(0) = -g_1 \tag{3}$$
$$F_N y_N(x_{N+1}) = g_{N+1} \tag{4}$$

(1) = *balance equation*, (2) = *intermediate condition*,
(3) = *initial condition*, (4) = *end condition*

Solution y(x)

Theorem (Picard Lindelöf, Superposition principle)

Solution of equation system (1) *with initial conditions* y_0 *is given by:*

$$y(x) = P(x) \cdot y_0 + q(x) \tag{5}$$

with:

Fundamental system

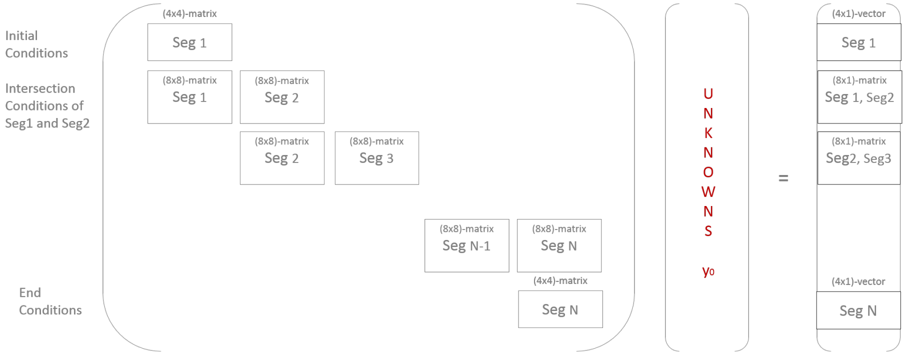
$$\begin{aligned} P(x) : \mathbb{R} &\to \mathbb{R}^{8\times 8} \\ x &\mapsto exp^{M\cdot x} \end{aligned}$$

Particular solution

$$\begin{aligned} q(x) : \mathbb{R} &\to \mathbb{R}^{8} \\ x &\mapsto -M^{-1} \cdot b \end{aligned}$$

The unknown y_0 in (5) are verified via the boundary conditions.

Final system of equations



Global solution for particle density $n(x)$

Solving the equation system and evaluating $y(x)$ in (5) with the unknowns y_0 gives us the particle density $n(x)$ at position x.

For segment k:

$$n_k(x) = [y_k(x)]_{1:4}$$

The global solution is therefore given by:

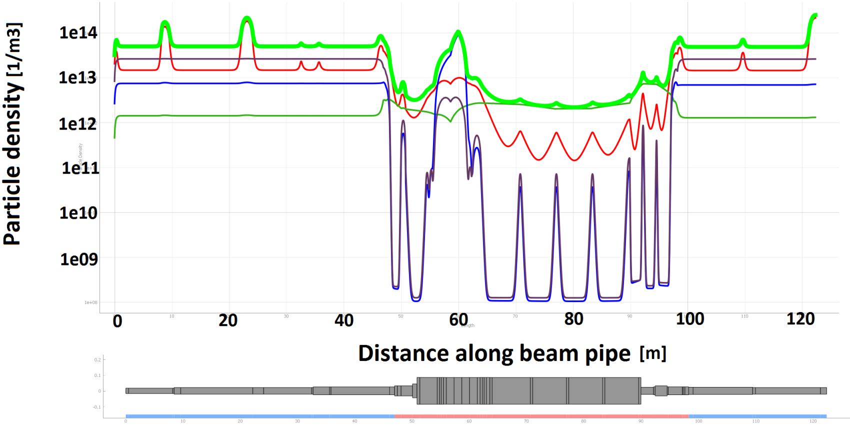
$$n(x) = \begin{cases} n_1(x) & x_1 \leq x \leq x_2 \\ n_2(x) & x_2 < x \leq x_3 \\ \vdots & \\ n_N(x) & x_N < x \leq x_{N+1} \end{cases}$$

Results

- **Algorithm is implemented in a Python environment**
- **Cross checked with *MolFlow+*[1] and LHC's data**
- **Delivers fast results, within one minute!**
- **Multi-gas model**
- **Is applicable to any vacuum system.**

[1] Monte-Carlo simulation program(R. Kersevan, M. Ady)

Q1 to Q4 - Quadrupoles in cryogenic region including a straight warm section



FCC forecast

Aim: 5 times better vacuum quality to guarantee a 100h beam lifetime (as it is now for LHC)

$$\rightarrow n \approx 2 \cdot 10^{14} \frac{\text{particles}}{\text{m}^3} \text{(in the arcs)}$$

Change of parameters:

- **aperture**
- **photon flux**
- **electron clouds**
- **different material**

Future work

- **Extension of the model**
  - Using experimentally results and simulations in Molflow+ $\rightarrow$ interpretate and implement it in analytical form
  - Dynamic effects, e.g. surface history
- **Error and sensitivity analysis**
- **Graphical User Interface**

- **Evaluate different designs for FCC**

Thank you for your attention!

. . . and thanks to the Vacuum Group at CERN,
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For questions and details: ida.aichinger@cern.ch