Improved model for transmission probabilities of edge-welded bellows based on TPMC simulations


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- Principle of vacuum simulations
- Simulation of edge-welded bellows
- Analysis of simulation results
- Improved model for edge-welded bellows
Principle of vacuum simulations

- **Test Particle Monte Carlo (TPMC) simulation** for free molecular flow
  - Molflow+

- **Surfaces** approximated by **mesh**
  - Individual properties of each surface element:
    - Sticking coefficient $\alpha_i$
    - Desorption probability and angular distribution $\cos^n(\Theta)$
    - Diffuse (Lambertian) reflection

- **Particle tracking** counts for each surface element
  - Number of **desorptions** $N_D$
  - Number of **hits** $N_H$
  - Number of **adsorptions** $N_A$
Principle of vacuum simulations: conductance

- Conductance of a tube: \( Q = C \cdot \Delta p \)
- Tube connects two large recipients

Simulation of the conductance with TPMC code

- **Entrance:** desorbing and adsorbing surface (\( \alpha_{\text{in}} = 100\% \)) \( N_{D,\text{in}}, N_{A,\text{in}} \)
- **Exit:** adsorbing surface (\( \alpha_{\text{out}} = 100\% \)) at exit \( N_{A,\text{out}} \)
- Conductance = inflow \( \times \) transmission probability \( W = \frac{N_{A,\text{out}}}{N_{D,\text{in}}} \)

\[
C = \frac{1}{4} \cdot \bar{c} \cdot A \cdot \frac{N_{A,\text{out}}}{N_{D,\text{in}}}
\]

\[
Q = C \cdot \Delta p = \frac{1}{4} \cdot \bar{c} \cdot A \cdot \frac{N_{A,\text{out}}}{N_{D,\text{in}}} \cdot \Delta p
\]
Vacuum simulation of edge-welded bellows

- Implementation of edge-welded bellows:
  - 2 straight tubes at each end
  - $n$ bellow elements approximated by mesh

- Entrance and exit tube surfaces: 30 surface elements per tube

- $n$ membrane elements: $60 \times n$ surface elements

  - Large increase in number of surface elements
  - Increase in simulation time by several orders of magnitude
  - Is it possible to replace the bellow with a straight tube?
Bellow parameters

- **Model geometry parameters:**
  - tube diameter: \( d = 100 \text{ mm} \)
  - tube length / tube diameter \( l/d \)
  - bellow length / tube length \( l_B/l \)
  - bellow height / tube diameter \( h/d \)
  - width of single bellow element \( w \)

- **Monte Carlo data:**
  - number of desorptions \( N_D \)
  - number of adsorptions \( N_A(E) \)

- **Analysis of simulation data:**
  - transmission probability
    \[
    W(l/d, l_B/l) = \frac{N_A(E)}{N_D}
    \]
Variation of opening angle $\alpha_B \left( \frac{h}{d} \right)$

- Variation of $\frac{h}{d}$ changes the transmission probability $W$ considerably
- Common bellow geometry: $W$ changes only by a few percent
  $\Rightarrow$ $\frac{h}{d}$ variance is acceptable for common bellow geometries
Variation of opening angle $\alpha_B (h/d)$

- **small angles (a):** bellow converging towards **straight tube**
- **large angles (c):** multiple reflections in one bellow element; **forward reflection reduced**
- **Minimum for angles around 55°:** bellow surfaces have perfect angle for backward reflection
Variation of bellow length $l_B/l$ and tube length $l/d$

- **Model geometry parameters:**
  - tube diameter: $d = 100$ mm
  - tube length / tube diameter $l/d$
  - bellow length / tube length $l_B/l$

- **Fixed parameters:**
  - bellow height / tube diameter $h/d = 0.25$
  - width of single bellow element $w/d = 0.025$

- **Analysis of simulation data:**
  - transmission probability $W(l/d, l_B/l) \equiv \frac{N_{A(E)}}{N_{D}}$
Variation of bellow length $l_B/l$ and tube length $l/d$

- **Transmission probabilities** for **straight circular tubes** from literature (no bellows, empirical):

  $$W(l/d, 0) = \frac{14 + 4\frac{l}{d}}{14 + 18\frac{l}{d} + 3\left(\frac{l}{d}\right)^2}$$

  *(K. Jousten et al, Handbook of Vacuum Technology, p. 136)*

- **Plot** of TPMC transmission probabilities $W$ versus $l/d$

- **Ansatz** for $W$ of the tube:

  $$W(l/d, 0) = \frac{1 + c_1\frac{l}{d}}{1 + c_2\frac{l}{d} + c_3\left(\frac{l}{d}\right)^2}$$

- The $c_i$ parameters were fitted with the TPMC results
Variation of bellow length $l_B/l$ and tube length $l/d$

- **Transmission probabilities of pure bellows**
  (no straight tube elements), i.e. $l_B/l = 1$

- **Plot** of the TPMC transmission probabilities $W$ versus $l/d$

- $l/d$ dependence follows the **same functional form** as before, but with **different** fit parameters

- **Ansatz** for $W$ of a pure bellow:

  $$W(l/d, 1) = \frac{1 + c_4 \frac{l}{d}}{1 + c_5 \frac{l}{d} + c_6 \left(\frac{l}{d}\right)^2}$$

- The $c_i$ parameters were fitted with the TPMC results

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**Fit function**

<table>
<thead>
<tr>
<th>Fit function</th>
<th>$(1 + c_4(l/d))/(1 + c_5(l/d) + c_6(l/d)^2)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$c_4$</td>
<td>$0.210 \pm 0.024$</td>
</tr>
<tr>
<td>$c_5$</td>
<td>$1.461 \pm 0.028$</td>
</tr>
<tr>
<td>$c_6$</td>
<td>$0.204 \pm 0.025$</td>
</tr>
</tbody>
</table>

$w/d = 0.025$

$h/d = 0.250$

$l_B/l = 1.0$
Variation of bellow length $l_B/l$ and tube length $l/d$

- **What is $W$ in general?**
  - Bellow length: $0 \leq l_B/l \leq l$
  - 2 tubes, central bellow

- Simulation shows **linear dependence** of $W$ on $l_B/l$

- **New ansatz** for $W$:

$$W \left( \frac{l}{d}, \frac{l_B}{l} \right) =$$

$$W_T \left( \frac{l}{d} \right) + \frac{l_B}{l} \cdot \left[ W_B \left( \frac{l}{d} \right) - W_T \left( \frac{l}{d} \right) \right]$$
Variation of bellow length $l_B/l$ and tube length $l/d$

**New ansatz** for the transmission probability of bellows:

$$W (l/d, l_B/l) = \left(1 - \frac{l_B}{l}\right) \frac{1 + c_1 \frac{l}{d}}{1 + c_2 \frac{l}{d} + c_3 \left(\frac{l}{d}\right)^2} + \frac{l_B}{l} \frac{1 + c_4 \frac{l}{d}}{1 + c_5 \frac{l}{d} + c_6 \left(\frac{l}{d}\right)^2}$$

**Fit results for parameters $c_i$:**

<table>
<thead>
<tr>
<th>parameter</th>
<th>fit value</th>
<th>standard error $\sigma$</th>
</tr>
</thead>
<tbody>
<tr>
<td>c1</td>
<td>0.2915</td>
<td>0.0020</td>
</tr>
<tr>
<td>c2</td>
<td>1.3018</td>
<td>0.0026</td>
</tr>
<tr>
<td>c3</td>
<td>0.2225</td>
<td>0.0015</td>
</tr>
<tr>
<td>c4</td>
<td>0.2707</td>
<td>0.0069</td>
</tr>
<tr>
<td>c5</td>
<td>1.5267</td>
<td>0.0077</td>
</tr>
<tr>
<td>c6</td>
<td>0.2777</td>
<td>0.0077</td>
</tr>
</tbody>
</table>

(M. Krause, J. Wolf, Vacuum 160 (2019), 402)
Comparison of straight tube results with literature

Case without bellows, i.e. **straight tubes**:

\[ W(l/d, 0) = \frac{1 + c_1 \frac{l}{d}}{1 + c_2 \frac{l}{d} + c_3 \left( \frac{l}{d} \right)^2} \]

For **very long tubes**, this becomes:

\[ W(l/d, 0) \bigg|_{(l/d) \to \infty} \rightarrow (1.322 \pm 0.013) \cdot \left( \frac{l}{d} \right)^{-1} \]

This is **in accordance** with literature for a **straight circular tube**:

\[ W(l/d) \bigg|_{(l/d) \to \infty} \rightarrow \frac{4}{3} \cdot \left( \frac{l}{d} \right)^{-1} \]

(K. Jousten et al, Handbook of Vacuum Technology, p. 136)

For **very long bellow** \((l_B/l = 1)\), the model converges to:

\[ W(l/d) \rightarrow \frac{c_4}{c_6} \cdot \frac{d}{l} = (0.97 \pm 0.04) \cdot \frac{d}{l} \approx \frac{d}{l} \]
Comparison of straight tube results with literature

- Case without bellows, i.e. **straight tubes**:

\[ W \left( \frac{l}{d}, 0 \right) = \frac{1 + c_1 \frac{l}{d}}{1 + c_2 \frac{l}{d} + c_3 \left( \frac{l}{d} \right)^2} \]

- For **very short tubes**, this becomes:

\[ W \left( \frac{l}{d}, 0 \right) \bigg|_{(l/d) \to 0} \rightarrow 1 - (1.0103 \pm 0.0025) \frac{l}{d} \]

- This is **in accordance** with literature for a **straight circular tube**:

\[ W \left( \frac{l}{d} \right) \bigg|_{(l/d) \to 0} \rightarrow 1 - \frac{l}{d} \]

*(K. Jousten et al, Handbook of Vacuum Technology)*
Comparison of straight tube results with literature

- **TPMC simulation:**

\[
W(l/d, 0) = \frac{1 + c_1 \frac{l}{d}}{1 + c_2 \frac{l}{d} + c_3 \left(\frac{l}{d}\right)^2}
\]

- **Literature:**

\[
W(l/d, 0) = \frac{14 + 4 \frac{l}{d}}{14 + 18 \frac{l}{d} + 3 \left(\frac{l}{d}\right)^2}
\]

(K. Jousten et al, Handbook of Vacuum Technology)

- **On average only 0.13% deviation**

**Fit function**

\[W_{\text{sim}} = s \cdot W_{\text{emp}} + y\]

<table>
<thead>
<tr>
<th>Intersection point y</th>
<th>8.28E-5 ± 5.41E-4</th>
</tr>
</thead>
<tbody>
<tr>
<td>Slope s</td>
<td>1.0013 ± 0.0004</td>
</tr>
</tbody>
</table>
Replacement of bellows in TPMC simulations

- **Objective:** replace a bellow with a straight tube
  - same transmission probability
  - same diameter
  - modified length $l'$

Transmission probability of the bellow:

$$W \left(l/d, l_B/l\right) = \left(1 - \frac{l_B}{l}\right) \frac{1 + c_1 \frac{l}{d}}{1 + c_2 \frac{l}{d} + c_3 \left(\frac{l}{d}\right)^2} + \frac{l_B}{l} \frac{1 + c_4 \frac{l}{d}}{1 + c_5 \frac{l}{d} + c_6 \left(\frac{l}{d}\right)^2}$$

Straight tube with modified length $l'$ and same transmission probability:

$$W \left(l'/d, 0\right) = 1 \frac{1 + c_1 \frac{l'}{d}}{1 + c_2 \frac{l'}{d} + c_3 \left(\frac{l'}{d}\right)^2}$$
Replacement of bellows in TPMC simulations

- **Ansatz:** \[ W \equiv W (l/d, l_B/l) = W (l'/d, 0) \]

\[
\frac{l'}{d} = \frac{c_1 - c_2 W + \sqrt{(c_1 - c_2 W)^2 + 4c_3 W (1-W)}}{2c_3 W}
\]

- **Proposed procedure** for replacing bellows in TPMC simulations:
  - calculate \( W \) with the model introduced here
  - calculate the effective length \( l'/d \)
  - replace the bellow in the simulation with a straight tube with length \( l'/d \)

- this procedure has been tested for a few bellows with different design parameters
  - error of a few percent
  - significant reduction in simulation time
Replacement of bellows in TPMC simulations

- Reduction in simulation time by several orders of magnitude

![Graph showing simulation time for 10^6 absorptions in s vs. \( \frac{l_B}{l} \)]

- \( l/d = 4 \)
- \( w/d = 0.025 \)
- \( h/d = 0.250 \)
Conclusion

- A wide range of bellow design parameters have been simulated.

- Variations in bellow widths and heights have no significant effect (for standard bellow parameters).

- A numerical model for transmission probabilities has been found, based on TPMC simulations.

- A simple approximation for the transmission probability of very long bellows is $W \approx d/l$.

- A procedure for replacing bellows by straight tubes in molecular flow simulations has been proposed.

Details and results:

M. Krause, J. Wolf: Improved model for transmission probabilities of edge-welded bellows based on TPMC simulations
Variation of opening angle $\alpha_B (h/d)$

**Variation of** $h/d$ **changes the transmission probability $W$ considerably**

**Common bellow geometry:** $W$ **changes only by a few percent**

$\Rightarrow$ **$h/d$ variance is acceptable** for common bellow geometries
Variation of opening angle $\alpha_B (w/d)$

- Variation of $w/d$ changes the transmission probability $W$ considerably.
- Common bellow geometry: $W$ changes only by a few percent.
  - $w/d$ variance is acceptable for common bellow geometries.