Maxwell velocity slip and Smoluchowski temperature jump boundary condition for ANSYS CFX

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Abstract. Multi-dimensional numeric flow simulation is a common but non-trivial approach to simulate the operation behavior of screw machines. Current challenges of computational fluid dynamics (CFD) simulations of screw machines are especially related to turbulence modelling and meshing. An adaption of CFD simulations to screw vacuum pumps is difficult since the Navier-Stokes equations have limited validity for low pressure regimes. However, the scope of application can be extended to higher Knudsen numbers (e.g. lower pressure regimes) by the use of velocity slip and temperature jump boundary conditions at solid surfaces. Even if the complete simulation of screw vacuum pumps is still challenging, these boundary conditions can be used to examine isolated effects like clearance flows or inhomogeneous pressure distributions in working chambers. A common commercial CFD-Solver is ANSYS CFX, which also has been successfully applied to screw machines, but it does not provide a Maxwell velocity slip and a Smoluchowski temperature jump boundary condition. In the presented work these boundary conditions are implemented in Ansys CFX using user-defined expressions in a similar way as it has been implemented in the rhoCentralFOAM solver of the open source toolbox OpenFOAM. The boundary conditions are validated by comparison with stationary OpenFOAM results, DSMC results and measurements for a hypersonic plate flow. In addition, the boundary conditions are verified by experimental and DSMC results of a gas flow in a clearance between a rotational shaft and a plane counter plate.

1. Introduction

Dry running screw vacuum pumps have become an important part of vacuum systems. In recent years, they replaced multistage roots pumps and oil-lubricated rotary vane pumps because they are compatible with soil and small amounts of liquid. Due to oil-free operation, sealing between different working chambers is realized by small clearances. Leakages through the clearances can be described as one of the major loss mechanisms of a screw vacuum pump. Screw vacuum pumps are mainly used as fore pumps, which means the suction pressure ranges from a few pascals up to the...
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atmospheric pressure. The circumferential speed of the pistons can reach up to 80 m/s. Considering that, the flow mechanism in the clearance can be mainly described as a pressure driven Poiseuille flow and a Couette flow driven by the rotation of the pistons. Rotatory positive displacement vacuum pumps are mainly simulated with chamber simulation tools whereby classic screw compressors can also be simulated by the use of computational fluid dynamics (CFD) solving the Navier-Stokes-Fourier (N-S-F) equations [1]. In order to augment the CFD-approach to vacuum pumps transitional non-equilibrium of rarefied gas flows need to be considered. The level of gas rarefaction is characterised by the Knudsen number, which is the ratio of gas molecular mean free path and a characteristic length. The N-S-F equations produces reasonable results for Knudsen numbers up to 0.01, for $Kn$ ranges up to 0.1 velocity slip and temperature jump boundary conditions should be applied at the walls. For larger $Kn$ numbers the N-S-F equations aren’t valid. The first-order conventional slip boundary condition was developed by Maxwell[2] in 1879. The temperature jump condition developed by Smoluchowski [3] is driven by the surface normal heat flux. Both boundary conditions has been implemented in the open source CFD software OpenFOAM, which is described in [4] and [5]. One of the most commonly used commercial CFD solvers which has been successfully used on screw machines is ANSYS CFX [6], which does not natively provide non-equilibrium boundary conditions for rarefied gases. However for subsequent research on screw vacuum pumps it is sensible to implement Maxwell velocity slip and Smoluchowski temperature jump boundary conditions into ANSYS CFX. In addition this is reasonable for detailed investigation of flow mechanisms in screw machines like it has been done in [7] and [8]. During the preparations of this paper several ways to implement the boundary conditions presented in [5] have been tried out. Therefore, the aim of the presented paper is to show the approach of best numerical stability. It’s realized with user defined expressions to calculate the coefficients for the finite-slip and the defined-heat-transfer-coefficient boundary conditions. The thermal slip is represented due to a fictional moving wall and a corrected wall heat flux. The boundary conditions are validated by comparison with stationary OpenFOAM results, DSMC results and measurements for a hypersonic plate flow provided by [9]. In addition, the boundary conditions are verified by experimental and DSMC results of a gas flow in a clearance between a rotational shaft and a plane counter plate presented in [10, 11].

2. Non-equilibrium boundary condition in CFX

The non-equilibrium slip/jump boundary conditions are implemented based on the equations for Maxwell slip and Smoluchowski jump presented in [4, 5]. Before getting into details some basic quantities are introduced, which are formulated in a way that these also work for incompressible flow. Since ANSYS CFX first solves the momentum and mass equation and in a second step the energy equation, it seems to be sensible to formulate the quantities based on density $\rho$ and static pressure $p$. The most important
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time for rarefied gases is the molecular mean free path which is, 
\[ \lambda = \frac{\pi \bar{c} \mu}{4 \bar{p}} \]  
(1) 
using the model of hard sphere molecules. It’s calculated from the static pressure \( p \), the 
dynamic viscosity \( \mu \) and the mean molecular velocity
\[ \bar{c} = \sqrt{\frac{8 \bar{p}}{\pi \bar{q}}} \]  
(2) 
of the gas.

2.1. Maxwell Viscous Slip

The Maxwell viscous slip depends on the wall shear stress and therefore can be calculated 
using the finite slip boundary condition, which is natively provided by ANSYS CFX [12]. Considering the CFX Modelling guide this boundary condition is available only 
for laminar flows. This option causes the fluid to slip at the wall when the wall shear 
stress is greater than a critical stress \( \tau_c \).
\[ |\tau_w| < \tau_c \rightarrow u_{\text{FiniteSlip}} = 0 \]  
(3) 
ANSYS CFX simulates the slip by using a moving wall with the wall speed computed 
as follows:
\[ u_{\text{FiniteSlip}} = U_S \cdot \frac{\tau_w}{|\tau_w|} \left( \frac{|\tau_w| - \tau_c}{\tau_n} \right)^m e^{-\frac{\tau_n}{\tau_c}} \]  
(4) 
where \( U_S \) is the slip speed, \( \tau_n \) is a normalising stress which is by default \( \tau_n = 1 \text{Pa} \), \( m \) is 
a positive power, \( B \) is a pressure coefficient, and \( p \) is the static pressure. As it is shown 
the finite-slip velocity vector \( u_{\text{FiniteSlip}} \) has the same direction as the wall shear stress 
vector \( \tau_w \).

The Maxwell viscous slip referring to [4] is given as follows
\[ u_{\text{MVS}} = \frac{\sigma_u - 2 \lambda}{\sigma_u} S \cdot (n \cdot \tau) = \frac{2 - \sigma_u \lambda}{\sigma_u} \tau_w \]  
(5) 
where \( \sigma_u \) is the tangential momentum accommodation coefficient, \( \tau \) the deviatoric stress 
tensor, \( n \) is the unit normal vector defined as positive in the direction pointing out of 
the flow domain and \( S = I - nn \) is the tensor which removes the normal components 
form every vector field. The tangential momentum accommodation coefficient normally 
is varying in-between 0 and 1. The tensor product \( -S \cdot (n \cdot \tau) \) is resulting into the wall 
 shear stress vector \( \tau_w \) tangential to the wall surface. Therefore Eq.5 can be represented 
by Eq.4 setting \( \tau_c = 0 \), \( m = 1 \) and \( B = 0 \). The slip speed is given with
\[ U_S = \frac{2 - \sigma_u \lambda}{\sigma_u} \cdot 1 \text{[Pa]} \]  
(6)
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2.2. Maxwell Thermal Slip

The thermal slip is modelled by an additional wall velocity added to the real wall velocity, thereby the Maxwell thermal velocity slip is calculated as follows considering the local gradient of the static temperature $T$:

$$\mathbf{u}_{MTS} = \frac{3 \mu \mathbf{S} \cdot \nabla T}{4 \varrho \frac{T}{T}}$$

Since the thermal slip is only a model for the fluid velocity in the Knudsen layer close to the wall and the real fluid velocity at the wall is still equal to the wall velocity, this modelling approach leads to inaccuracy in the conservation of energy. The N-S-F energy equation is

$$\frac{\partial}{\partial t} (\varrho E) + \nabla \cdot (\varrho \mathbf{u} (E + \frac{p}{\varrho})) = \nabla \cdot (\tau \cdot \mathbf{u} - \mathbf{q}) + Q - \varrho \mathbf{u} \cdot \mathbf{g}$$

where $E = e + \frac{1}{2} |\mathbf{u}|^2 + G$, is the total energy, $e$ is the thermal energy, $\varrho$ the fluid density, $G$ the specific potential energy, $\mathbf{q}$ the heat flux vector, $Q$ a volumetric energy source and $\mathbf{g}$ the specific gravity force. All other quantities have already been shown. As the energy equation shows, the additional modelled wall velocity is resulting in an additional friction work due to wall shear stress, which should be compensated to fulfill the conservation of energy. The compensation is done by an additional heat flux at the wall which is calculated as follows from wall shear stress and thermal slip velocity.

$$q_{MTS} = \mathbf{u}_{MTS} \cdot \mathbf{\tau}_w = \mathbf{u}_{MTS} \cdot \frac{\mathbf{u}_{\text{FiniteSlip}}}{U_S} \cdot 1 \text{ [Pa]}$$

If the finite-slip model is used, the wall shear stress variable wall shear is not calculated in CFX and can not be use in the user defined expressions and therefore a workaround is needed which recalculates the wall shear stress from the finite-slip solution. In [5] the additional viscous heat generation is modelled with a modified wall temperature such as the Smoluchowski temperature jump. For ANSYS CFX this approach does not work since the dynamic viscosity and thermal conductivity at the wall depends on the wall temperature so that the wall temperature would depend on itself due to the Smoluchowski temperature jump and viscous heat boundary condition. For this reason the modelling approach of the Smoluchowski temperature jump does also differ from [4, 5].

2.3. Smoluchowski Temperature Jump

In order to simulate the temperature jump the defined heat exchange parameter option of ANSYS CFX is used. This option models a heat exchange from an environment temperature to the fluid domain with a given heat exchange coefficient. In this approach the environment temperature is set to the wall temperature and the heat transfer coefficient is calculated in order to ensure that the Smoluchowski temperature jump occurs. In reference to Smoluchowski the temperature jump depending on the wall heat flux $q_w$ is given as follows

$$T - T_w = \frac{2 - \sigma_T}{\sigma_T} \frac{2 \gamma \lambda}{(\gamma + 1) Pr} \mathbf{n} \cdot \mathbf{q} = \frac{2 - \sigma_T}{\sigma_T} \frac{2 \gamma \lambda}{(\gamma + 1) Pr} q_w$$
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where Pr is the Prandtl number, \( \gamma \) is the ratio of specific heat and \( \sigma_T \) is the thermal accommodation coefficient which is in-between 0 and 1. The equation can be rearranged to the following form

\[
q_w = k \cdot (T - T_w)
\]

where \( k \) is the heat transfer coefficient given by

\[
k = \frac{\sigma_T \cdot (\gamma + 1) \cdot Pr}{2 - \sigma_T \cdot 2 \cdot \gamma \cdot \lambda}.
\]

The ratio of specific heat is calculated as follows from the specific heat capacity \( C_p \) at constant pressure, universal gas constant \( \mathcal{R} \) and the molar mass \( M \)

\[
\gamma = \frac{C_p}{C_p - \frac{\mathcal{R}}{M}}
\]

to allow a calculation also for incompressible fluids. It may be sensible to limit \( k \) for \( \lambda \to 0 \) to improve numerical stability since \( k \) otherwise becomes infinity, however in this paper it was not necessary.

### 3. Results

The presented boundary conditions are validated by two exemplary test cases. The first one is a hypersonic flow over a flat plate and the second one is a clearance between a rotating shaft and a plane counter plate. Both simulations are performed with perfect gases of constant ratio of specific heat capacities \( \gamma \), constant Prandtl number \( Pr \) and temperature depending dynamic viscosity \( \mu(T) \). The dynamic viscosity is modelled with the Sutherland-Model which reads as follows

\[
\mu(T) = \mu_0 \frac{T_0 + T_S}{T + T_S} \left( \frac{T}{T_0} \right)^{\frac{\gamma}{2}}
\]

where \( \mu_0 \) is the reference viscosity at reference temperature \( T_0 \) and \( T_S \) is the Sutherland temperature. All CFD simulations with the Maxwell/Smoluchowski boundary conditions use the values \( \sigma_u = \sigma_T = 1.0 \).

#### 3.1. Hypersonic flat plate

The mesh and the boundary conditions applied on the flat plate case are shown in Fig. 1. The dimensionless boundary conditions and dimensions of the fluid domain are shown in Tab. 1. The boundary conditions, such as free stream Mach number \( Ma_\infty \) wall temperature \( T_w \) and fluid parameters are set equal to those in the experiment in \[9\]. The applied gas is nitrogen. The results are presented for the reverse Knudsen number \( Kn_{-1} = x/\lambda_\infty \), where \( x \) is the distance from the leading edge and \( \lambda_\infty \) the mean free path of the gas at free stream conditions. The angle of attack of the free stream is zero. The mesh has 80000 cells with a grading to the leading edge and to the plate resulting into a minimal cell dimension of \( \Delta x/\lambda_\infty = \Delta y/\lambda_\infty = 0.14 \). The results of ANSYS CFX including the boundary conditions are compared to experiments of \[9\].
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Table 1. Hypersonic flat plate - geometry and boundaries

| $Kn_x^{-1}$ | $Ma_\infty$ | $\frac{L_u}{T_\infty}$ | $\frac{L_T}{T_\infty}$ | $\gamma$ | $Pr$ | $\sigma_u$ | $\sigma_T$ | $\frac{L_u}{\theta}$ | $\frac{L_T}{\theta}$ |
|-------------|--------------|-----------------|-----------------|-------|-----|---------|---------|----------------|----------------|
| 0...250     | 6.1          | 3.575           | 1.331           | 1.4   | 0.71| 1       | 1       | 0.1            | 0.5            |

and to dsmcFOAM+ [13] and rhoCentralFoam [14] results. For that the results shown in [4] have been reproduced including the viscous heating presented in [5]. Thereby it has been noticed that the sign of the thermal creep has been presented wrongly in [4, 5] and in OpenFOAM [14]. The thermal creep has to be calculated with a positive signed temperature gradient, since it represents a flow from the cold to the warm regions in the fluid. However for this publication the sign has been fixed in a local fork of the OpenFOAM source code in which also the viscous heating has been implemented. Changing the sign does effect the presented results only in minor way, since these are less affected by thermal creep CFX and rhoCentralFoam simulations have been done for the same mesh. For the DSMC simulation no grading has been used, the collision cell size is $\Delta x = \Delta y = \Delta z = 0.5 \lambda_\infty$.

Figure 1. Metcalf et al. case [9], computational mesh and boundary conditions

The results for the static pressure $p(y = 0)$ at plate surface are shown in Fig. 2. The pressure is normalized to the pressure $p_\infty$ of the free stream. No clear differences between CFX and rhoCentralFoam can be observed. However the deviation to DSMC results are distinctly higher, whereby the DSMC are closer to measurements, which has also been observed in [4].

In Fig. 3 the near wall temperature distribution is shown. The temperature is normalized to the free stream. Again CFX is compared to DSMC, rhoCentralFOAM and measurement results. If the results are compared to the wall temperature (Tab. 1), a temperature jump can be detected. In the opposite to the pressure distribution a deviation between CFX and rhoCentralFoam occurs, which possibly leads back to the different implementation of the viscous heat term. However the CFX results are
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closer to those of DSMC. In general all simulations do not give a good agreement to the measurements even for DSMC, which has also been observed in [4].

For the slip velocity, shown in Fig. 4, there are only minor differences between CFX and rhoCentralFOAM, where CFX is slightly closer to DSMC. Measurements for the velocity slip are not provided in [9].

3.2. Rotating Shaft

In order to verify the boundary conditions for clearance flows in screw vacuum pumps, simulations are compared to measurements of Huck et al. [10]. Huck set up an experiment with a clearance formed by a rotating shaft with a radius of \( R = 75 \text{ mm} \) on the one side and a plane contour on the other side. The clearance height between the plane contour and the shaft was set to \( h = 0.3 \text{ mm} \). The inlet and outlet pressure of the clearance as well as the circumferential speed of the shaft could be varied.
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while the mass flow rate \( \dot{m} \) through the clearance was measured. For details of the experimental setup and methods of measurement, see Ref. [10]. The comparison of simulation and experimental results is done for a variation of a dimensionless wall velocity \( U_0 = \frac{U_{shaft}}{\bar{c}_in} \) at a constant pressure ratio \( \Pi = \frac{p_{in}}{p_{out}} \). In addition the DSMC results from [11] are shown. The mesh and the applied boundary conditions for CFX are shown in Fig. 5. A grading is applied normal to the walls and the minimal cross sectional flow area leading to a minimal cell dimension of \( \Delta x/h = 0.02 \), \( \Delta y/h = 0.00277 \) and 32830 cells. In front and behind of the shaft a channel of height \( H \) is modelled. The overall length of the fluid domain is given with \( L \). The width of the quasi-2D fluid domain is given width \( \Delta z = 1\text{mm} \). On the surface of the shaft a wall velocity \( U_{shaft} \) is applied. In order to allow mass flow in both directions at the inlet as well as on the outlet an opening boundary condition is applied. The dimensionless boundary conditions as well as the geometry parameters are given in Tab 2. The measurements and simulations have been done with dry air.

The results are presented as dimensionless reduced mass flow rate,

\[
C_0 = \frac{\pi \bar{c}_{in}}{2 p_{in} h \Delta z} \dot{m}
\]

as a function of the Knudsen number \( Kn_h = \frac{\lambda_{in}}{h} \) and for different dimensionless wall velocities \( U_0 \). The wall temperature is set to the inlet temperature since all measurements have been done at environment temperature. In the case of a back flow, the outlet temperature is also set to the inlet value. All results are shown in Fig 6 with the classifications of the different flow regimes of rarefied gas flows. The diagram is split into a logarithmic and a linear part since negative values have to be shown also. The N-S-F results using Maxwell/Smoluchowski boundary conditions are giving a good agreement with the measurements in continuum and slip flow regime for Knudsen numbers upto \( 3 \cdot 10^{-2} \). For higher Knudsen numbers deviations occur though it is the slip regime considering the nominal Knudsen number \( Kn_h \). This is explained due to higher local Knudsen number downstream of the clearance where the slip boundary condition is not valid any more. However this effect is reduced for higher shaft velocities leading to a good agreement of the CFX results over the full shown range of Knudsen number for the maximum rotational speed. Considering the DSMC results it can be observed
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Table 2. Rotating shaft - geometry and boundaries

| $\frac{R}{h}$ | $\frac{L}{h}$ | $\frac{H}{h}$ | $Kn_h$ | $\Pi$ | $U_0$ | $\frac{T_{out}}{T_{in}}$ | $\frac{P_{ex}}{P_{in}}$ | $\gamma$ | $Pr$ | $\sigma_u$ | $\sigma_T$ |
|---------------|--------------|---------------|--------|-------|------|-----------------|-----------------|-------|------|--------|--------|
| 250           | $1e^{3}$     | 120           | $1e^{-3} - 1$ | 8     | $-8.64e^{-2}...8.64e^{-2}$ | 1               | 0.379 | 1.4  | 0.71  | 1      | 1      |

that these perfectly merge with CFX results in the slip regime, which also confirms the quality of the boundary condition in CFX.

Figure 6. Huck et al. case [10], dimensionless mass flow for varying Knudsen numbers and circumferential speeds

4. Conclusion

This paper does provide an approach to implement a Maxwell velocity slip and Smoluchowski temperature jump boundary condition into ANSYS CFX. The approach has been validated with simulations of the rhoCentralFoam solver of the open source CFD Software OpenFOAM and verified with DSMC simulations and measurements of two test cases. The first test case verifies the boundary condition for hypersonic flow, where thermal creep and the temperature jump can not be neglected. In this case both N-S-F solvers are giving similar results with minor deviations in temperature jump due to different modelling of viscous heat generation. The second case verifies
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the boundary condition for the usage in screw vacuum pumps especially for moderate Knudsen numbers and high positive wall velocities. Since the circumferential speed of screw vacuum pumps is typically high a usage of ANSYS CFX for such machines could be possible, if the shown boundary conditions are used. Especially inside the working chamber minor uncertainties are expected compared to the clearance flows since the Knudsen number in working chambers is smaller. However the wall velocity in the clearances is higher and so the boundary conditions should work for a wide range of machine suction pressure. Detached from the simulation of a complete screw machine the boundary condition in CFX can be used to improve models for clearances and working chamber in a chamber model simulation. Exemplary applications are mentioned in [15] and [8]. Finally one restriction of boundary condition should be mentioned, which has not been proved in this work. The used finite slip boundary condition is restricted to laminar flow, however in vacuum pumps also turbulences can occur so a turbulence modelling is needed. The presented approach may work if a shear stress turbulence model is used and the near wall laminar sub layer is resolved, but this has not been tested yet. This is not a major restriction since the laminar sub layer should always be resolved for accurate clearance modelling [7]. At least it could be sensible to limit the heat transfer coefficient for low mean free paths for improved numerical stability of the temperature jump.

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