Simulation of Residual Gas Particles in an Ultrahigh Vacuum System

Theory behind the Analytical Solution Approach

Ida Aichinger

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Outline

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   Mass-balance differential equation with boundary conditions
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   Analytical approach
4. Results
   How good is the model matching in comparison to measured LHC data?
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Introduction - Simulation program

- **Aim:** Fulfil FCC-hh vacuum requirement: Ultra high vacuum for FCC \( \iff n < 2 \cdot 10^{14} \text{ particles/m}^3 \)

- 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:

$$V \frac{dn(x, t)}{dt} = c_{\text{spec}}(x, t) \cdot \frac{d^2 n(x, t)}{dx^2}$$

$$+ Q(x, t) - S(x, t) \cdot n(x, t)$$

Flow into system

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:

$$Q(x, t) = \eta_{ph} \cdot \dot{\Gamma}_{ph} + \eta_i \cdot \dot{i}_i + \eta_e \cdot \dot{N}_e + q$$

- **Photon-stimulated desorption**: $\eta_{ph} \cdot \dot{\Gamma}_{ph}$
- **Ion-induced desorption**: $\eta_i \cdot \dot{i}_i$
- **Electron-induced desorption**: $\eta_e \cdot \dot{N}_e$
- **Thermal outgassing**: $q$

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:

\[
S(x, t) = \alpha \cdot \frac{A \cdot v_{\text{gas}}}{4}
\]

with:

\(\alpha\) ... 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:

$$n_{k-1}(x_k) = n_k(x_k)$$

$$-a_{k-1}n'_{k-1}(x_k) + a_k n'_k(x_k) = S_k n_k(x_k) - g_k$$
Boundary conditions

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

\[ a_1 n'_1(x_1) = \frac{S_1}{2} n_1(x_1) - \frac{g_1}{2} \]

\[ -a_N n'_N(x_{N+1}) = \frac{S_{N+1}}{2} n_N(x_{N+1}) - \frac{g_{N+1}}{2} \]
System of 1\textsuperscript{st}-order differential equation:

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

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

Boundary conditions:

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

\[ H_{k-1}y_{k-1}(L) - (H_k + S_k)y_k(0) = G_k \]  \tag{2}

\[ F_1y_1(0) = -g_1 \]  \tag{3}

\[ F_Ny_N(x_{N+1}) = g_{N+1} \]  \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:*

\[
y(x) = P(x) \cdot y_0 + q(x)
\]  

(5)

with:

**Fundamental system**

\[
P(x) : \mathbb{R} \rightarrow \mathbb{R}^{8 \times 8}
\]

\[x \mapsto \exp^{M \cdot x}\]

**Particular solution**

\[
q(x) : \mathbb{R} \rightarrow \mathbb{R}^8
\]

\[x \mapsto -M^{-1} \cdot b\]

The unknown \( y_0 \) in (5) are verified via the boundary conditions.
Final system of equations

\[ \text{Initial Conditions} \]
- Seg 1
- Seg 2
- Seg 3
- Seg N
- Seg N

\[ \text{Intersection Conditions of Seg1 and Seg2} \]
- (4x4)-matrix
- Seg 1
- Seg 2

\[ \text{End Conditions} \]
- (8x8)-matrix
- Seg 1
- Seg 2
- Seg N

\[ \text{Unknowns} = \begin{bmatrix} \text{Seg 1} \\ \text{Seg 2} \\ \text{Seg N} \end{bmatrix} \]

\[ \text{Resultant} = \begin{bmatrix} \text{Segment 1} \\ \text{Segment 2} \\ \text{Segment N} \end{bmatrix} \]
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* and LHC’s data
- Delivers fast results, within one minute!
- Multi-gas model
- Is applicable to any vacuum system.

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1. Monte-Carlo simulation program (R. Kersevan, M. Ady)
Q1 to Q4 - Quadrupoles in cryogenic region including a straight warm section

Particle density [1/m³]

Distance along beam pipe [m]
FCC forecast

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

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

Change of parameters:
- aperture
- photon flux
- electron clouds
- different material
Future work

- **Extension of the model**
  - Using experimentally results and simulations in Molflow+ → 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!

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For questions and details: ida.aichinger@cern.ch