Heat transfer modeling of a solar parabolic through receiver by direct simulation Monte Carlo method

Author(s):
Good, Philipp

Publication Date:
2011

Permanent Link:
https://doi.org/10.3929/ethz-a-007249969

Rights / License:
In Copyright - Non-Commercial Use Permitted
HEAT TRANSFER MODELING OF A SOLAR PARABOLIC TROUGH RECEIVER BY DIRECT SIMULATION MONTE CARLO METHOD

AUTHOR
Philipp Good

PROFESSORSHIP OF RENEWABLE ENERGY CARRIERS ETH
Prof. Aldo Steinfeld

SUPERVISOR
Dr. Matt Roesle

November 2, 2011
ABSTRACT

In this project the conduction heat loss through the rarefied gas in a solar parabolic trough receiver with actively controlled pressure in the annular gap between the absorber and vacuum jacket tubes is analyzed using the Direct Simulation Monte Carlo (DSMC) method. These simulations are coupled to an overall heat transfer model including convection, conduction and thermal radiation, and the non-uniform concentrated solar radiation incident on the receiver is treated using Monte Carlo ray tracing. This modeling approach is valid also for high Knudsen numbers as encountered in the target range of operating pressure around 1 Pa, and the results are compared to that obtained from a previous study using a continuum model of the rarefied gas with slip boundary conditions.

For krypton in the annular gap a high consistency between the two models is observed over the whole Knudsen number range from the free-molecular up to the continuum regime, whereas two-dimensional DSMC simulations for air predict slightly higher conduction heat transfer rates than the continuum approach, with the highest deviation occurring at 1 Pa. The change in average glass temperature is usually below 1 °C and the difference in total heat loss between the two models is mainly due to different heat conduction rates. Three-dimensional DSMC simulations of axial flow predict a gas conductance that is as much as 20 % higher than the values provided by the continuum model in the pressure range of interest. This has a significant effect on the specifications of the vacuum system.

The reliability of the DSMC results is verified by a sensitivity analysis to the main computational parameters and by comparison to one-dimensional analytical solutions. The model parameters match the specifications of current state-of-the-art solar receivers and validation through experiments is still required.
# CONTENTS

Abstract .................................................................................................................................................. ii

Contents .............................................................................................................................................. iii

List of figures ....................................................................................................................................... v

List of tables ......................................................................................................................................... vii

List of symbols ..................................................................................................................................... viii

1 Introduction ......................................................................................................................................... 1

1.1 The HITECO project ....................................................................................................................... 1

1.2 Knudsen number and rarefied flow regimes .................................................................................... 3

1.3 Objectives ....................................................................................................................................... 7

2 The Direct Simulation Monte Carlo method ....................................................................................... 9

2.1 Basic Concept ................................................................................................................................. 9

2.1.1 Discretization in time and space ............................................................................................... 9

2.1.2 Area of applicability .................................................................................................................. 11

2.1.3 Sampling of macroscopic properties ......................................................................................... 11

2.1.4 Sampling of collisions ............................................................................................................... 13

2.2 Binary elastic collisions and molecular models ............................................................................... 15

2.2.1 Conservation of momentum and energy .................................................................................... 15

2.2.2 Impact parameters and collision cross-section .......................................................................... 17

2.2.3 Requirement of molecular models for DSMC simulations ....................................................... 18

2.2.4 The variable hard sphere model ............................................................................................... 20

2.2.5 The variable soft sphere model ............................................................................................... 22

2.3 Inelastic collisions and rotational relaxation ................................................................................. 23

2.3.1 Internal degrees of freedom ..................................................................................................... 24

2.3.2 The Larsen-Borgnakke model .................................................................................................. 24

2.3.3 Rotational relaxation ................................................................................................................. 25

2.4 Surface interactions ......................................................................................................................... 27

2.5 The DS2V/DS3V programs ............................................................................................................. 28

2.5.1 Nearest-neighbor collisions ...................................................................................................... 28

2.5.2 Variable time step ...................................................................................................................... 30

2.5.3 Separate sampling and collision cells ....................................................................................... 31

2.5.4 Geometry definition .................................................................................................................. 32
Preface

3 Overall heat transfer model of solar receiver .................................................................................. 34
  3.1 Energy balances ......................................................................................................................... 35
  3.2 Flow diagram of the overall model ............................................................................................ 38
  3.3 Radiation heat transfer .............................................................................................................. 40
    3.3.1 Solar radiation ..................................................................................................................... 40
    3.3.2 Radiation heat transfer between the absorber and the glass jacket ........................................ 41
  3.4 Convection heat transfer ............................................................................................................ 47
    3.4.1 From the glass jacket to the environment .............................................................................. 47
    3.4.2 From the absorber to the HTF ............................................................................................ 47
  3.5 Conduction heat transfer ............................................................................................................ 48
    3.5.1 Absorber tube ....................................................................................................................... 48
    3.5.2 Glass jacket .......................................................................................................................... 49

4 Results ............................................................................................................................................ 51
  4.1 Two-dimensional heat transfer simulations .................................................................................. 52
    4.1.1 Off-sun configuration .............................................................................................................. 52
    4.1.2 On-sun configuration ............................................................................................................. 57
  4.2 Three-dimensional axial flow simulations .................................................................................... 60
    4.2.1 Conductance of receiver segments ......................................................................................... 61
    4.2.2 Pressure distribution along the receiver ................................................................................. 63
    4.2.3 Effect of axial flow on conduction heat transfer .................................................................... 65

5 Discussion ...................................................................................................................................... 67
  5.1 Accuracy and sensitivity of simulation results ............................................................................. 67
    5.1.1 Errors due to scattering .................................................................................................... 67
    5.1.2 Effect of number of molecules ........................................................................................... 71
  5.2 Comparison to analytical solutions ............................................................................................ 73
    5.2.1 Conduction heat transfer .................................................................................................. 73
    5.2.2 Axial flow ............................................................................................................................. 76

6 Conclusion ..................................................................................................................................... 82

Acknowledgement ............................................................................................................................ 84

References .......................................................................................................................................... 85

Appendix ............................................................................................................................................ 87
  A Gas properties ................................................................................................................................. 87
  B Calculation of configuration factors .............................................................................................. 89
  C Geometry of support structure .................................................................................................... 93
LIST OF FIGURES

Figure 2-1: Binary collision in the center of mass frame of reference (Bird 1994) ........................................ 16
Figure 2-2: Impact parameters and collision cross-section (Bird 1994)......................................................... 17
Figure 2-3: Angle of deflection in a binary collision of rigid spheres (Bird 1994) .............................................. 19
Figure 2-4: Flow domain of 2-D heat transfer simulations. ................................................................................. 32
Figure 2-5: Surface triangles specifying the geometry of a 1 meter long glass tube segment ...................... 33
Figure 3-1: Radial heat transfers in a solar parabolic trough receiver ............................................................... 35
Figure 3-2: Radial and circumferential heat exchange between segments in the 2-D model ....................... 37
Figure 3-3: Flowchart of the overall heat transfer model of the solar receiver ............................................... 39
Figure 3-4: Configuration factors from reference segment (3,k) on inner glass surface to absorber tube segments (2,i) .................................................................................................................. 43
Figure 3-5: Configuration factors between inner glass tube segments ............................................................ 43
Figure 3-6: Radiative heat transfers at semi-transparent glass jacket ............................................................... 45
Figure 4-1: Gas conduction heat loss for air in the vacuum chamber at various pressures in off-sun configuration ........................................................................................................................................ 53
Figure 4-2: Gas conduction heat loss for krypton in the vacuum chamber at various pressures in off-sun configuration ........................................................................................................................................ 54
Figure 4-3: Surface temperatures predicted by the ANSYS CFX model and by the 1-D and 2-D Matlab models in off-sun configuration ........................................................................................................... 56
Figure 4-4: Surface temperatures and conduction heat fluxes at the outer absorber and inner glass tubes at 1 Pa ........................................................................................................................................ 57
Figure 4-5: Temperature profile of inner glass surface predicted by ANSYS CFX and 2-D Matlab models at pressures of 0.1 Pa, 1 Pa and 10 Pa ................................................................................................................ 58
Figure 4-6: Heat fluxes at the vacuum jacket and average glass temperature at 1 Pa .......................................... 59
Figure 4-7: Average temperature of glass jacket, gas conduction and total heat loss in on-sun configuration at various pressures .............................................................................................................. 60
Figure 4-8: 3-D simulation domain of 1 meter long receiver segment with different pressure boundaries at inlet and outlet ........................................................................................................................................ 61
Figure 4-9: 1 meter long section with support structure in the middle .................................................................. 61
Figure 4-10: Conductance of a 1 meter long tube segment without and with support in the middle as a function of reference pressure ........................................................................................................... 63
Figure 4-11: Solar Collector Element (SCE) of the HITECO receiver ................................................................. 63
Figure 4-12: Pressure distribution along a semi Solar Collector Assembly for three different pressure levels at the intake of the vacuum pump. ................................................................. 65
Figure 4-13: Conduction heat loss through air in axial flow as a function of pressure.................. 65
Figure 5-1: Deviation between heat transfer rates at absorber and glass jacket for VSS model with constant Zr ........................................................................................................ 69
Figure 5-2: Pressure distribution along solar receiver segment with air in on-sun configuration.... 71
Figure 5-3: Heat transfer rate and MCS/MFP ratio as a function of number of simulated molecules. 72
Figure 5-4: Mass flow rate and MCS/MFP ratio as a function of number of simulated molecules....... 73
Figure 5-5: Conduction heat transfer through air in off-sun configuration compared to 1-D analytical solutions in slip regime. ........................................................................................................ 76
Figure 5-6: Conductance of 1 meter long segment without support for air in on-sun arrangement compared to analytical solutions. ............................................................................... 79
Figure 5-7: Conductance of 1 meter long segment without support for isothermal xenon at 300 K compared to analytical solutions. ....................................................................................... 80
Figure 5-8: Ratio of flow conductance of 1 m receiver tube section with support structure in the middle to that without support........................................................................... 81
Figure B-1: Configuration factors between circumferential cylinder segments.......................... 89
Figure C-1: Geometry of the support structure .............................................................................. 93
LIST OF TABLES

Table 1-1: Knudsen number in annular gap for air, krypton and xenon at 213 °C.............................. 5
Table 1-2: Rarefied gas flow regimes. .................................................................................................. 6
Table 2-1: Characteristic temperatures of rotation and vibration for nitrogen and oxygen (Bird 1994). ......................................................................................................................... 24
Table 2-2: Values for the rotational relaxation collision number according to Parker (1959).......... 26
Table 3-1: Radii of the PTR 70 receiver manufactured by Schott .......................................................... 36
Table 3-2: Spectral properties of glass jacket and absorber tube (Roesle and Coskun 2011).......... 40
Table 4-1: Simulation conditions of the overall heat transfer model .................................................. 51
Table 4-2: Molecular models and rotational relaxation collision number ....................................... 52
Table 4-3: Conductance of a semi Solar Collector Element at different outlet pressures .............. 64
Table 5-1: Statistical errors of various DS2V calculations in off-sun configuration ......................... 68
Table 5-2: Temperature jump coefficients utilized in the 1-D slip solutions .................................. 75
Table 5-3: Dimensionless flow rate as a function of rarefaction for completely diffuse reflection and radius ratio of 0.6 (Breyiannis, Varoutis et al. 2008) ................................................................. 78
Table A-1: Gas properties under standard conditions (101,325 Pa and 0°C) and model parameters used in DSMC simulations (Bird 1994) ................................................................................................. 87
Table A-2: Viscosity and thermal conductivity of air calculated according to (Lemmon and Jacobsen 2004) ........................................................................................................................................ 88
Table B-1: Configuration factors as a function of circumferential displacement used in the 2-D model ........................................................................................................................................ 92
## List of Symbols

### Roman letters

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Meaning</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A$</td>
<td>cross-sectional area; absorptivity</td>
</tr>
<tr>
<td>$a_c$</td>
<td>thermal accommodation coefficient</td>
</tr>
<tr>
<td>$B$</td>
<td>constant in slip solution of radial heat transfer</td>
</tr>
<tr>
<td>$b$</td>
<td>distance of closest approach</td>
</tr>
<tr>
<td>$C$</td>
<td>flow conductance</td>
</tr>
<tr>
<td>$c$</td>
<td>molecular velocity vector</td>
</tr>
<tr>
<td>$c_0$</td>
<td>macroscopic velocity vector</td>
</tr>
<tr>
<td>$c'$</td>
<td>thermal velocity vector</td>
</tr>
<tr>
<td>$c_m$</td>
<td>center of mass velocity vector</td>
</tr>
<tr>
<td>$c_{mean}$</td>
<td>mean thermal speed</td>
</tr>
<tr>
<td>$c_{mp}$</td>
<td>most probable thermal speed</td>
</tr>
<tr>
<td>$c_p$</td>
<td>specific heat at constant pressure</td>
</tr>
<tr>
<td>$D$</td>
<td>diffusion coefficient</td>
</tr>
<tr>
<td>$d$</td>
<td>diameter</td>
</tr>
<tr>
<td>$E$</td>
<td>emissivity; value of expectation</td>
</tr>
<tr>
<td>$F_{\Delta T}$</td>
<td>blackbody fractional function</td>
</tr>
<tr>
<td>$F_{i-k}$</td>
<td>configuration factor between surfaces $i$ and $k$</td>
</tr>
<tr>
<td>$F_N$</td>
<td>number of real molecules represented by each simulated molecule</td>
</tr>
<tr>
<td>$G$</td>
<td>dimensionless flow rate</td>
</tr>
<tr>
<td>$h$</td>
<td>convective heat transfer coefficient; axial length of receiver section</td>
</tr>
<tr>
<td>$i$</td>
<td>an integer</td>
</tr>
<tr>
<td>$K$</td>
<td>thermal conductivity</td>
</tr>
<tr>
<td>$k$</td>
<td>Boltzmann constant; an integer</td>
</tr>
<tr>
<td>$Kn$</td>
<td>Knudsen number</td>
</tr>
<tr>
<td>$L$</td>
<td>characteristic length</td>
</tr>
<tr>
<td>$l$</td>
<td>an integer</td>
</tr>
<tr>
<td>$\dot{M}$</td>
<td>mass flow rate</td>
</tr>
<tr>
<td>$m$</td>
<td>molecular mass</td>
</tr>
<tr>
<td>$N$</td>
<td>number of molecules/surface segments</td>
</tr>
</tbody>
</table>
number density

Nusselt number

pressure; probability

Prandtl number

total heat transfer per unit length of the receiver

heat transfer rate per unit length of a circumferential segment

heat flux

pV-flow

reflectivity; flow resistance; gas constant

radius; intermolecular distance

temperature

time

axial velocity component

volume; transmissivity

axial coordinate

rotational relaxation collision number

VSS parameter

specific heat ratio

mean molecular spacing; rarefaction parameter

angle between collision and reference planes

number of rotational degrees of freedom

temperature jump coefficient

exponent in the inverse power law model

constant in the inverse power law model

fraction of inelastic collisions

mean free path; wavelength

viscosity coefficient

collision frequency

VHS parameter

density

differential collision cross-section; Stefan-Boltzmann constant; standard deviation
\( \sigma_p \)  viscous slip coefficient
\( \sigma_T \)  total collision cross-section
\( \tau \)  relaxation time
\( \chi \)  deflection angle
\( \Omega \)  solid angle
\( \omega \)  temperature exponent of the coefficient of viscosity

**Subscripts**

- \( \text{abs} \)  absorber tube
- \( \text{c} \)  cell; continuum regime
- \( \text{cond} \)  conduction in solids
- \( \text{conv} \)  convection
- \( \text{e} \)  equilibrium; emitted
- \( \text{ext} \)  external
- \( \text{gas} \)  gas conduction
- \( \text{glass} \)  glass jacket
- \( i \)  inner
- \( \text{in} \)  Incoming; inlet
- \( \text{leave} \)  leaving
- \( \text{max} \)  maximum
- \( o \)  outer
- \( \text{out} \)  outgoing; outlet
- \( r \)  relative; real; reduced; rotational; reflected
- \( \text{rad} \)  thermal radiation
- \( \text{ref} \)  reference
- \( s \)  slip regime
- \( \text{solar} \)  solar radiation
- \( \text{sky} \)  sky temperature
- \( T \)  total
- \( t \)  transitional regime
- \( v \)  vibrational
- \( w \)  wall
- \( 0 \)  heat transfer fluid
1 inner absorber surface; first molecule
2 outer absorber surface; second molecule
3 inner glass jacket surface
4 outer glass jacket surface
5 environment
∞ ambient

**Acronyms**

CFD computational fluid dynamics
CFX ANSYS CFX program
CSP concentrating solar power
CV coefficient of variation
DSMC Direct Simulation Monte Carlo
DTS desired time step
HITECO high temperature efficient collector project
HS hard sphere
HTF heat transfer fluid
MCS mean collision separation
MFP mean free path
MCT mean collision time
MTT mean transit time
NTC no time counter
SCA solar collector assembly
SCE solar collector element
VeGaS Very General Monte Carlo Ray-Trace Simulation
VHS variable hard sphere
VSS variable soft sphere
1 INTRODUCTION

Facing the imminent issue of global warming the European Union is committed to the “20-20-20” objectives by 2020, i.e. reducing greenhouse gas emissions by at least 20% from 1990 levels, achieving a 20% share of renewables in the overall energy mix and saving 20% of energy consumption by improving energy efficiency. In order to meet these targets different fields of research have to be explored, as no single technology is considered capable of solving the problem. In areas with elevated solar irradiation such as Southern Europe, Northern Africa and the Middle East a viable and high-potential way of electricity production is concentrated solar power (CSP). With further industrial development and high levels of energy efficiency this technology could meet up to 7% of the world’s power needs by 2030 and one quarter by 2050. Among the various CSP designs the parabolic-trough solar collector is currently the most mature and promising technology for large-scale electricity production, with a currently installed world-wide capacity of 1’000 MW and more than 3’000 MW under construction or planned to be commissioned within the next five years (Richter, Teske et al. 2009). Nevertheless, in order to accelerate its implementation, the costs of electricity generated by this technology have to be reduced.

1.1 The HITECO project

For this purpose the European Commission has launched a three-years project in November 2010 under the title “New solar collector for high temperature operation in CSP applications”, in the following referred to as HITECO (High Temperature Efficient Collector). This project aims at lowering the electricity cost by raising the operating temperature of the heat transfer fluid to 600 °C and hence increasing the overall efficiency of the power cycle. Actual state-of-the-art collector systems are designed to work at a maximum operating temperature of 400 °C. This limit is imposed by several key components and a significant drop in efficiency would occur at higher temperatures. In the course of the HITECO project the critical limitations of present collector designs are re-
assessed and solutions are elaborated to develop and validate a new receiver tube concept that allows the heat transfer fluid to reach 600 °C. For this purpose new materials are researched that stay stable at such temperatures while maintaining the optical, mechanical and thermal performance of the receiver, new heat transfer fluids are explored and new supports, union systems and contact points are developed in order to better accommodate the varying thermal expansion of the steel and glass tubes. Moreover the new design is assessed from a manufacturing point of view to obtain a product that is easier and cheaper to fabricate, to assemble and to commission and a solution is chosen showing optimal energy cost (€/kWh). The HITECO project brings together nine industrial partners and research organizations from four European countries. The role of ETH Zurich in the project consists of modeling the thermal performance of the receiver tube and the collector system, assessing its sensitivity to key parameters and validating the models through experiments to help determine the optimal design.

In the following two particular limitations of existing designs are discussed on the basis of the “PTR 70” solar receiver manufactured by the German company Schott, which is regarded as the state-of-the-art technology throughout this thesis and is briefly described below. Basically the PTR 70 receiver is composed of two coaxial, cylindrical cavities with a length of 4 meters. The inner tube is made of stainless steel and carries the heat transfer fluid. It is covered with a selective coating on the outside which allows a high fraction of sunlight to be absorbed while preventing infrared radiation to be emitted. The inner pipe is surrounded by a glass cover that is transparent to solar radiation. In the chamber confined between the two tubes a high vacuum (0.001 Pa) is established for thermal insulation purposes and to activate the getter systems. The getters limit conductive and convective heat losses by capturing the molecular hydrogen that is dissociated due to the temperature increase of the heat transfer fluid and permeates through the stainless steel walls into the vacuum chamber. In order to maintain the vacuum in the enclosure the glass jacket is linked to metallic bellows seals at both ends of the tube by means of glass to metal welds that require a high degree of air tightness. Finally three of these elements are joined by inner tube welding to form 12 meter long collector modules. A general one-dimensional model predicting the heat loss of such a receiver has been implemented by Forristall (2003) in Engineering Equation Solver.

One problem arising from this design is encountered in manufacturing due to welding in vacuum. This results in a complex fabrication process and high costs, since the vacuum chamber needs to be sealed and tested in the assembly line. Another issue evolves during operation and concerns the getters whose ability to absorb hydrogen decreases significantly at higher temperatures.
these systems are not capable of absorbing any other gases produced by desorption processes or leaks such as helium and argon. Furthermore getter systems reach saturation after absorbing a certain amount of hydrogen, which might be exceeded in 20 years of operation, thus reducing strongly the performance of the receiver. Moreover the pressure level is not monitored and can only be estimated by comparing the temperature measured at the glass tube to the theoretical value under these conditions.

Therefore one improvement of the HITECO receiver design is a continuous vacuum jacket for each collector. The pressure is actively maintained by means of a vacuum pump, and the gas composition may be controlled as well (e.g. air or heavy inert gases). The vacuum system will operate at moderate pressures in the range between 0.1 Pa and 10 Pa, rather than the high vacuum required in existing designs. Additionally, the introduction of purge gases may induce a flow along the length of the vacuum jacket, which cannot occur in the present state-of-the-art receivers. In order to decide on the optimal pressure and composition of the gas, their influence on the heat loss through the vacuum jacket due to thermal conduction and convection needs to be quantified. Furthermore the pressure drop along the tubes during gas evacuation has to be modeled to determine the specifications of the vacuum system. Coskun (2011) has developed a two-dimensional model of combined conductive, convective and radiative heat transfer for the HITECO receiver including the effects of non-uniform solar flux on the receiver tubes. The model is implemented in the commercial CFD software ANSYS CFX that deals with conduction and convection. Radiation is treated separately by means of a Monte Carlo ray-tracing code and the net radiative heat transfer to the absorber tube and glass cover is included in the CFX model as energy sources.

1.2 Knudsen number and rarefied flow regimes

The first step in the analysis of the gas consists in determining the degree of rarefaction in the vacuum chamber. This is expressed by means of the Knudsen number, which is defined as the ratio of the molecular mean free path $\lambda$ to the characteristic flow length $L$,

$$Kn = \frac{\lambda}{L} \quad (1.1)$$

$L$ may be chosen either as a universal length parameter to calculate a global Knudsen number of the flow or as the scale length of a macroscopic flow gradient, e.g. $L = \rho/(\partial \rho/\partial x)$, for local Knudsen
numbers. This number is important because the conventional continuum model, whose mathematical description is generally provided by the Navier-Stokes equations, is only applicable for Knudsen numbers up to 0.1 and errors become significant at values around 0.2. The reason for this is that the transport terms in the Navier-Stokes formulation lose their validity if the density of the gas is very low or if the gradients of the macroscopic properties are so steep that their scale length becomes comparable to the mean free path of the molecules. More precisely, the shear stresses, heat fluxes, and diffusion velocities can no longer be expressed as linear functions of the gradients in velocity, temperature, and species concentration. It is noted that the limits on the range of validity are imposed by the assumption about the transport terms rather than the continuum approach itself. The conservation equations of mass, momentum and energy still hold under rarefied conditions, but they do not form a determinate set (Bird 1994).

To calculate the overall Knudsen number in the annular gap between the absorber tube and the vacuum jacket the hydraulic diameter is chosen as the characteristic length of the flow in this thesis,

\[
L = d_h = d_{glass,i} - d_{abs,o}. \tag{1.2}
\]

The mean free path is the average distance traveled by a gas molecule between two consecutive collisions. Generally the velocity \( c \) of a gas molecule is composed of two parts, the macroscopic stream velocity \( c_0 \) and the thermal velocity \( c' \),

\[
c = c_0 + c'. \tag{1.3}
\]

The mean free path is defined in the reference frame of the stream and may be related to the molecular mean collision frequency \( \nu \) by

\[
\lambda = \frac{c_{mean}}{\nu}, \tag{1.4}
\]

where \( c_{mean} \) is the average magnitude of the thermal velocity vector. The reciprocal of the mean collision rate is called mean collision time, which may be regarded as the time scale of macroscopic processes. From kinetic theory the collision frequency in a homogeneous gas can be calculated by

\[
\nu = n \bar{\sigma}_{Tc_r}, \tag{1.5}
\]

where \( n \) is the number density and \( \bar{\sigma}_{Tc_r} \) denotes the mean product of the total collision cross-section of molecules and their relative speed. The bar indicates the average over all molecules in the gas. The difficulty in this formula lies in the correct definition of the collision cross-section, which varies with the molecular model and is, in general, a function of relative velocity. A slightly unrealistic but nevertheless useful model in this case is the hard sphere (HS) molecule because its
total collision cross-section \( \sigma_r = \pi d^2 \) is constant and independent of \( c_r \). In the following a gas in equilibrium-state is considered, i.e. there are neither spatial nor temporal gradients in the macroscopic flow properties. In an equilibrium gas there is no preferred direction, i.e. the velocity distribution of the molecules is isotropic and the mean thermal and relative speeds are related to each other by \( \bar{c}_r = \sqrt{2} c_{\text{mean}} \) (Bird 1994). By using the ideal gas law

\[
P = k n T
\]

the mean free path in a hard sphere gas in equilibrium may be written as

\[
\lambda = \frac{1}{\sqrt{2\pi d^2}} = \frac{k T}{\sqrt{2\pi d^2} P}
\]

(1.7)

where \( P \) is the scalar pressure, \( T \) the thermodynamic temperature and \( k \) the Boltzmann constant. However, this expression depends on the collision cross-section of molecules, which is essentially not measurable and varies, as noted above, with the molecular model. Therefore an alternative definition in terms of measurable quantities is used here for the calculation of the Knudsen number. In the literature the mean free path is mostly defined via the viscosity coefficient \( \mu \),

\[
\lambda = \frac{\mu c_{mp}}{P}
\]

(1.8)

where \( c_{mp} = \sqrt{2kT/m} \) is the most probable thermal speed of molecules with mass \( m \) in an equilibrium gas at temperature \( T \). Using the dimensions of the PTR 70 receiver \((d_{\text{abs, o}} = 70 \text{ mm}, d_{\text{glass, i}} = 115 \text{ mm})\) the Knudsen number in the vacuum chamber can be calculated for various gases at different pressures (cf. table 1-1).

<table>
<thead>
<tr>
<th>Pressure [Pa]</th>
<th>Air</th>
<th>Krypton</th>
<th>Xenon</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.1</td>
<td>3.1</td>
<td>2.5</td>
<td>1.9</td>
</tr>
<tr>
<td>1</td>
<td>0.31</td>
<td>0.25</td>
<td>0.19</td>
</tr>
<tr>
<td>10</td>
<td>0.031</td>
<td>0.025</td>
<td>0.019</td>
</tr>
</tbody>
</table>

These values are obtained for a gas temperature corresponding to the average of the outer absorber and inner glass surfaces, \( T = \left( T_{\text{abs, o}} + T_{\text{glass, i}} \right) / 2 \), and unless otherwise stated the Knudsen number in this thesis is calculated in this manner. Here the values \( T_{\text{abs, o}} = 400 ^\circ \text{C} \) and \( T_{\text{glass, i}} = 25 ^\circ \text{C} \) are utilized.
Based on the value of $Kn$ four flow regimes are distinguished in the theory of rarefied gas dynamics, which are summarized in table 1-2 (Shen 2005).

<table>
<thead>
<tr>
<th>Range of $Kn$</th>
<th>Flow name</th>
<th>Mathematical description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$Kn &lt; 0.01$</td>
<td>Continuum regime</td>
<td>Navier-Stokes and energy equations</td>
</tr>
<tr>
<td>$0.01 &lt; Kn &lt; 0.1$</td>
<td>Slip regime</td>
<td>Navier-Stokes and energy equations with velocity slip and temperature jump boundary conditions</td>
</tr>
<tr>
<td>$0.1 &lt; Kn &lt; 10$</td>
<td>Transitional regime</td>
<td>Boltzmann equation</td>
</tr>
<tr>
<td>$Kn &gt; 10$</td>
<td>Free molecular regime</td>
<td>Collision-less Boltzmann equation</td>
</tr>
</tbody>
</table>

In the slip regime some discrete effects such as velocity slip and temperature jump manifest themselves at the boundaries of the flow, which cannot be observed in the continuum regime. However, the Navier-Stokes equations can still be utilized with adapted boundary conditions. At very high Knudsen numbers beyond 10 the collisions of the gas molecules with surfaces prevail and the reflected molecules travel across a large distance before colliding with other molecules. Hence the velocity distribution function of molecules in the oncoming flow is not affected by the presence of a body and can be assumed to correspond to the equilibrium Maxwell distribution. Consequently the calculation of energy and momentum transfer from the oncoming flow to the surface is straightforward in free molecular flow. In the transitional regime gas-surface interactions and collisions between gas molecules within the flow are of similar importance and the gas behavior is uniquely described by the Boltzmann equation (Shen 2005).

A comparison of tables 1-1 and 1-2 shows that in the pressure range of interest in the HITECO project the gas is likely to be in the transitional regime. Consequently the continuum assumption is not valid and a model on the molecular level is required in this thesis to analyze the behavior of the gas in the HITECO receiver. In the microscopic approach the discrete structure of the gas is considered as a large number of particles and information is provided on the position, velocity and state of the molecules at any time. The mathematical model is given by the Boltzmann equation, which is an integro-partial differential equation for the fraction of molecules in a given location and state. The density function is the only dependent variable, as the set of independent variables is extended by the physical variables defining the state of a molecule. In a monoatomic gas the state is fully determined by the three translational velocity components. For diatomic and polyatomic molecules with internal degrees of freedom additional variables are required to account for the rotational and vibrational energies. Thus for a monoatomic gas, a steady flow problem that is three-
dimensional in physical space becomes six-dimensional in phase space. For this reason and due to

the presence of an integral part – also referred to as collision integral – the Boltzmann equation
cannot be solved analytically in non-trivial cases. Furthermore the additional dimensions in phase
space cause overwhelming difficulties for conventional numerical procedures because a bounded
grid has to be specified in the velocity space. Therefore the application of CFD techniques to the
Boltzmann equation is restricted to simple geometries and monoatomic gases. However, the
discrete structure of the gas allows circumvention of these problems by simulating individual
molecules directly according to physical principles (Bird 1994).

Bird proposed the Direct Simulation Monte Carlo (DSMC) method, a probabilistic procedure for the
simulation of gas flows, and showed its consistency with the Boltzmann equation (Bird 1970). The
method is flexible compared to the underlying analytical model and facilitates the implementation
of complex physical effects, a property that is common to other Monte Carlo procedures such as the
ray tracing technique in radiation heat transfer. Additionally, in contrast to conventional CFD
techniques, direct physical simulations are immune to numerical instabilities. A drawback of DSMC
is that despite the enhancements in processing power and memory the method is still expensive in
terms of computer resources. The computation time is generally proportional to the number of
simulated molecules, which hinders the utilization of the method in the continuum regime. A wide
variety of problems has been successfully analyzed by means of DSMC simulations, ranging from the
formation of shock waves at re-entering spacecrafts to heat transfer in micro-electro-mechanical
systems (MEMS). However, the method has not been applied to parabolic trough receivers yet. (Bird
1994).

1.3 Objectives

The goal of this project is to study the behavior of the gas within the HITECO vacuum jacket by
means of the Direct Simulation Monte Carlo method. There is no commercial DSMC software and the
only freely available DSMC codes are those from G.A. Bird1, who invented the method, and those
included in the open source CFD toolbox OpenFOAM2. The DS2V/DS3V codes developed by Bird
(Bird 2005) for the simulation of two- and three-dimensional flows respectively have been
optimized for computational efficiency and allow for more sophisticated boundary conditions than

1 http://www.gab.com.au (1.11.2011)
2 http://www.openfoam.com (1.11.2011)
the DSMC solver. Therefore this project evaluates the applicability of the DS2V/DS3V programs before attempting to develop a new DSMC code.

Two-dimensional simulations for conductive heat transfer shall be performed from the free-molecular flow limit (0.01 Pa) up to the continuum regime (100 Pa). The errors of the continuum model (Roesle and Coskun 2011) are assessed over the entire transitional and slip flow regimes and convergence of the two models in the continuum limit is to be verified. In addition a general two-dimensional model of the HITECO receiver is developed that considers all three modes of heat transfer. This model is utilized for the prediction of surface temperatures, which serve as boundary conditions in the DSMC simulations, and for the estimation of total heat loss of the absorber. Furthermore three-dimensional axial flow simulations through a receiver tube segment are intended to simulate the situation when the vacuum pump is running. The obtained mass flow rates at a given pressure difference are again compared to CFD results.
2 THE DIRECT SIMULATION MONTE CARLO METHOD

The Direct Simulation Monte Carlo (DSMC) method enables gas flows to be modeled on a molecular level by simulating the motion of individual particles according to physical principles. In this chapter the main concepts of direct simulations are explained, the most important models for intermolecular collisions and gas-surface interactions utilized in DSMC procedures are described and finally the DS2V/DS3V programs will be tested for their applicability in this project.

2.1 Basic Concept

To initialize a DSMC calculation the flow domain needs to be divided into volume elements, like in conventional CFD. Then a large number of representative molecules are introduced into the domain according to some initial distribution. These molecules have the correct physical size and the term “representative” indicates that for reasons of computational feasibility one simulated molecule typically represents a very large number of real molecules. As the simulation is started the motion of each molecule is tracked (direct simulation). Periodically, random pairs of molecules within the same volume element are chosen for collisions (Monte Carlo simulation). The position coordinates, velocity components and internal energies of all simulated molecules are stored in the computer and modified with time. It is noted that these molecular quantities are exactly conserved in all the collisions and boundary interactions and hence the DSMC method satisfies the conservation of mass, momentum and energy within the range of round-off errors of the computer.

2.1.1 Discretization in time and space

The essential approximation made in DSMC simulations is that over a small time interval or step Δt the molecular motion is independent of intermolecular collisions. Accordingly, each molecule is
moved by its corresponding distance traveled in this time interval, taking interactions with flow boundaries into account. After the calculation of the molecular moves the time variable is advanced by one time step and an appropriate set of intermolecular collisions is selected. By alternating moving and colliding the flow develops from its initial state with time in a physically realistic manner. Usually a uniform flow is chosen as the initial state of the gas, which is specified by means of the macroscopic stream velocity and two state variables, e.g. number density and temperature. Accordingly, neither an initial estimate of the flow field nor any kind of iteration is needed. All simulations are unsteady in the sense that they employ a time parameter which may be identified with physical time in the real flow. However, if the boundary conditions allow for the formation of a steady flow, the steady state may be attained as an average of the unsteady flow over time. The uncoupling of molecular motion and intermolecular collisions is valid as long as the time step is small compared to the local mean collision time, and if this condition is met the results are independent of its actual value (Bird 1994).

The grid in physical space is utilized for the appropriate choice of collision partners within each volume element and to sample macroscopic flow properties. The more molecules are employed in a simulation, the finer is the grid and the shorter gets the separation distance between colliding molecules. This leads to a more accurate representation of the real flow behavior and thus improves the quality of the calculation. However, as the computation time of DSMC routines is generally proportional to the number of simulated molecules, this is at the cost of higher computational efforts. This tradeoff gains importance at low Knudsen numbers and shorter mean free paths e.g. in the continuum regime. Bird (2005) proposed the ratio of the mean collision separation (MCS) to the mean free path (MFP) as the most important quality criterion for DSMC simulations and recommended an upper limit of

$$\frac{MCS}{MFP} < 0.2,$$

as higher values would cause distortions of the results. Advantage may be taken of flow symmetries that reduce the number of dimensions of a problem. The cell grid is simply required in the spatial directions with varying flow properties and the mean collision separation is measured in these dimensions only. Consequently the number of molecules needed and also the number of position coordinates that have to be stored can be reduced in such a simulation, while the flow domain itself and the collisions are still three-dimensional (Bird 1994).
2.1.2 Area of applicability

The procedures for the probabilistic choice of appropriate collisions are based directly on relations from classical kinetic theory. Therefore the DSMC method is subject to the same limitations as the Boltzmann equation. The principal requirements for its applicability are a dilute gas and molecular chaos. The general definition of a dilute gas is given by

\[ \delta \gg d, \]  

where \( \delta = n^{-1/3} \) is the mean molecular spacing and \( d \) the diameter of the molecules. In such a gas the fraction of volume that is occupied by the gas molecules is very small and the motion of each molecule is unaffected by other molecules for the most part. In addition, if there is a collision between molecules, it is overwhelmingly probable that only two molecules are involved, so binary collisions need to be considered only. The assumption of molecular chaos basically requires that the molecules move independently of each other and that thus the probability of finding two molecules in a certain two particle configuration is simply the product of the probabilities of finding each molecule in its corresponding one particle configuration. Consequently the DSMC method cannot be applied to dense gases or to plasmas with a high portion of ionized particles that are affected by long-range interactions. In addition the DSMC method utilizes models of gas molecules and boundary interactions developed in kinetic theory, which provide only an approximation to real physics. An important difference to the Boltzmann equation is that the DSMC method does not rely on inverse collisions. Furthermore the boundary conditions in direct simulations are defined by the behavior of individual molecules rather than by means of a distribution function. This enables the incorporation of complex flow phenomena such as chemical reactions, which cannot be considered in the analytical model (Bird 1994).

2.1.3 Sampling of macroscopic properties

The DSMC method provides information on the position, velocity and state of every molecule at all times, which enables the sampling of macroscopic flow properties such as density, pressure and temperature at any location in the flow. Accordingly, the simulation results can be expressed in terms of quantities that are well known from continuum analyses. The relations between microscopic and macroscopic quantities may be found in any book on kinetic theory and are not recapitulated here. For more information the reader is referred to (Bird 1994; Shen 2005). In this
subsection some general issues related to the calculation of macroscopic properties from molecular quantities are illustrated and two averaging techniques are introduced.

Macroscopic quantities are associated with a spatial location in the flow and have to be based on the state of the molecules in a small volume element enclosing this particular point. In a volume element $V$ with number density $n$ there are $N_r$ real molecules and this number follows a Poisson distribution about the mean value $nV$ with standard deviation $\sqrt{nV}$,

$$P(N_r) = \frac{(nV)^{N_r}}{N_r!} e^{-(nV)}.$$ \hfill (2.3)

A normalized measure of dispersion in statistics is the coefficient of variation, which is defined as the ratio of the standard deviation to the mean value,

$$CV(N_r) = \frac{\sqrt{\text{Var}(N_r)}}{E(N_r)} = \frac{1}{\sqrt{nV}}.$$ \hfill (2.4)

The number of simulated molecules within the same volume $V$ is denoted by $N$ and is Poisson-distributed with mean value and variance equal to $nV/F_N$,

$$P(N) = \frac{(nV/F_N)^N}{N!} e^{-(nV/F_N)},$$ \hfill (2.5)

where $F_N$ is the number of real molecules represented by each simulated molecule. Its variation coefficient is given by

$$CV(N) = \frac{F_N}{\sqrt{nV}}.$$ \hfill (2.6)

From equations (2.4) and (2.6) it is seen that the statistical fluctuations in real gases are amplified by the factor $\sqrt{F_N}$ in DSMC simulations, and as $F_N$ can easily be in a range of $10^{10}$ to $10^{12}$, this effect is significant. Using the definition of the mean molecular spacing $n\delta$ can be written as $V/\delta^3$. Consequently, in order to limit the level of scatter to a reasonable level, the linear dimensions of the cell, over which the instantaneous macroscopic properties are sampled, should satisfy the condition

$$V^{1/3} \gg F_N^{1/3} \delta.$$ \hfill (2.7)

In addition the linear dimensions of the volume element in every spatial direction should be small compared the local scale length of the macroscopic gradients in the gas in that particular direction, to ensure a good resolution of the flow. In practical applications of the DSMC method this is usually not possible without violating the scattering condition stated above. However, equation (2.7) needs
to be met only for *instantaneous averages* and can thus be mitigated by alternative averaging techniques.

The first one is called *time average* and is established by summing the properties of the molecules in the volume element over a certain time interval. This enables any steady flow to be described in terms of macroscopic quantities. The second average is built from the instantaneous averages over the molecules in the corresponding volume element in a large number of similar systems. By means of this so-called *ensemble average* the macroscopic quantities of an unsteady flow may be established by repeating the experiment for many times. Time and ensemble averages can be used to establish macroscopic quantities of practically any flow. However, both techniques are stochastic and thus subject to fluctuations. The standard deviation is inversely proportional to the square root of the sample size and may thus be reduced to any desired level by increasing the sampling interval for time averaging or the number of repetitions for ensemble averaging respectively. The accomplishment of a certain accuracy of the results is sometimes referred to as convergence, which is not to be confused with the convergence of conventional CFD procedures from an initial approximation to the exact solution (Bird 1994).

### 2.1.4 Sampling of collisions

The proper implementation of the collision sampling, i.e. the appropriate choice of collision pairs and the realization of the correct number of collisions, is crucial to the consistency of the simulation with the physical flow processes. Considered is a cell of volume $V_c$ and number density $n$. This cell contains $nV_c$ real molecules and the average number of simulated molecules is given by $\bar{N} = nV_c/F_N$. The actual number of simulated molecules is denoted by $N$, which is a stochastic variable. According to kinetic theory the total number of collisions $N_T$ in a time step $\Delta t$ within this cell may then be calculated by means of equation (1.5),

$$
N_T = \frac{1}{2} N \nu \Delta t = \frac{1}{2} N n \bar{\sigma}_r \bar{c}_r \Delta t.
$$

Various procedures for the random sampling of collisions within a cell have been developed over the years and here only the most efficient and widely used technique is briefly described, namely the no time counter (NTC) method proposed by Bird.
No time counter method

The probability of collision between two particular simulated molecules in time interval $\Delta t$ can be calculated as the ratio of the volume swept out by their total cross section $F_N\sigma_T$ at relative speed $c_r$ to the cell volume,

$$P = \frac{F_N\sigma_T c_r \Delta t}{V_c}. \quad (2.9)$$

One sampling possibility is to compute this value for all $N(N - 1)/2$ potential collision pairs and to select each collision with its corresponding probability of occurrence. However, the efficiency of this so-called direct method is low, because $P$ is usually very small and the computation time is proportional to the square of the number of molecules in the cell. Therefore the NTC method considers only a fraction of all possible collision pairs and their probability is increased by dividing equation (2.9) by this fraction. In order to achieve maximum efficiency the fraction is chosen such that the maximum probability equals unity, i.e. the fraction is given by

$$P_{\text{max}} = \frac{F_N(\sigma_T c_r)_{\text{max}} \Delta t}{V_c}. \quad (2.10)$$

Initially the maximum product of collision cross-section and relative speed $(\sigma_T c_r)_{\text{max}}$ can be chosen sufficiently large and is then altered as higher values are encountered during the simulation. The number of collision pairs considered per time step is obtained by multiplication of (2.10) by $N(N - 1)/2$. However, as $N$ is subject to statistical fluctuations it is recommended to replace $N(N - 1)$ by the product of the instantaneous value and a time or ensemble averaged value $N \bar{N}$. Accordingly the number of molecule pairs considered for collision per time step in the NTC method is equal to

$$\frac{1}{2} N \bar{N} F_N(\sigma_T c_r)_{\text{max}} \Delta t \quad (2.11)$$

and the collision is selected with probability

$$P = \frac{\sigma_T c_r}{(\sigma_T c_r)_{\text{max}}}. \quad (2.12)$$

The number of collisions that are realized per time step is not affected by the exact value of $P_{\text{max}}$ and amounts to

$$N_{T,\text{NTC}} = \frac{1}{2} \frac{N \bar{N} F_N \sigma_T c_r \Delta t}{V_c} = \frac{1}{2} N n \bar{\sigma_T} c_r \Delta t. \quad (2.13)$$
This number is in agreement with the theoretical value of equation (2.8) and it is seen that the procedure yields a computation time that is linear in \( N \) (Bird 1994).

### 2.2 Binary elastic collisions and molecular models

As mentioned in the beginning of this chapter, the probability of occurrence of ternary and higher-particle collisions in a dilute gas is so small that they can be neglected and only binary collisions need to be considered in DSMC routines. The objective of this section is to calculate the post-collision velocities \( c_1' \) and \( c_2' \) of two molecules with masses \( m_1 \) and \( m_2 \) from their initial velocities \( c_1 \) and \( c_2 \) before the collision. It will be seen that assumptions about the behavior of molecules are required to completely determine these velocities and the molecular models that are relevant to this thesis will be introduced.

#### 2.2.1 Conservation of momentum and energy

The conservation equations of energy and momentum constitute the starting point of the analysis. The term “elastic” indicates that no energy is exchanged between translational and internal modes. Hence the conservation of linear momentum

\[
m_1 c_1 + m_2 c_2 = m_1 c_1' + m_2 c_2' = (m_1 + m_2) c_m
\]

and energy

\[
m_1 c_1'^2 + m_2 c_2'^2 = m_1 c_1^2 + m_2 c_2^2
\]

must be satisfied in the collision. Here \( c_m \) denotes the velocity of the center of mass of the molecule pair. This velocity remains constant in the collision and can be calculated from the pre-collision velocities according to

\[
c_m = \frac{m_1 c_1 + m_2 c_2}{m_1 + m_2}
\]

The relative velocities between the molecules before and after the collision are defined by
The Direct Simulation Monte Carlo method

\[ c_r = c_1 - c_2, \]
\[ c_r^* = c_1^* - c_2^*. \]  \hfill (2.17)

Using these definitions the pre- and post-collision velocities can be written as

\[ c_1 = c_m + \frac{m_2}{m_1 + m_2} c_r \]
\[ c_2 = c_m - \frac{m_1}{m_1 + m_2} c_r \]  \hfill (2.18)

\[ c_1^* = c_m + \frac{m_2}{m_1 + m_2} c_r^* \]
\[ c_2^* = c_m - \frac{m_1}{m_1 + m_2} c_r^* \]  \hfill (2.19)

Consequently the three-dimensional trajectories can be reduced to two-dimensions by a coordinate transformation into a reference frame moving with velocity \( c_m \). The conservation of angular momentum requires that the projected distance \( b \) between the trajectories is not affected by the collision (cf. figure 2-1).

![Figure 2-1: Binary collision in the center of mass frame of reference (Bird 1994).](image)

The reduced mass \( m_r \) is given by

\[ m_r = \frac{m_1 m_2}{m_1 + m_2} \]  \hfill (2.20)
and due to the conservation of total kinetic energy in the collision the magnitude of the relative velocity stays constant, i.e.

\[ c_r' = c_r. \quad (2.21) \]

Hence the problem of determining the post-collision velocities is reduced to finding the directional change \( \chi \) of the relative velocity vector. The conservation of energy and momentum delivers four scalar equations for six unknowns and hence further relations are required to completely determine a binary collision. Commonly two so-called impact parameters are chosen, which are described below. In addition the angle of deflection \( \chi \) needs to be specified (Bird 1994).

### 2.2.2 Impact parameters and collision cross-section

The two impact parameters are the distance of the closest approach \( b \) of the undisturbed trajectories in the center of mass frame of reference (also referred to as miss distance) and the angle \( \varepsilon \) between the collision plane in which these trajectories lie and some reference plane (cf. figure 2-2).

![Figure 2-2: Impact parameters and collision cross-section (Bird 1994).](image)

The differential cross-section \( \sigma d\Omega \) specified by the two impact parameters \( b \) and \( \varepsilon \) in the plane normal to \( c_r \) may be defined as
2. The Direct Simulation Monte Carlo method

\[ \sigma d\Omega = b b d \varepsilon, \]  

where \( d\Omega = \sin \chi d\chi d\varepsilon \) is the unit solid angle about the post-collision relative velocity vector \( \mathbf{c}^r \). The total collision cross-section is then defined as the integral of the differential area over all solid angles, i.e.

\[ \sigma_T = \int_0^{4\pi} \sigma d\Omega = 2\pi \int_0^\pi \sigma \sin \chi d\chi. \]  

This is a key quantity in DSMC procedures because it is utilized in equation (2.13) to establish the correct collision rate. The impact parameters \( b \) and \( \varepsilon \) are then sampled from uniformly distributed random numbers \( R_b \) and \( R_\varepsilon \) between 0 and 1 according to

\[ R_b = \frac{\pi b^2}{\sigma_T}, R_\varepsilon = \frac{\varepsilon}{2\pi}. \]  

The last quantity needed to calculate the post-collision velocities is the deflection angle \( \chi \), which is determined by the definition of a molecular model (Bird 1994; Shen 2005).

2.2.3 Requirement of molecular models for DSMC simulations

From a computational point of view it is required that the utilized molecular model provides a well-defined total collision cross-section because otherwise the collision rate cannot be determined properly by the DSMC procedure. Experience has also shown that for an accurate representation of the real gas behavior it is crucial that the model reproduces the correct coefficient of viscosity and also its temperature dependence. The exact solutions for the coefficients of viscosity, conductivity and diffusion of a monoatomic gas are provided by the Chapman-Enskog theory. In literature, usually their first approximation is utilized, which involves a single term of the Sonine polynomial series. The corresponding expressions for the dynamic viscosity, the thermal conductivity and the diffusion coefficient are stated in (Bird 1994).

Realistic molecular models in kinetic theory are usually defined by an intermolecular force or potential. A frequently used model neglecting the attractive part of the intermolecular potential is the inverse power law model, whose force is given by

\[ F = \frac{\kappa}{r^n}. \]  

18
Here \( r \) is the distance between the molecules and \( \kappa \) and \( \eta \) are two model parameters which may be utilized for the specification of realistic gas properties. However, it can be seen from equation (2.25) that for any finite value of \( \eta \) the extension of the force field is infinite and hence the integral for the total collision cross-section in equation (2.23) diverges, a problem that is common to other classical models. Accordingly, a finite cut-off of the deflection angle \( \chi \) or alternatively of the miss distance \( b \) is utilized in practical applications. However, as this truncation is arbitrary, the resulting total collision cross-section is not suitable for the calculation of the collision rate in DSMC simulations. For this reason, phenomenological models were developed that retain the essential properties of gas molecules while showing a finite total collisional cross-section.

The simplest approach is to treat the molecules as perfectly elastic, rigid spheres. This so-called hard sphere (HS) model was already used in the introduction of this thesis to calculate the molecular mean free path of gas molecules in equilibrium. It may be regarded as a special case of the inverse power law model with \( \eta = \infty \). A collision of two hard sphere molecules with diameters \( d_1 \) and \( d_2 \) is shown schematically in figure 2-3.

Define the mean diameter of the molecule pair

\[
d_{12} = (d_1 + d_2)/2,
\]

the miss distance and the angle of deflection can be related to each other by

\[
\theta_A + \theta_A' = \chi
\]

\[
b = \frac{d_{12}}{2} \sin \left( \frac{\chi}{2} \right)
\]

\[
\sin \theta_A = \frac{d_{12}}{2b} \sin \chi
\]

\[
\cos \theta_A = \frac{d_{12}}{2b} \cos \chi
\]

\[
\theta_A' = \theta_A + \frac{\pi}{2}
\]

\[
\sin \theta_A' = \frac{d_{12}}{2b} \sin \chi
\]

\[
\cos \theta_A' = \frac{d_{12}}{2b} \cos \chi
\]

Figure 2-3: Angle of deflection in a binary collision of rigid spheres (Bird 1994).
The Direct Simulation Monte Carlo method

\[
\frac{b}{a_{12}} = \cos \left( \frac{X}{2} \right). \tag{2.27}
\]

The total collision cross-section of a HS molecule is found to be

\[
\sigma_T = \pi d_{12}^2, \tag{2.28}
\]

and the viscosity coefficient of a hard sphere gas is given by the theory of Chapman and Enskog,

\[
\mu = \frac{5}{16} \frac{1}{\sigma_T} \sqrt{\frac{m k T}{\pi}}. \tag{2.29}
\]

The diameter of HS molecules is usually chosen such that expression (2.29) produces realistic viscosity coefficients. If a real gas shows a viscosity \( \mu_{ref} \) at a reference temperature \( T_{ref} \), the HS diameter may be determined by

\[
d = \left( \frac{5}{16} \frac{1}{\mu_{ref}} \sqrt{\frac{m k T_{ref}}{\pi}} \right)^{\frac{1}{5}}. \tag{2.30}
\]

The HS model provides a coefficient of viscosity that is proportional to the square root of temperature. However, real gases usually show a viscosity-temperature power law of the form

\[
\mu \propto T^\omega, \tag{2.31}
\]

where the exponent \( \omega \) typically lies in a range near 0.75. Therefore the hard sphere model is generally not a good approximation to a real gas. Temperature exponents \( \omega \) and reference viscosities \( \mu_{ref} \) of various gases are found in (Bird 1994).

### 2.2.4 The variable hard sphere model

The variable hard sphere (VHS) model developed by Bird is based on the observation that the effective collision cross-section of real molecules decreases with increasing relative speed between the molecules. Analytical and numerical studies of gas flows revealed that this behavior strongly affects the results, whereas the force field and the resulting scattering distribution have a minor impact. Accordingly the VHS model is usually defined by an inverse power law

\[
d = d_{ref} \left( \frac{c_{ref}}{c_r} \right)^\xi, \tag{2.32}
\]
where \( d_{\text{ref}} \) corresponds to the effective diameter at relative speed \( c_{r,\text{ref}} \) and \( \xi \) is the VHS parameter, while the angle of deflection is still given by the isotropic scattering law of the HS model, i.e.

\[ \chi = 2 \cos^{-1} \left( \frac{b}{d} \right). \]  

(2.33)

The total collision cross-section of such a molecule is still given by equation (2.28), i.e. \( \sigma_T = \pi d^2 \).

For the coefficient of viscosity of a VHS gas the Chapman-Enskog theory yields

\[ \mu = \frac{15 \sqrt{\pi mk (4kT_{\text{ref}})^{\xi} T_{\text{ref}}^{1+\xi}}} {8 \Gamma(4-\xi) \sigma_{T,\text{ref}} c_{r,\text{ref}}^{2\xi}} \]  

(2.34)

Thus \( \mu \propto T_{\text{ref}}^{1+\xi} \) and for a gas with viscosity \( \mu_{\text{ref}} \) at reference temperature \( T_{\text{ref}} \) and obeying equation (2.31), the VHS model establishes the correct coefficient of viscosity by setting

\[ \xi = \omega - \frac{1}{2} \]  

(2.35)

and calculating the effective diameter as a function of the relative kinetic energy \( E_{t} = \frac{1}{2} m_r c_r^2 = \frac{1}{4} m c_r^2 \) in the collision, i.e.

\[ d = \frac{15 \sqrt{\pi m/(kT_{\text{ref}})^{\xi+1/2}}} {8 \Gamma(4-\xi) \mu_{\text{ref}} E_{t}^{\xi}} \]  

(2.36)

It is recommended to use this diameter to set the total collision cross-section of VHS molecules (Bird 1994; Shen 2005).

In a gas mixture composed of species 1 and 2 the diameter is calculated separately for each molecule and the effective diameter of the cross-collision may be obtained by equation (2.26). However, it might be more appropriate to determine the total cross-section of collisions between different molecules by means of the diffusion coefficient \( D_{12} \),

\[ D_{12} = \frac{3 \sqrt{\pi} (\frac{2kT}{m_r})^{1+\xi_{12}}} {8 \Gamma(3-\xi_{12}) n \sigma_{T,\text{ref},12} c_{r,\text{ref}}^{2\xi_{12}}}. \]  

(2.37)

The VHS parameter \( \xi_{12} \) can be determined directly by equation (2.35), if values are available for the exponent \( \omega_{12} \) of the gas mixture, or alternatively set as the mean of the individual parameters. For a
binary gas mixture with diffusion coefficient $D_{12,\text{ref}}$ at reference temperature $T_{\text{ref}}$ the cross-collisional diameter may be obtained again as a function of the relative translational energy,

$$d_{12} = \sqrt{\frac{3}{8} \frac{(2kT)^{\frac{1}{2}+\xi_{12}}}{\Gamma(3 - \xi_{12})} \sqrt{\pi m_n D_{12,\text{ref}} (2E_t)^{\xi_{12}}}}$$  \hspace{1cm} (2.38)

As there is, in general, a difference between the mean of the viscosity based diameters and the cross-collision diameter defined by the diffusion coefficient, the ability of the VHS model to reproduce the correct transport properties in a gas mixture might be limited (Bird 1994).

2.2.5 The variable soft sphere model

For this reason Koura and Matsumoto introduced the variable soft sphere (VSS) model. While the dependence of the variable soft sphere diameter with relative speed is equivalent to relation (2.32) for the VHS model, the deflection angle is modified to

$$\chi = 2 \cos^{-1} \left( \left( \frac{b}{d} \right)^{1/\alpha} \right).$$  \hspace{1cm} (2.39)

Here $\alpha$ is the VSS scattering parameter. The total collision cross section of a variable soft sphere molecule is again given by $\sigma_t = \pi d^2$. This leads to the following expression for the viscosity of a VSS gas,

$$\mu = \frac{5}{16} \frac{(\alpha + 1)(\alpha + 2) \sqrt{\pi mk (\frac{4k}{m})^\xi} T^{\frac{1}{2}+\xi}}{a\Gamma(4 - \xi) \sigma_t \sigma_{T,\text{ref}} c_{r,\text{ref}}^{2\xi}}.$$  \hspace{1cm} (2.40)

Like in a variable hard sphere gas, the coefficient of viscosity is proportional to $T^{\frac{1}{2}+\xi}$ and the parameter $\xi$ is chosen as in the VHS case. Similarly, the diffusion coefficient in a VSS gas mixture is given by

$$D_{12} = \frac{3}{16} \frac{(\alpha_{12} + 1) \sqrt{\pi} \left( \frac{2kT}{m_n} \right)^{\frac{1}{2}+\xi_{12}}}{\Gamma(3 - \xi_{12}) \sigma_{T,\text{ref},12} c_{r,\text{ref}}^{2\xi_{12}}}.$$  \hspace{1cm} (2.41)

For a simple gas with viscosity $\mu_{\text{ref}}$ and self-diffusion coefficient $D_{11,\text{ref}}$ at reference temperature $T_{\text{ref}}$ the effective diameters $d$ and $d_{11}$ based on viscosity and diffusion are given by
2. The Direct Simulation Monte Carlo method

\[ d = \frac{5}{16} \frac{(\alpha + 1)(\alpha + 2)^{1/2}}{a \Gamma(4 - \xi) \mu_{ref} E_t^{\xi}} \sum_{i=1}^{\xi+1/2} \frac{m}{\pi(kT_{ref})} \]  

(2.42)

and

\[ d_{11} = \frac{3}{8} \frac{(\alpha + 1)^{1/2}}{\Gamma(3 - \xi) \sqrt{m\pi nD_{11,ref} E_t^{\xi}}} \]  

(2.43)

respectively, and by requiring equality for the two diameters \( \alpha \) may be determined by

\[ \alpha = \frac{10 \rho D_{11,ref}}{6(3 - \xi) \mu_{ref} - 5 \rho D_{11,ref}}. \]  

(2.44)

Consequently the VSS model reflects diffusion processes in gas mixtures more precisely than the VHS model and is thus favorable for the analysis of diffusion phenomena. A limitation of the model is that constant values for \( \alpha \) are generally only valid in a certain temperature range. Typical values for the VSS scattering parameter \( \alpha \) of various gases at 0 °C are given in (Bird 1994).

It is noted that the VHS and VSS models both approximate the realistic inverse power law model, i.e. they neglect the attractive potential at large intermolecular distances and show a finite total collision cross-section. A popular model in kinetic theory including the attractive component is the Lennard-Jones potential, and similarly the generalized hard sphere (GHS) and the generalized soft sphere (GSS) models were developed to consider this effect in DSMC simulations. More information on these models is available in (Bird 1994; Shen 2005). As the gas in the HITECO receiver will never reach temperatures far below standard conditions, the attractive force is neglected in this thesis and the VHS and VSS models are used to simulate the gas behavior in the vacuum jacket.

2.3 Inelastic collisions and rotational relaxation

Besides the three translational velocity components diatomic and polyatomic molecules have rotational and vibrational degrees of freedom, which are also referred to as internal modes. If two molecules are involved in an inelastic collision, energy is exchanged between the different modes and in this section it is explained briefly how this effect is included in DSMC procedures.
2.3.1 Internal degrees of freedom

The characteristic temperatures of rotation $\Theta_r$ and vibration $\Theta_v$ indicate the point at which the corresponding degrees of freedom are excited. Typical values for the dominating diatomic species in air, i.e. nitrogen and oxygen, are summarized in Table 2-1.

Table 2-1: Characteristic temperatures of rotation and vibration for nitrogen and oxygen (Bird 1994).

<table>
<thead>
<tr>
<th>Gas</th>
<th>Rotation $\Theta_r$ [K]</th>
<th>Vibration $\Theta_v$ [K]</th>
</tr>
</thead>
<tbody>
<tr>
<td>$N_2$</td>
<td>2.88</td>
<td>3'371</td>
</tr>
<tr>
<td>$O_2$</td>
<td>2.07</td>
<td>2'256</td>
</tr>
</tbody>
</table>

Apparently, at ambient temperature (300 K) the rotational degrees of freedom may be assumed to be fully excited while the vibrational modes are mostly inactive. Recalling the target of the HITECO project to raise the temperature of the heat transfer fluid to 600 °C (873 K) and taking this value as an upper limit to the gas temperature inside the annulus, it may be concluded that it is sufficient to consider rotational excitation while vibrational effects may be neglected. Accordingly, only rotational degrees of freedom are further discussed in this section.

Basically energy can only be stored in the rotation about an axis with high moment of inertia. Hence diatomic molecules generally have two rotational degrees of freedom because there is no rotation about the internuclear axis. Similar to the problem of elastic collisions, phenomenological models are used in DSMC routines to simulate the energy exchange between rotational and translational modes, as the classical polyatomic models from kinetic theory, such as the two centers of repulsion model, are impractical if millions of collisions have to be calculated. The most widely used phenomenological model is that of Larsen and Borgnakke, which is briefly described below (Bird 1994).

2.3.2 The Larsen-Borgnakke model

The Larsen-Borgnakke model reallocates the total energy in an inelastic collision between the translational and internal degrees of freedom by sampling from the equilibrium distributions of these modes corresponding to the total energy. The appropriate relaxation time, i.e. the time
2. The Direct Simulation Monte Carlo method

required by a molecule to accomplish equilibrium between translational and internal energies, is established by regarding only a fraction \( \Lambda \) of collisions as inelastic. The other collisions are treated as completely elastic and are calculated according to the underlying monoatomic model. This approach has proved to reproduce a realistic relaxation behavior. The implementation of the Larsen-Borgnakke model in DSMC simulations is described in detail in (Bird 1994).

### 2.3.3 Rotational relaxation

A gas with collision rate \( \nu \) is considered in which the rotational temperature \( T_r \) of a particular molecule differs from the overall temperature of the gas. Applying the Larsen-Borgnakke method to a fraction \( \Lambda \) of the collisions leads to a relaxation process that may be characterized by

\[
\frac{dT_r}{dt} = \nu \Lambda (T_e - T_r),
\]

where \( T_e \) is the final equilibrium temperature in the gas. Integration yields

\[
T_r = T_e - (T_e - T_{r,0})e^{-\nu \Lambda t},
\]

where \( T_{r,0} \) is the initial rotational temperature at zero time and both \( \nu \) and \( \Lambda \) are generally a function of temperature. The time in which a disturbance from equilibrium decreases by a factor of \( 1/e \) is defined as the relaxation time \( \tau \), and obviously (Bird 1994)

\[
\tau = \frac{1}{\nu \Lambda},
\]

The difficulty in DSMC simulations consists of specifying an appropriate value \( \Lambda \) for the fraction of inelastic collisions such that the correct relaxation rate is achieved. Some data is available in literature on the rotational relaxation collision number \( Z_r \), which may be regarded as the average number of collisions required to establish equilibrium. An approximate relation between \( Z_r \) and \( \Lambda \) is given by the simple formula

\[
Z_r = \frac{1}{\Lambda},
\]

Haas et al. (1994) recommended the utilization of a more accurate result,
2. The Direct Simulation Monte Carlo method

\[ Z_r = \frac{3\zeta_r(5 - 2\omega + \zeta_r)}{(3 + \zeta_r)(5/2 - \omega)(5/2 - \omega + \zeta_r)\left(1 - \left(1 - \frac{\zeta_r\Lambda}{5/2 - \omega + \zeta_r}\right)^{2}\right)} \]  

(2.49)

where \( \zeta_r \) is the number of rotational degrees of freedom. Parker (1959) calculated the rotational and vibrational relaxation collision numbers for some gases composed of diatomic molecules. For the rotational relaxation collision number he obtained the expression

\[ Z_r = \frac{Z_r^{\infty}}{1 + \frac{\pi^{3/2}}{2} \left(\frac{T^*}{T}\right)^{1/2} + \left(\frac{\pi^2}{4} + \pi\right) \left(\frac{T^*}{T}\right)} \]  

(2.50)

and for \( Z_r^{\infty} \) and \( T^* \) he proposed the following values for oxygen and nitrogen.

<table>
<thead>
<tr>
<th>Gas</th>
<th>( Z_r^{\infty} )</th>
<th>( T^* )</th>
</tr>
</thead>
<tbody>
<tr>
<td>N(_2)</td>
<td>15.7 collisions</td>
<td>80 K</td>
</tr>
<tr>
<td>O(_2)</td>
<td>14.4 collisions</td>
<td>90 K</td>
</tr>
</tbody>
</table>

The values stated by Parker may be regarded as appropriate for hard sphere molecules and an overview of generalizations to other molecular models may be found in (Wysong and Wadsworth 1998). Hash et al. (1994) proposed an extension to the variable hard sphere model,

\[ Z_r = \frac{Z_r^{\infty}}{1 + \frac{4\pi}{3} \frac{\Gamma(3 - \omega)}{\Gamma(3/2 - \omega)} \left(\frac{T^*}{T}\right)^{1/2} + \frac{2(\pi^2/4 + 2)}{5/2 - \omega} \left(\frac{T^*}{T}\right)} \]  

(2.51)

where \( \Gamma \) is the gamma function. A generalization to the variable soft sphere model was presented by Koura (1996),

\[ Z_r = \frac{m}{2m_r}Z_r^{\infty} \frac{\Gamma(1 + \alpha)}{\Gamma(3/2 + \alpha)} \frac{\Gamma(1 + \alpha)}{\Gamma(5/2 - \omega)} \left(\frac{T^*}{T}\right)^{1/2} + \left(\frac{\pi^2}{4} + 2\right) \left(\frac{T^*}{T}\right) \]  

(2.52)

which also considers collisions between different types of molecules. It is noted that the letter \( \omega \) represents the exponent in the viscosity-temperature power law throughout this text. In literature sometimes also the VHS parameter \( \xi = \omega - 1/2 \) is denoted by \( \omega \), and hence the formulae above may appear differently in different sources.
2.4 Surface interactions

Maxwell proposed two fundamental models for the interaction of a stationary gas with surfaces in equilibrium, namely diffuse reflection and specular reflection. In specular reflection the velocity component normal to the surface is reversed while the tangential velocity remains unchanged. Thus a specular reflecting boundary is perfectly elastic and acts as a plane of symmetry. In diffuse reflection the post-reflection velocities of the molecules are independent of the velocities before the surface interaction, and they are distributed according to the half-space equilibrium or Maxwell distribution. For equilibrium diffuse reflection the temperature corresponding to the Maxwell distribution of the reflected molecules and the surface temperature need to be equal to the gas temperature. However, in practical applications the gas molecules generally have a stream velocity relative to the surface that is not zero and thus the gas near the surface is not in equilibrium. A useful generalization of the equilibrium diffuse reflection model is obtained by considering different temperatures for the incident molecules $T_i$ and the wall $T_w$ and allowing exchange of energy such that the temperature of the Maxwell distribution of the reflected molecules $T_r$ is equal to the wall temperature $T_w$. In the following this gas-surface interaction model is referred to as completely diffuse reflection with full accommodation to the surface temperature (Bird 1994).

In real flows the extent, to which the reflected molecules have adapted their temperature to that of the surface, may be measured by the thermal accommodation coefficient

$$a_c = \frac{q_i'' - q_r''}{q_i'' - q_w''}$$  \hspace{1cm} (2.53)

Here $q_i''$ and $q_r''$ are the incident and reflected energy fluxes respectively, and $q_w''$ is the hypothetic energy flux that would leave the surface by diffuse reflection and complete adaption of the molecules to the wall ($T_r = T_w$). Similarly the accommodation coefficients of normal and tangential momentum could be defined.

The simplest approach to modeling partial accommodation effects is to consider a fraction $\alpha_d$ of the molecules to be reflected diffusely and specular reflection for the other molecules. A more elaborate phenomenological model for incomplete accommodation was developed by Cercignani, Lampis and Lord and is explained in detail in (Shen 2005). The CLL model includes separate accommodation coefficients for the normal energy and tangential momentum and is therefore superior to diffuse-specular reflection.
Experiments with gases in contact with surfaces showed that the reflection behavior is well approximated by the diffuse reflection model with complete thermal accommodation for the majority of practical flow problems. Therefore, this boundary condition is used most frequently in numerical studies. However, in certain cases the thermal accommodation can be significantly lower than unity and Bird (1994) mentions three conditions under which the assumption of full adaption to the wall temperature needs to be carefully validated:

- Smooth metal surface that has been outgassed by exposure to high vacuum;
- Small ratio of the molecular weight of the gas to that of the surface molecules;
- Very high translational energy of the gas molecules relative to the surface.

As none of these issues clearly applies to the vacuum chamber of the HITECO receiver diffuse reflection with full accommodation to the surface temperature is employed in all the calculations in this project. For polyatomic molecules additional coefficients for the accommodation of internal modes need to be specified. In this thesis only rotation is considered and the corresponding accommodation coefficient is set to unity. Hence the velocity and rotational energy of the reflected molecules are both sampled from their equilibrium distribution at the surface temperature.

### 2.5 The DS2V/DS3V programs

The DS2V/DS3V programs developed by Bird are very general DSMC codes that have been optimized for computational efficiency over several years. In this section some features are highlighted and the applicability of the programs to the HITECO receiver is evaluated.

#### 2.5.1 Nearest-neighbor collisions

As mentioned in section 2.1, short separation distances between colliding molecules lead to a more realistic representation of the collisions occurring in a real gas, which results in more accurate simulations. In the following two procedures are described that aim at reducing the mean collision separation between molecules at the lowest possible computational cost.
Transient-adaptive subcells

Instead of selecting collision pairs randomly from within a cell by means of a collision sampling technique such as the NTC method, the cell is divided into subcells and collision partners are chosen from the same or neighboring subcells. Using a fine grid of subcells such that maximally two molecules are located within the same subcell and applying a search algorithm in neighboring subcells leads to a preferred selection of nearest neighbors for collision, thus reducing the mean collision separation to the minimum for the given number of simulated molecules. The microscopic quantities required by the collision routine, e.g. the collision rate, are still collected from the whole cell which reduces statistical noise and saves memory. In addition the transient-adaptive subcell technique considers the subcell structure only during the collision phase. If a cell is considered for collisions, it is temporarily subdivided and the molecule simulators are allocated to the corresponding subcells. After the collisions have been performed the information about the molecule indexing is discarded again. This causes minimum memory cost because the grid of subcells is only considered for a single cell at the time. The transient-adaptive subcell technique aims at a single molecule per subcell and was originally implemented in Bird's DS2 program (Bird, Gallis et al. 2009).

Virtual subcells

The idea of the virtual subcell technique is to sort all $N$ molecules within a cell and to select for every molecule its nearest neighbor as collision partner. This is an $N^2$ operation and was initially considered infeasible to be utilized in DSMC procedures. However, its implementation in the DS2V/DS3V programs showed that virtual subcells are computationally faster than transient-adaptive subcells if the number of molecules per cell is less than 35. An issue related to nearest neighbor selection evolves if multiple collisions take place within a cell in a single time step and one molecule involved in a preceding collision is chosen again as the first molecule. As no moving sequence has taken place the other molecule in the preceding collision is still nearest and will be chosen again, which would lead to highly unrealistic collisions because after a collision, molecules move away from each other. Therefore it is necessary to remember for each molecule its last collision partner and if the same molecule is chosen again, to exclude it from the collision and to select the second nearest neighbor instead (Bird, Gallis et al. 2009).

Transient-adaptive and virtual subcells are two alternatives for the efficient choice of collision pairs in DSMC simulations. The virtual subcell technique is deterministic in the sense that for a randomly
chosen molecule it selects its nearest neighbor as potential collision partner, while the selection process in the transient-adaptive subcell technique is stochastic. Hence virtual subcells are more accurate but their time penalty increases from 5 % for a number of 8 simulators per cell up to 100 % for 256 molecules in a single cell, whereas the transient-adaptive subcell technique induces a constant penalty in computation time of about 12 % irrespectively of the number of molecules per cell. Bird’s DS2V/DS3V codes automatically employ virtual subcells for less than 40 molecules per cell and transient-adaptive subcells if this number is exceeded (Bird 2005).

2.5.2 Variable time step

In every cell the time step should be small compared to the local mean collision time. Consequently, if the ratio of minimum to maximum density in the flow is small, the utilization of a single time parameter and one universal time step throughout the domain becomes inefficient because the low-density regions would allow for much longer time intervals. Ideally the time step should automatically be adapted to the local mean collision time (MCT) of molecules within a cell and to the mean transit time (MTT) of molecules across the cell. Therefore the DS2V/DS3V program suite uses global and cell-based time steps along with global, cell- and molecule-based time parameters. In each cell a desired time step (DTS) is defined as the minimum of a fixed fraction of the local MCT and a fixed fraction of the local MTT, and its value is updated continuously. Using the default computational settings the program calculates the cell-based time steps by

\[ DTS = \min(0.2 \cdot MCT, 0.5 \cdot MTT). \] (2.54)

The global time step is typically set to a fraction of the minimum DTS in the flow domain, and the global time parameter is gradually advanced by this interval. If in a particular cell with local time step DTS the time parameter of a molecule lags behind the global time by DTS/2, its value is advanced by DTS and the molecule is moved by a corresponding distance. Similarly, if the time parameter of a cell falls behind the global time by DTS/2, its value is augmented by DTS and an appropriate number of collisions between molecules within the cell are realized.

The smaller the global time step is chosen, the more uniformly are the collisions distributed over time. This reduces the error due to time discretization, which arises from the fact that collisions are performed at discrete times while in a real gas they occur continuously over time. A computational penalty is introduced by the variable time step because the code runs through all molecules and
cells, although only a fraction of them are chosen for moving and collisions. This time penalty is proportional to the ratio of the maximum to the minimum time step employed in the simulation. Therefore the ratio of the average to the minimum time step is typically set to a value below 10 (Bird, Gallis et al. 2009).

2.5.3 Separate sampling and collision cells

As mentioned above the time penalty caused by the virtual subcell technique increases with the number of molecules per cell and the best results in terms of computation time and accuracy are obtained with 5 to 10 particles per cell. Therefore the default average number of molecules per collision cell is set to 8 in the DS2V/DS3V programs. The sampling of macroscopic quantities for these cells would lead, in general, to excessively large memory cost and to an unnecessarily high level of scattering. The sole requirement of the sampling cells is that their linear dimensions are small compared to the scale length of the gradients of the macroscopic properties in the corresponding direction in order to ensure a good resolution of the flow. Hence the sampling cells usually contain 3 to 5 collision cells and the average number of molecules per sampling cell lies in the range of 30.

In order to achieve completely independent collision and sampling cells the average number of molecules $\bar{N}$ that is calculated for sampling cells only needs to be eliminated in equation (2.11), which is evaluated in each collision cell. As the instantaneous number of molecules $N$ in a cell is Poisson-distributed the expectation of $N\bar{N}$ is equal to the expected value of $N(N - 1)$ and hence the former expression is replaced by the latter. Therefore the only quantities that have to be stored for each collision cell are the cell time and volume, the number of molecules $N$ and the maximum product of total collision cross-section and relative speed $(\sigma_T c_r)_{max}$ (Bird 2005).

Initially the cell volumes are uniformly sized over the flow domain and each one contains the same number of molecules. As the flow develops from its initial state, the density changes and the DS2V/DS3V programs enable adaption of the collision and sampling cells to the flow, which allows maintaining a constant average number of molecules per cell. In addition the codes generate output files containing the macroscopic properties of each sampling cell, which have proven to be adequate for the application in this thesis.
2.5.4 Geometry definition

The DS2V code already includes an environment for the definition of flow geometries and a variety of boundary types are available, such as solid surfaces, flow boundaries, plane of symmetry, etc. Due to the low pressure in the vacuum chamber heat through the gas is purely transferred by conduction, so gravitation need not to be considered and the problem may be regarded as symmetric. Consequently, only half the annular gap is simulated and a specular surface of symmetry is utilized to reduce the computational effort. A snapshot of the simulation domain is shown in the figure below. For the solid absorber and glass jacket diffuse boundaries with complete accommodation to the surface temperature are applied. As the program does not allow specifying curved surfaces, the circular shapes have to be approximated by straight line segments. Here the absorber and glass tubes are both represented by 60 surface intervals, resulting in segment angles of 3° and relative errors in surface area of 0.0114 %, which is tolerable in this application.

![Diffuse reflection](image)

In the three-dimensional version the surfaces are specified by means of triangles and as there is no geometry generation tool included in the program suite commercial software is generally required to define complicated flow configurations. However, for the simple geometry of a cylinder the points defining each triangle may be calculated using e.g. Matlab and written to a text file, which can then be read by the surface definition program DS3DG to set the boundary types (cf. figure 2-5).
2. The Direct Simulation Monte Carlo method

![Figure 2-5: Surface triangles specifying the geometry of a 1 meter long glass tube segment.](image)

The DS2V/DS3V programs sample the macroscopic quantities at solid surfaces such as pressure and heat flux separately for each surface interval/triangle and produce detailed data output files. Therefore the routines are considered to be appropriate for the analysis in this project.
3 Overall Heat Transfer Model of Solar Receiver

For the specification of appropriate boundary conditions in the direct simulations of the gas an overall heat transfer model of the solar receiver is required to calculate realistic surface temperatures for the absorber tube and the glass jacket. A two-dimensional heat transfer model of the HITECO absorber was developed by Coskun (2011) in ANSYS CFX, which treats the rarefied gas in the annulus as a continuum. The wall temperatures predicted by this model may be used as a first estimate in the DSMC simulations to assess the difference in gas conduction between the molecular and the continuum approach. However, heat conduction through the gas influences the glass temperature and conversely depends itself on the temperature difference between absorber and glass tube. Therefore a new heat transfer model is developed in this project that utilizes the gas conduction results obtained by the Direct Simulation Monte Carlo method for the prediction of surface temperatures and for the calculation of total heat loss of the solar receiver. The temperature data output may then be used to set up another DSMC simulation with new boundary conditions. This procedure can be repeated until the deviation of the newly calculated surface temperatures from that used in the simulation is smaller than a desired level of accuracy. The final surface temperatures and heat losses are then compared to the CFX results and will be validated by experiments in a later stage of the HITECO project.

Generally there are two different experimental set-ups to measure the heat loss of a solar receiver. In off-sun tests electric heaters inside the steel tube bring the inner absorber tube surface to a desired temperature. After a certain heating-up time the system reaches a steady state and the thermal energy required to maintain a constant temperature corresponds to the total heat loss of the receiver. These measurements are performed indoors in a laboratory environment. Hence the receiver is not irradiated by sunlight and the heat fluxes on the tubes are uniform. In on-sun tests the receiver is located in the focal line of a parabolic trough collector and is supplied with heat transfer fluid at a desired temperature. The operating temperatures of the glass envelope, which serve as a comparative measure for the heat loss of the absorber, may then be measured by means
of infrared pyrometers or cameras. In this kind of experiment the concentrated solar irradiation causes a non-uniform heat flux distribution over the receiver tubes.

To produce results that are comparable to measurements, a one-dimensional heat transfer model is developed to simulate the lab-scale off-sun experiments. This model is then extended to two dimensions in order to precisely predict the temperature profile of the glass jacket in the irradiated case, considering the non-uniformity of heat fluxes.

### 3.1 Energy balances

Figure 3-1 shows a cross-section of a linear absorber with all relevant modes of heat transfer occurring in radial direction.

![Figure 3-1: Radial heat transfers in a solar parabolic trough receiver.](image)
As the geometry of the HITECO absorber has not been completely specified yet, the dimensions of the state-of-the-art PTR 70 receiver are utilized in the model.

Table 3-1: Radii of the PTR 70 receiver manufactured by Schott.

<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>$r_1$</td>
<td>33 mm</td>
</tr>
<tr>
<td>$r_2$</td>
<td>35 mm</td>
</tr>
<tr>
<td>$r_3$</td>
<td>57.5 mm</td>
</tr>
<tr>
<td>$r_4$</td>
<td>60 mm</td>
</tr>
</tbody>
</table>

The axial temperature gradient along the absorber in existing parabolic trough power plants is typically below 1 °C/m (Forristall 2003). Therefore heat transfer in this direction is not considered by the model and all heat losses are expressed as heat transfer rate $Q'$ per unit length of the receiver, W/m. The inner boundary condition of the model is specified by the temperature $T_1$ of the inner absorber tube surface in the un-irradiated lab-scale tests and by convection to a heat transfer fluid at uniform temperature $T_0$ in the on-sun field tests. The outer boundary condition is given by the ambient temperature $T_0$, which is assumed to be uniform in both cases.

For the one-dimensional model the receiver is divided into four cylindrical surfaces that are assigned different temperatures (cf. figure 3-1):

1. Inner absorber tube ($r_1, T_1$);
2. Outer absorber tube ($r_2, T_2$);
3. Inner glass tube ($r_3, T_3$);
4. Outer glass tube ($r_4, T_4$).

The heat transfers may then be expressed through the surface temperatures and by means of figure 3-1 the energy balance can be formulated for each surface. As the temperature of the inner absorber tube is fixed in the un-irradiated case, this results in three simultaneous equations that are nonlinear in the surface temperatures due to the radiation terms:

\[ Q'_{2,rad} + Q'_{23,\text{gas}} - Q'_{12,\text{cond}} = 0, \]  
\[ (3.1) \]

\[ Q'_{3,rad} + \frac{1}{2} Q'_{34,rad} + Q'_{34,\text{cond}} - Q'_{23,\text{gas}} = 0, \]  
\[ (3.2) \]
3. Overall heat transfer model of solar receiver

\[ Q_{45,conv} + Q_{45,rad} + \frac{1}{2} Q_{34,rad} - Q_{34,cond} = 0. \] \hspace{1cm} (3.3)

The extension to a two-dimensional model is accomplished by dividing each surface into \( N \) angular segments and including also convection to the HTF, concentrated solar irradiation from the mirrors and circumferential heat conduction between the segments of each surface (cf. figure 3-1).

\[ \text{Figure 3-2: Radial and circumferential heat exchange between segments in the 2-D model.} \]
3. Overall heat transfer model of solar receiver

Here \( q' \) is still expressed in W/m, but it denotes the heat transfer rate per unit length of a single circumferential segment, whereas \( Q' \) indicates the heat transfer rate per unit length over the full perimeter. Accordingly, the total heat transfer rate in the 2-D model is obtained by

\[
Q' = \sum_{i=1}^{N} q'_i.
\]

(3.4)

The conservation of energy at all segments yields a non-linear system of \( 4N \) equations for the surface segment temperatures:

\[
q'_{10,\text{conv}} + q'_{12,\text{cond}} + q'_{1,\text{cond}} - q'_{3,\text{ambient}} = 0,
\]

(3.5)

\[
q'_{2,\text{gas}} + q'_{2,\text{rad}} + q'_{2,\text{cond}} - q'_{2,\text{ambient}} - q'_{12,\text{cond}} - q'_{2,\text{solar}} = 0,
\]

(3.6)

\[
q'_{3,\text{rad}} + \frac{1}{2} q'_{3,\text{gas}} + q'_{34,\text{cond}} + q'_{3,\text{cond}} - q'_{3,\text{ambient}} - q'_{3,\text{gas}} - \frac{1}{2} q'_{3,\text{solar}} = 0,
\]

(3.7)

\[
q'_{45,\text{conv}} + \frac{1}{2} q'_{45,\text{rad}} + q'_{45,\text{cond}} + q'_{4,\text{cond}} - q'_{4,\text{ambient}} - q'_{34,\text{cond}} - \frac{1}{2} q'_{34,\text{solar}} = 0.
\]

(3.8)

Both models are implemented in Matlab, which provides computationally efficient algorithms to solve non-linear sets of equations numerically. In this project the Matlab function “fsolve” is used, which allows for a quite quick calculation of the surface temperatures also in the two-dimensional case. In the following sections the input data required by the model is described, the heat transfers indicated in figure 3-2 are analyzed in detail and their modeling equations are given.

3.2 Flow diagram of the overall model

Figure 3-3 shows the flowchart of the overall heat transfer model developed in this thesis. The initial DSMC simulation is run with the surface temperatures \( T_{\text{CFX}} \) predicted by the continuum model, and the simulated rates of conduction heat transfer \( q'_{\text{gas}} \) across the gas serve as an input to the Matlab model. In on-sun configuration additional information about the distribution of solar radiation on the receiver is provided by a Monte Carlo ray tracing simulation. The solar energy \( q'_{\text{solar}} \) absorbed by the absorber and glass tube segments is independent of the surface temperatures and needs to be determined only once. This calculation is performed with VeGaS (Very General Monte Carlo Ray-Trace Simulation), the in-house code developed at the lab “Professorship of Renewable Energy Carriers” at ETH Zurich. The Matlab model and the DSMC
3. Overall heat transfer model of solar receiver

Simulation are then solved iteratively to find the definite surface temperatures $T$ and heat transfers $q'$. In this project the values are accepted if the temperature difference $|T_{\text{Mat}} - T_{\text{DSMC}}|$ is below 1 °C for all surface segments.

**Initialization:**

![Initialization Diagram]

**Iteration:**

![Iteration Diagram]

**Termination:**

![Termination Diagram]

Figure 3-3: Flowchart of the overall heat transfer model of the solar receiver.

The DSMC simulations constitute the most time-consuming part in the analysis and it is therefore desirable to achieve convergence in a few iteration steps. Due to the accurate initial surface temperatures available from the CFX model, and as the contribution of gas conduction to the total heat loss is small in the target range of operating pressure, it is expected to reach convergence by a single iteration of the DSMC simulation in most cases.

Two-dimensional DSMC simulations of conductive heat transfer are performed at various pressures for both, the off-sun and the on-sun configuration using the DS2V program. The final surface temperatures predicted for these cases are further utilized as boundary conditions in three-dimensional DSMC simulations carried out with the DS3V program. The purpose of these simulations is to assess the effect of axial flow on conduction heat loss and to quantify the flow rate as a function of pressure difference when the vacuum pump is operating.
3. Overall heat transfer model of solar receiver

3.3 Radiation heat transfer

Although the emphasis in this thesis is on the behavior of the rarefied gas in the vacuum chamber, the overall heat transfer is dominated by radiation and a detailed treatment of radiative heat transfer is necessary to provide realistic boundary conditions of the gas conduction problem. While thermal radiation due to emission from the absorber tube and the glass jacket depends on surface temperatures and is dealt with by the Matlab model, as explained in the subsequent subsections, the solar flux distribution incident on the receiver may be determined a priori using a Monte Carlo ray tracing approach.

3.3.1 Solar radiation

In the VeGaS simulation sunrays of solid angle $\theta_{\text{sun}} = 6.72 \cdot 10^{-5}$ sr hit the parabolic mirrors, corresponding to the solid angle subtended by the sun as observed from the earth. A typical parabolic trough collector with a rim angle of 80° and geometric concentration ratio of 26.2 (ratio of concentrator aperture width to absorber tube outer diameter) is chosen (Roesle and Coskun 2011). Its optical error is modeled by a random angular fluctuation from perfect specular reflection for each ray, sampled from a Gaussian distribution with zero mean and standard deviation of 8 mrad. The non-gray surfaces of the absorber and the glass tube are modeled by the gray band approximation using five spectral bands.

<table>
<thead>
<tr>
<th>Spectral Band</th>
<th>Wavelength [(\mu m)]</th>
<th>$E_{\text{glass}}/A_{\text{glass}}$</th>
<th>$R_{\text{glass}}$</th>
<th>$V_{\text{glass}}$</th>
<th>$E_{\text{abs}}/A_{\text{abs}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\Delta\lambda_1$</td>
<td>0-0.3</td>
<td>0.935</td>
<td>0.065</td>
<td>0</td>
<td>0.98</td>
</tr>
<tr>
<td>$\Delta\lambda_2$</td>
<td>0.3-2.4</td>
<td>0.019</td>
<td>0.065</td>
<td>0.916</td>
<td>0.98</td>
</tr>
<tr>
<td>$\Delta\lambda_3$</td>
<td>2.4-2.7</td>
<td>0.019</td>
<td>0.065</td>
<td>0.916</td>
<td>0.08</td>
</tr>
<tr>
<td>$\Delta\lambda_4$</td>
<td>2.7-8</td>
<td>0.978</td>
<td>0.022</td>
<td>0</td>
<td>0.08</td>
</tr>
<tr>
<td>$\Delta\lambda_5$</td>
<td>8-(\infty)</td>
<td>0.82</td>
<td>0.18</td>
<td>0</td>
<td>0.08</td>
</tr>
</tbody>
</table>

Table 3-2: Spectral properties of glass jacket and absorber tube (Roesle and Coskun 2011).

The properties of the vacuum jacket are typical for a 2.5 mm thick layer of BK7 borosilicate glass. The selective coating of the absorber tube is modeled with approximate values for the absorptivity at short and long wavelengths and a sharp cut-off at $\lambda = 2.4 \ \mu m$. This wavelength is chosen to obtain
an absorptance of 0.95 and emittance of 0.1 for the PTR 70 receiver at 400 °C operating temperature, as specified by the manufacturer Schott (Roesle and Coskun 2011). The VeGaS simulation includes Fresnel reflection and refraction at the vacuum jacket as well as absorption in the glass tube and assumes diffuse reflection at the outer absorber surface.

Generally, parabolic mirrors are made of a glass with the reflecting surface at the bottom, such that incoming solar radiation passes through the glass layer before and after reflection. As glass strongly absorbs radiation at wavelengths below 0.3 μm and above 2.7 μm, this energy never arrives at the receiver and only radiation in bands 2 and 3 needs to be considered in the simulation. The spectrum of the solar radiation is modeled as thermal emission from a blackbody at $T_{solar} = 5780$ K and the fractions of total solar power emitted in the corresponding spectral bands are $F_{\lambda}T_{solar} = 0.93$ and $F_{\lambda}T_{solar} = 0.01$ respectively. To account also for the small fraction of radiation absorbed by the concentrators in this range of wavelengths, the product of incident solar flux on the collectors and mirror reflectivity is set to 800 W/m².

To include Fresnel reflection and refraction as well as absorption for the semi-transparent glass jacket in the VeGaS simulation, the glass tube is represented by two perfectly transparent Fresnel surfaces with an absorbing surface in the middle. The outer absorber tube surface is assumed to be diffusely reflecting. To match the division of surfaces with that used in the DSMC simulations the absorber and the glass jacket are both divided into 120 circumferential segments and the solar energy absorbed by each segment is included in the Matlab model as heat source. Surface absorption occurs at the absorber tube and thus $q_{2,\text{solar}}^i$ is allocated to the outer absorber segments, whereas in the semi-transparent vacuum jacket solar energy is actually absorbed along the full path of the rays through the glass. The attenuation of radiation in an absorbing medium is exponential, but due to the small fraction that is absorbed in this case it may be approximated by a linear function and thus $q_{34,\text{solar}}^i$ is divided equally between the inner and the outer glass surfaces.

### 3.3.2 Radiation heat transfer between the absorber and the glass jacket

Radiative heat exchange due to thermal emission from the absorber and the glass tube is treated by the radiosity method for an enclosure. Emission and reflection from the surfaces are assumed to be diffuse and the gray band approximation with spectral properties of table 3-2 is used. The thermal emission from the absorber in the first band at very short wavelengths may be written as
3. Overall heat transfer model of solar receiver

\[ Q'_{e,\text{abs},\Delta \lambda_1} = 2\pi r_2 E_{\text{abs},\Delta \lambda_1} F_{\Delta \lambda_1, r_2} \sigma T^4_2, \]  

where \( \sigma \) is the Stefan-Boltzmann constant and \( F_{\Delta \lambda_1, r_2} \) denotes the fraction of the hemispherical total emissive power emitted by a blackbody at temperature \( T_2 \) in the spectral band \( \Delta \lambda_1 \). Plugging in the maximum operating temperature of 873.15 K aimed at in the HITECO project, the thermal radiation emitted by the absorber at wavelengths below 0.3 \( \mu \)m amounts to 9.37e-18 W/m. This is a negligible amount and thus thermal radiation from the absorber and the glass jacket is only considered in the last four spectral bands. In wavelength bands 2 and 3, for which the glass tube is partially transparent to radiation, the radiosity method is applied to an enclosure with semi-transparent windows. For bands 4 and 5, in which the vacuum jacket is opaque, the basic radiosity method is used and thermal emission from the outer glass surface to the environment is considered separately.

**Opaque glass jacket**

In the one-dimensional model the radiosity method is applied to an enclosure composed of two diffuse surfaces, namely the outer absorber (2) and the inner glass (3) surface. The configuration factors are obtained by means of the reciprocity relation

\[
\begin{align*}
F_{2-2} &= 0, & F_{2-3} &= 1; \\
F_{3-2} &= \frac{r_2}{r_3} = 0.609, & F_{3-3} &= 1 - \frac{r_2}{r_3} = 0.391. 
\end{align*}
\]  

The radiative heat exchange between the absorber and the glass tube may then be expressed in the closed form

\[ Q'_{2,\text{rad},\Delta \lambda_1} = -Q'_{3,\text{rad},\Delta \lambda_1} = \frac{2\pi r_2 (F_{\Delta \lambda_1, r_2} \sigma T^4_2 - F_{\Delta \lambda_1, r_3} \sigma T^4_3)}{E_{\text{abs},\Delta \lambda_1}} + F_{3-3} \left( \frac{1}{E_{\text{glass},\Delta \lambda_1}} - 1 \right). \]  

The enclosure in the two-dimensional model is composed of \( 2N \) surfaces and the configuration factors between all segments need to be determined analytically. Due to the axially symmetric arrangement of the tubes it is sufficient to calculate the configuration factors \( F_{3,k-2,i} \) and \( F_{3,k-3,i} \) from a particular segment \( (3,k) \) located on the inner glass surface to all segments on the absorber \( (2,i) \) and the glass \( (3,i) \) respectively. The configuration factors for a specific absorber segment \( (2,k) \) are then obtained by
The results for \( N = 120 \) segments, i.e. each segment spanning an angle of 3\(^\circ\), are shown in the figures below and are in excellent agreement with a Monte Carlo ray-tracing simulation performed with VeGaS.

Figure 3-4: Configuration factors from reference segment \((3,k)\) on inner glass surface to absorber tube segments \((2,i)\).

Figure 3-5: Configuration factors between inner glass tube segments.
The angular displacement measures the circumferential angle between the reference segment (k) and the other segments (i). It is seen that the view between segments is blocked by the absorber tube and the corresponding configuration factors are zero if the angular displacement is higher than \( \cos^{-1}(r_2/r_3) = 52.5^\circ \) for the absorber segments (2,i) and greater than \( 2\cos^{-1}(r_2/r_3) = 105^\circ \) for the glass segments (3,i) respectively. The pattern looks similar for all segments and the detailed calculation may be found in the appendix B.

The radiosity equations for the opaque glass bands \( (l = 4,5) \) may then be formulated for the \( k = 1, ..., N \) absorber tube segments

\[
\frac{1}{E_{\text{abs},\Delta t}} q''_{2,k,rad,\Delta t} - \sum_{i=1}^{N} F_{2,k-3,i} \frac{1 - E_{\text{glass},\Delta t}}{E_{\text{glass},\Delta t}} q''_{3,i,rad,\Delta t} = F_{\Delta t,\tau_{2,k}} \sigma T_{2,k}^4 - \sum_{i=1}^{N} F_{2,k-3,i} F_{\Delta t,\tau_{3,i}} \sigma T_{3,i}^4
\]

and for the \( k = 1, ..., N \) vacuum jacket segments

\[
- \sum_{i=1}^{N} F_{3,k-2,i} \frac{1 - E_{\text{abs},\Delta t}}{E_{\text{abs},\Delta t}} q''_{2,l,rad,\Delta t} + \sum_{i=1}^{N} \left( \frac{\delta_{kl}}{E_{\text{glass},\Delta t}} - F_{3,k-3,i} \frac{1 - E_{\text{glass},\Delta t}}{E_{\text{glass},\Delta t}} \right) q''_{3,i,rad,\Delta t} = - \sum_{i=1}^{N} F_{3,k-2,i} F_{\Delta t,\tau_{3,i}} \sigma T_{2,i}^4 + \sum_{i=1}^{N} \left( \delta_{kl} - F_{3,k-3,i} \right) F_{\Delta t,\tau_{3,i}} \sigma T_{3,i}^4
\]

where \( \delta_{ki} \) is equal to 1 for \( i = k \) and 0 otherwise. This yields a linear system of equations for the \( 2N \) net radiative heat fluxes leaving the segments and the heat transfers may be expressed through the surface segment temperatures by a simple matrix inversion.

To calculate the radiative heat transfer between the outer vacuum jacket surface and the surroundings, the sky temperature \( T_{\text{sky}} \) is assumed to be equal to that of the environment. The external radiation from the environment incident on the receiver may then be calculated by

\[
Q_{4,\text{ext,}\Delta t} = 2\pi r_4 F_{\Delta t,\tau_5} \sigma T_{5}^4.
\]

For an ambient temperature of 25 °C this amounts to 0.456e-3 W/m and 2.59e-3 W/m in the wavelength bands 2 and 3 respectively, and thus radiation from the surroundings is only considered at longer wavelengths in bands 4 and 5. The radiation heat exchange rate with the environment is then given by

\[
q_{\Delta t,\text{rad}} = \frac{2\pi r_4}{N} \sum_{i=4}^{5} E_{\text{glass},\Delta t} \left( F_{\Delta t,\tau_{4,i}} \sigma T_{4,i}^4 - F_{\Delta t,\tau_5} \sigma T_{5}^4 \right).
\]
Semi-transparent glass jacket

A section of the semi-transparent glass envelope is shown in the figure below. In bands 2 and 3 the outer surfaces of the enclosure are semi-transparent windows at radius \( r_{34} = (r_3 + r_4)/2 \) and temperatures \( T_{34,i} = (T_{3,i} + T_{4,i})/2 \). As indicated above, radiation from surroundings may be neglected at short wavelengths and the solar radiation is dealt with in the VeGaS simulation, so the external energy arriving at the receiver at wavelengths below 2.7 μm is zero, \( q'_{34,i,ext} = 0 \).

Figure 3-6: Radiative heat transfers at semi-transparent glass jacket.

The configuration factors between surface segments are then calculated using the mean radius \( r_{34} \) of the glass jacket, and for the 1-D model the following values are obtained:

\[
F_{2-2} = 0, \quad F_{2-34} = 1; \quad F_{34-2} = \frac{r_2}{r_{34}} = 0.596, \quad F_{34-34} = 1 - \frac{r_2}{r_{34}} = 0.404.
\]

Applying the radiosity method for an enclosure with windows yields the following closed-form expressions for the net radiative energy leaving the absorber and the glass tube for uniform surface temperatures,

\[
Q'_{2,\text{rad,Δ}_i} = 2\pi r_2 F_{\text{abs,Δ}_i} \left( \frac{1 - R_{\text{glass,Δ}_i}}{1 - R_{\text{glass,Δ}_i}(1 - F_{34-2} F_{\text{abs,Δ}_i})} \right) \left( 1 - \frac{F_{\text{abs,Δ}_i}}{T_{34,i}} \sigma T_{34,i}^4 - \frac{E_{\text{glass,Δ}_i} F_{\text{abs,Δ}_i}}{R_{\text{glass,Δ}_i}} \sigma T_{34,i}^4 \right).
\]

(3.18)
3. Overall heat transfer model of solar receiver

\[
Q'_{34,rad,\Delta \lambda_l} = \frac{2\pi r_{34} E_{\text{glass},\Delta \lambda_l}}{1 - R_{\text{glass},\Delta \lambda_l} (1 - F_{34-2} E_{\text{abs},\Delta \lambda_l})} \left[ \right. \left( \frac{2}{(2R_{\text{glass},\Delta \lambda_l} + E_{\text{glass},\Delta \lambda_l}) (1 - F_{34-2} E_{\text{abs},\Delta \lambda_l})} F_{\Delta \lambda_l T_{34}} \sigma T_{34}^4 \right. \\
\left. - F_{34-2} E_{\text{abs},\Delta \lambda_l} F_{\Delta \lambda_l r_{2} \sigma T_{2}^4} \right]. 
\]

In the two-dimensional model the 2N radiosity equations may again be formulated for the \( k = 1, ..., N \) absorber segments

\[
\frac{1}{E_{\text{abs},\Delta \lambda_l}} q''_{2,k,rad,\Delta \lambda_l} = \sum_{i=1}^{N} F_{2,k-34,i} \frac{R_{\text{glass},\Delta \lambda_l}}{E_{\text{glass},\Delta \lambda_l}} q''_{34,i,rad,\Delta \lambda_l} \\
= F_{\Delta \lambda_l T_{2,k}} \sigma T_{2,k}^4 - \sum_{i=1}^{N} F_{2,k-34,i} (2R_{\text{glass},\Delta \lambda_l} + E_{\text{glass},\Delta \lambda_l}) F_{\Delta \lambda_l T_{34,i}} \sigma T_{34,i}^4 
\]

and for the \( k = 1, ..., N \) glass jacket segments

\[
- \sum_{i=1}^{N} F_{34,k-2,i} \frac{1}{E_{\text{abs},\Delta \lambda_l}} q''_{2,i,rad,\Delta \lambda_l} + \sum_{i=1}^{N} \left( \frac{\delta_{k,i}}{E_{\text{glass},\Delta \lambda_l}} - F_{34,k-34,i} \frac{R_{\text{glass},\Delta \lambda_l}}{E_{\text{glass},\Delta \lambda_l}} \right) q''_{34,i,rad,\Delta \lambda_l} \\
= - \sum_{i=1}^{N} F_{34,k-2,i} F_{\Delta \lambda_l T_{2,i}} \sigma T_{2,i}^4 \\
+ \sum_{i=1}^{N} (2\delta_{k,i} - F_{34,k-34,i} (2R_{\text{glass},\Delta \lambda_l} + E_{\text{glass},\Delta \lambda_l}) F_{\Delta \lambda_l T_{34,i}} \sigma T_{34,i}^4 
\]

The only modification in the above formulae as compared to equations (3.13) and (3.14) for the opaque case occurs in the last term to account also for the energy \( q''_{34,i,leave} \) leaving the enclosure. Thermal emission from the glass jacket to the outside is already included here and needs no further treatment. Finally the radiation heat transfer rates for the energy balances are obtained by

\[
q'_{2,i,rad} = \frac{2\pi r_2}{N} \sum_{l=2}^{5} q''_{2,i,rad,\Delta \lambda_l} 
\]

\[
q'_{3,i,rad} = \frac{2\pi r_3}{N} \sum_{l=4}^{5} q''_{3,i,rad,\Delta \lambda_l} 
\]

\[
q'_{34,i,rad} = \frac{2\pi r_{34}}{N} \sum_{l=2}^{3} q''_{34,i,rad,\Delta \lambda_l} 
\]

and like the solar energy \( q'_{34,i,solar} \) the net energy leaving the transparent vacuum jacket \( q'_{34,i,rad} \) is equally divided between the inner and the outer glass tube segments.
3.4 Convection heat transfer

3.4.1 From the glass jacket to the environment

Heat transfer to the environment by convection is modeled using Newton’s law of cooling, which yields

\[ Q'_{45,\text{conv}} = 2\pi r_4 h_\omega (T_4 - T_5) \]  \hfill (3.25)

in the one-dimensional case and

\[ q'_{45,i,\text{conv}} = \frac{2\pi r_4}{N} h_\omega (T_{4,i} - T_5) \]  \hfill (3.26)

in the 2-D model. The coefficient of convective heat transfer between the vacuum jacket and the surrounding air may be expressed by

\[ h_\omega = N u_{d_4} \frac{K_\omega}{d_4} \]  \hfill (3.27)

where \( d_4 \) is the diameter of the outer glass tube, \( K_\omega \) is the thermal conductivity of ambient air and \( N u_{d_4} \) is the Nusselt number based on \( d_4 \). Here the same value is chosen as in (Roesle and Coskun 2011),

\[ h_\omega = 10 \text{ W/(m}^2 \text{ °C).} \]  \hfill (3.28)

This corresponds to the convective heat transfer coefficient predicted by the Churchill-Bernstein correlation for a cylinder in cross flow, when the wind speed amounts to 1 m/s. The ambient temperature \( T_5 \) is assumed as uniform at 25 °C.

3.4.2 From the absorber to the HTF

Convective heat transfer to the HTF is treated similarly to convection to the environment,

\[ q'_{10,i,\text{conv}} = \frac{2\pi r_4}{N} h_{\text{HTF}} (T_{1,i} - T_0), \]  \hfill (3.29)
3. Overall heat transfer model of solar receiver

and Nusselt number correlations for the convective heat transfer coefficient between the absorber tube and the HTF in different flow regimes may be found in (Forristall 2003). However, as the flow of the heat transfer fluid through the steel tube has not been modeled in detail in the HITECO project yet, a uniform bulk temperature $T_0$ is assumed for the HTF and the convective heat transfer coefficient is again taken from (Roesle and Coskun 2011),

$$h_{HTF} = 5'000 \, W/(m^2 \cdot ^\circ C).$$

(3.30)

This corresponds to a typical value in current parabolic trough power plants.

3.5 Conduction heat transfer

3.5.1 Absorber tube

In the 1-D model only radial conduction through the absorber wall needs to be considered and the one-dimensional equation of heat conduction in cylindrical coordinates yields

$$Q_{12,\text{cond}} = K_{abs} \frac{2\pi}{\ln(r_2/r_1)} (T_1 - T_2),$$

(3.31)

where $K_{abs}$ is the thermal conductivity of the absorber tube. This is a material-dependent property and in this thesis the correlation given in (Forristall 2003) for stainless steel 321H is utilized,

$$K_{abs} = 0.0153 \cdot T + 14.775,$$

(3.32)

with $K_{abs}$ in units $W/(m \cdot ^\circ C)$ and temperature $T$ in $^\circ C$. This formula neglects the conductive resistance of the selective coating. In equation (3.31) a constant thermal conductivity is used, corresponding to the mean temperature $(T_1 + T_2)/2$ of the absorber tube.

In the 2-D model heat conduction also occurs in circumferential direction and approximations are necessary in order to avoid solving the partial differential equation of heat conduction and to express the heat transfer rates as a function of segment temperatures. Therefore, for dealing with conduction in the absorber tube the segments are regarded as rectangular elements, which is reasonable if the number $N$ is large enough such that each segment spans a small angle. The conductive heat transfer rates may then be written in their one-dimensional Cartesian form.
3. Overall heat transfer model of solar receiver

\[ q'_{\text{cond}} = K \frac{A}{l} \left( \frac{\Delta T}{\Delta x} \right) \]

where \( \frac{A}{l} \) is the area of heat exchange per unit length and \( \frac{\Delta T}{\Delta x} \) is the temperature gradient. This yields the following expressions for conduction in the absorber tube:

\[ q'_{1,2,i,\text{cond}} = K_{\text{abs},i} \frac{\pi(r_1 + r_2)}{N(r_2 - r_1)} (T_{1,i} - T_{2,i}), \tag{3.33} \]

\[ q'_{1,i,\text{cond}} = K_{\text{abs},i} \frac{N(r_2 - r_1)}{\pi(3r_1 + r_2)} (T_{1,i} - T_{1,i+1}), \tag{3.34} \]

\[ q'_{2,i,\text{cond}} = K_{\text{abs},i} \frac{N(r_2 - r_1)}{\pi(r_1 + 3r_2)} (T_{2,i} - T_{2,i+1}). \tag{3.35} \]

Here the thermal conductivity \( K_{\text{abs},i} \) is calculated for each conductive heat transfer in the absorber wall according to equation (3.32) using the mean temperature of the two segments involved in the heat exchange.

3.5.2 Glass jacket

Conduction in the glass tube is treated equally to conductive heat transfer in the absorber wall. Accordingly the heat loss through the glass jacket by conduction in the 1-D model is calculated by

\[ Q'_{34,\text{cond}} = K_{\text{glass}} \frac{2\pi}{\ln(r_4/r_3)} (T_3 - T_4), \tag{3.36} \]

where \( K_{\text{glass}} \) is the thermal conductivity of the glass. The vacuum jacket in state-of-the-art receivers is made of borosilicate glass and like in the CFX model (Roesle and Coskun 2011) its thermal conductivity is assumed to be a constant,

\[ K_{\text{glass}} = 1.09 \text{ W/(m °C)}. \tag{3.37} \]

Here the conductive resistance of the anti-reflective coating is neglected.

In analogy to equations (3.33)-(3.35) the radial and circumferential heat transfers in the 2-D model are obtained by

\[ q'_{34,i,\text{cond}} = K_{\text{glass}} \frac{\pi(r_3 + r_4)}{N(r_4 - r_3)} (T_{3,i} - T_{4,i}). \tag{3.38} \]
3. Overall heat transfer model of solar receiver

\[ q'_{3,\text{i,cond}} = K_{\text{glass}} \frac{N(r_3 - r_4)}{\pi(3r_3 + r_4)} (T_{3,i} - T_{3,i+1}). \]  \hspace{0.5cm} (3.39)

\[ q'_{4,\text{i,cond}} = K_{\text{glass}} \frac{N(r_4 - r_3)}{\pi(r_3 + 3r_4)} (T_{4,i} - T_{4,i+1}). \]  \hspace{0.5cm} (3.40)
4 RESULTS

In this chapter the gas conduction and axial flow results obtained by the Direct Simulation Monte Carlo method as well as their effect on overall heat transfer and pressure drop in the solar receiver are presented and compared to the continuum ANSYS CFX model (Roesle and Coskun 2011). All DSMC simulations employ the diffuse reflection model with full accommodation to the surface temperature for molecules colliding with the absorber and the glass tube and the model parameters utilized in the calculation of the temperature boundary conditions are summarized in the table below.

Table 4-1: Simulation conditions of the overall heat transfer model.

<table>
<thead>
<tr>
<th>Quantity</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$d_1$</td>
<td>66 mm</td>
</tr>
<tr>
<td>$d_2$</td>
<td>70 mm</td>
</tr>
<tr>
<td>$d_3$</td>
<td>115 mm</td>
</tr>
<tr>
<td>$d_4$</td>
<td>120 mm</td>
</tr>
<tr>
<td>$T_1, T_0$</td>
<td>400 °C</td>
</tr>
<tr>
<td>$h_{HTF}$</td>
<td>5000 W/(m$^2$°C)</td>
</tr>
<tr>
<td>$T_5$</td>
<td>25 °C</td>
</tr>
<tr>
<td>$h_{\infty}$</td>
<td>10 W/(m$^2$°C)</td>
</tr>
<tr>
<td>$k_{abs}$</td>
<td>(14.775 + 0.0153 $T$/°C) [W/(m°C)]</td>
</tr>
<tr>
<td>$k_{glass}$</td>
<td>1.09 W/(m °C)</td>
</tr>
</tbody>
</table>

DSMC simulations are primarily performed for air, which is freely available in the atmosphere and is thus considered as the most competitive solution in terms of cost. In all DSMC simulations air is represented by a gas mixture composed of 78 % nitrogen, 21 % oxygen and 1 % argon and for each chemical species the default properties in the DS2V and DS3V programs are utilized, which may be found in appendix A.
### 4.1 Two-dimensional heat transfer simulations

In order to assess the effect of the molecular collision model on the conduction heat transfer, two-dimensional DS2V calculations are first carried out for the un-irradiated case using the VHS and VSS models. The most suitable molecular model for the simulation of heat transfer is then identified and further utilized in the on-sun and axial flow simulations.

#### 4.1.1 Off-sun configuration

Conduction heat transfer simulations in off-sun arrangement are performed at gas pressures ranging from 0.01 Pa (free-molecular regime) up to 100 Pa (continuum regime), covering the full transitional and slip regime. The VHS and VSS parameters are set to the default values in the DS2V code, and the rotational relaxation collision number $Z_r$ of oxygen and nitrogen may either be set to a constant (5 is the default value in the program) or to a second order polynomial in temperature, $Z_r = aT^2 + bT + c$. This yields four different combinations to be utilized in the analysis, the VHS and VSS models both with constant and temperature dependent $Z_r$.

<table>
<thead>
<tr>
<th>Monoatomic model</th>
<th>Rotational relaxation collision number</th>
<th>Nitrogen $Z_r$</th>
<th>Oxygen $Z_r$</th>
</tr>
</thead>
<tbody>
<tr>
<td>VHS</td>
<td>$Z_r = \text{const.}$</td>
<td>$Z_r = 5$</td>
<td>$Z_r = 5$</td>
</tr>
<tr>
<td>VHS</td>
<td>$Z_r = f(T)$</td>
<td>$a = -4.559e-6$</td>
<td>$a = -3.924e-6$</td>
</tr>
<tr>
<td></td>
<td>$= aT^2 + bT + c$</td>
<td>$b = 9.576e-3$</td>
<td>$b = 8.421e-3$</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$c = 1.605$</td>
<td>$c = 1.290$</td>
</tr>
<tr>
<td>VSS</td>
<td>$Z_r = \text{const.}$</td>
<td>$Z_r = 5$</td>
<td>$Z_r = 5$</td>
</tr>
<tr>
<td>VSS</td>
<td>$Z_r = f(T)$</td>
<td>$a = -5.673e-6$</td>
<td>$a = -4.968e-6$</td>
</tr>
<tr>
<td></td>
<td>$= aT^2 + bT + c$</td>
<td>$b = 1.223e-2$</td>
<td>$b = 1.100e-2$</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$c = 1.832$</td>
<td>$c = 1.487$</td>
</tr>
</tbody>
</table>

One way to determine the coefficients $a$, $b$ and $c$ is by fitting the polynomial to equations (2.51) and (2.52) for the VHS and VSS models respectively. As the exact expressions for the rotational relaxation collision number are composed of a constant, a square root and a linear term, the approximation by a second order polynomial is quite accurate over a limited temperature range.
Here the coefficients are calculated by means of the Matlab function “polyfit” for temperatures between 300 K and 673 K, which is considered a reasonable range of gas temperature in this application. The corresponding values are given in table 4-2.

Figure 4-1 shows the DSMC results of conductive heat transfer through air in the annulus over the full pressure range, corresponding to $32 \geq Kn \geq 0.0033$. At high Knudsen numbers the heat transfer rates predicted by the DSMC method are consistent and the values obtained by the different intermolecular collision models all lie within 0.7 W/m at 1 Pa, which corresponds to a relative deviation of 1.4 %. As the gas pressure exceeds 1 Pa ($Kn = 0.33$) the divergence among the molecular models becomes significant and amounts to 28 W/m or 20 % at 100 Pa. This behavior is not unexpected because at high Knudsen numbers heat transfer is predominantly driven by gas-surface interactions, which are modeled by diffuse reflection with full adaption to the wall temperature in all simulations, whereas at decreasing $Kn$ the number of collisions between gas molecules increases and hence the molecular models gain importance.

![Graph of Heat Transfer Rate vs Pressure](image)

Figure 4-1: Gas conduction heat loss for air in the vacuum chamber at various pressures in off-sun configuration.

To decide on the most suitable molecular model for the simulation of conduction heat loss, the values obtained by the continuum CFX model (Coskun 2011) are also shown here. At 100 Pa the Knudsen number amounts to 0.0033 and the condition for the validity of the Navier-Stokes and
energy equations, $Kn < 0.01$, is easily satisfied. Therefore all curves in the figure above should converge to the value of one-dimensional heat conduction through an annular gap in the continuum regime. This value amounts to 156.3 W/m and is indicated by the results of the ANSYS simulations at 50 Pa and 100 Pa, in which a temperature-dependent thermal conductivity for air and zero temperature slip conditions at the boundaries are utilized. It may be observed that both variants of the variable hard sphere model underestimate the conduction heat loss at 100 Pa, whereas it is overpredicted by the variable soft sphere model with constant rotational relaxation collision number. Accordingly, convergence is only achieved by means of the VSS model with temperature-dependent $Z_r$ and therefore this molecular model is utilized in all succeeding simulations for air. This is in conformity with the theory of chapter 2, which states that the VHS model might not reproduce the exact transport phenomena of a gas mixture and describes the rotational relaxation parameter as a function of temperature.

To evaluate the difference between the VHS and the VSS model in the absence of the effect of rotational relaxation the DSMC method is applied to a monoatomic gas with no internal degrees of freedom. For this analysis the heavy inert gas krypton is chosen, which is considered for use in the HITECO receiver due to its low thermal conductivity.

![Figure 4-2: Gas conduction heat loss for krypton in the vacuum chamber at various pressures in off-sun configuration.](image-url)
Besides the substantially smaller absolute values of conduction heat loss the behavior of the molecular models is similar to that observed for air, i.e. they start to deviate from each other at pressures above 1 Pa ($Kn = 0.27$) and the difference amounts to 5.4 W/m or 9.4 % at 100 Pa ($Kn = 0.0027$). Again the heat transfer rates predicted by the ANSYS CFX model are shown for comparison. Apparently, the VSS model overestimates the thermal conductivity of the gas at high pressures while the VHS model is in close agreement with the continuum model over a wide range of Knudsen numbers, although it might slightly underestimate conductive heat transfer in the continuum regime. The error of the VSS model is almost certainly caused by the VSS parameter $\alpha$, which is set to a constant value of 1.32 corresponding to a reference temperature of 0 °C, although it is mentioned in (Bird 1994) that $\alpha$ might change with temperature. Consequently the VHS model is recommended here to simulate conduction heat transfer through pure krypton. However, it is noted that an appropriate VSS parameter for this application might be determined by decreasing $\alpha$ successively from 1.32 to 1 (VHS value) and identifying the simulation that reproduces the radial heat conduction rate in continuum regime most precisely.

The heat conduction rates of air obtained by the VSS model with $Z_r$ a function of temperature may be further utilized to calculate the surface temperatures by means of the one-dimensional overall heat transfer model as explained in chapter 3. Figure 4-3 shows a comparison of the outer absorber and inner glass temperatures determined by the ANSYS CFX model, which are used as boundary conditions in the DSMC simulations, and the new surface temperatures predicted by the 1-D Matlab model. Due to the high thermal conductivity of the steel tube the effect of heat loss on the absorber temperature is negligible, while the outer glass temperature and the temperature difference to the inner glass surface increase at rising gas pressures to enable higher conductive heat transfer rates through the vacuum jacket and to dissipate the additional energy to the environment by convection and radiation.
As expected the outer absorber tube temperatures predicted by the different models coincide with each other, whereas the pattern of the inner glass temperature is similar to that of gas conduction heat loss shown in figure 4-1. The maximum difference in average temperature of the vacuum jacket amounts to 0.94 °C and occurs at 1 Pa, which corresponds to the pressure for which the highest deviation in gas conduction heat loss is observed (6.1 W/m). Accordingly the variance in glass temperature is mainly due to different gas conduction rates, which confirms the consistency of the ANSYS CFX and the 1-D Matlab models. To assess the effect of the approximations made in the two-dimensional Matlab model for the heat conduction in the absorber and the glass tube and to verify the implementation of the 240 radiosity equations, the results obtained by the 2-D model for the off-sun case are also shown in the figure above. Neglecting solar irradiation and convection to the heat transfer fluid the 2-D model delivers uniform surface temperatures that are in excellent agreement with that of the 1-D model, thus justifying its utilization to predict surface temperatures in the irradiated case.
4. Results

4.1.2 On-sun configuration

Simulations in on-sun arrangement are performed exclusively for air using the VSS model with variable $Z_r$ and the gas pressure in the annular gap is varied between 0.01 Pa and 10 Pa, which encompasses the range of interest of operating pressures in the HITECO receiver. Figure 4-4 shows the surface temperature and conduction heat flux profiles on the absorber and the vacuum jacket at 1 Pa. The scatter in the heat flux results is due to the probabilistic nature of the DSMC method and is reduced to an acceptable level by time averaging over a long sampling interval. It is noted here that the total heat loss by gas conduction rather than its circumferential distribution is of interest from a receiver technology point of view, which is only marginally affected by scattering.

![Figure 4-4: Surface temperatures and conduction heat fluxes at the outer absorber and inner glass tubes at 1 Pa.](image)

The ANSYS CFX temperatures serve as boundary conditions in the first DSMC simulation and the resulting conductive heat fluxes are utilized to calculate new surface temperatures by the two-dimensional Matlab model. The maximum deviations between the different temperature profiles amount to 3.9 °C and 4.4 °C at the outer absorber and inner glass tubes respectively, and thus another DSMC simulation is set up using the Matlab temperatures as boundary conditions. As a
4. Results

consequence of the less pointed surface temperature profiles the second simulation yields flatter heat flux distributions on the vacuum jacket and to a lesser extent also on the absorber. However, the differences between the DSMC results are very small and lead to further changes of maximally 0.006 °C and 0.085 °C in the absorber and glass segment temperatures respectively. Consequently convergence is achieved after a single iteration of the DSMC simulation and a similar behavior is observed at all pressure levels analyzed here.

The final temperature profiles of the inner glass tube surface determined in this thesis by means of the DSMC method and the 2-D Matlab model are compared in figure 4-5 to those predicted by ANSYS CFX at three different pressures. It is seen that conduction heat loss through the gas affects the average temperature level of the vacuum jacket while its influence on the shape of the temperature distribution is negligible.

![Figure 4-5: Temperature profile of inner glass surface predicted by ANSYS CFX and 2-D Matlab models at pressures of 0.1 Pa, 1 Pa and 10 Pa.](image)

The deviation of the temperature profiles is mainly due to different assumptions in the radiation heat transfer model. Most importantly, a normally-distributed random error in specular reflection at the parabolic mirrors is included in the VeGaS simulation provided to the 2-D Matlab model, which leads to a smooth solar flux distribution on the receiver as indicated by $q'_{\text{solar}}$ in figure 4-6. This optical error is neglected in the VeGaS calculation utilized as input by the ANSYS model, which causes sharper peaks in the incident solar radiation and surface temperature profiles.
Besides surface temperatures the Matlab model may also be used to determine the various heat transfers occurring in the solar receiver. Figure 4-6 shows the circumferential variation of all heat transfer rates that are present in the consolidated energy balance of the vacuum jacket, i.e. the sum of the energy balances of surfaces 3 and 4. The heat fluxes arriving at the glass tube are plotted in red colors, the leaving energy fluxes are indicated in green and the profile of the average glass temperature $T_{34} = (T_3 + T_4)/2$ is also shown (blue).

![Figure 4-6: Heat fluxes at the vacuum jacket and average glass temperature at 1 Pa.](image)

It is noted that like the conductive heat exchange $q_{3,\text{gas}}''$ arriving at the vacuum jacket the thermal radiation $q_{3,\text{rad}}''$ absorbed by the opaque glass tube is governed by the temperature difference between the outer absorber and inner glass surfaces rather than their absolute temperatures. Accordingly the two-dimensional thermal radiation model implemented in Matlab has an additional smoothing effect on the glass temperature profile as compared to the CFX model in which the radiosity method is only applied to two surfaces using average temperatures of the absorber and the vacuum jacket, which results in uniform heat fluxes.

The effects of the results presented above on heat conduction in the annulus, mean glass tube temperature and total heat loss of the solar receiver at various gas pressures are shown in figure 4-7.
4. Results

As in the un-irradiated case the differences in vacuum jacket temperature and overall heat loss are mainly caused by different gas conduction rates predicted by the DSMC method and the continuum model. Again the maximum deviations in mean glass temperature (0.5 °C) and conduction heat loss (5.8 W/m) coincide with each other at a pressure of 1 Pa. It is noted that despite the differences in the radiation models and the resulting deviations of the circumferential temperature distribution the two models deliver consistent results for average and total quantities.

4.2 Three-dimensional axial flow simulations

Three-dimensional DS3V simulations of a 1 meter long receiver section with an axial pressure gradient are performed for air under on-sun conditions, i.e. circumferentially varying temperature boundary conditions are applied. As the axial temperature gradient in parabolic trough power plants is usually lower than 1 °C/m, the temperature variation in this direction is neglected and the 2-D temperature profile corresponding to the outlet pressure as calculated by the overall heat transfer model is set over the full length of the absorber and glass tubes. The outlet pressure is
varied between 0.1 Pa and 1 Pa and different pressure gradients are applied. Two different cases are analyzed: the mass flow rate through a 1 meter long annular duct that is empty and through the same section with a ring structure in the middle, as proposed to be placed every 6 meters in the HITECO receiver to support the absorber tube (cf. figure 4-9).

![Flow entry boundaries](image)

**Figure 4-8:** 3-D simulation domain of 1 meter long receiver segment with different pressure boundaries at inlet and outlet.

**Figure 4-9:** 1 meter long section with support structure in the middle.

The ratio of the flow cross-section at the support to that without support amounts to 42.2 % and a description of the geometry may be found in appendix C. As the surface temperature of the support is not known a priori, the triangles are specified as adiabatic surfaces in the DS3V code. The program then calculates the temperature of the support structure progressively during the simulation such that the net heat transfer to the surface is zero.

### 4.2.1 Conductance of receiver segments

Any pipe offers a resistance to gas flows, which causes a pressure drop in flow direction and depends on the cross-section geometry and the gas itself. The inverse of the flow resistance is called conductance, which is defined as

\[
C = \frac{1}{R} = \frac{q}{\Delta P}
\]  

(4.1)

where \( q \) is the gas flow rate through the duct. In vacuum technology applications usually the pV-flow
4. Results

\[ q_{pv} = \frac{d(PV)}{dt} \]  \hspace{1cm} (4.2)

is used in the definition of the conductance, which has units Watts and reflects the energy required to transport the gas particles across a certain pipe cross-section. If the temperature in the cross-section is known, this can be related to the mass flow rate by

\[ \dot{M} = \frac{q_{pv}}{R_s T'} \]  \hspace{1cm} (4.3)

where \( R_s = k/m \) is the mass specific gas constant. However, in a steady rarefied gas flow through a concentric annular tube with a radial temperature gradient, the temperature distribution in the flow field and thus pV-flow vary along the axial coordinate due to the pressure gradient. Therefore the conductance of an axial section of the HITECO collector is defined here by means of the mass flow rate that is constant,

\[ C = \frac{\dot{M}}{P_{in} - P_{out}} \]  \hspace{1cm} (4.4)

In figure 4-10 the results of the axial flow simulations with and without support in the middle are plotted as a function of reference pressure, which is defined as the mean of the inlet and outlet pressures,

\[ P_{ref} = (P_{in} + P_{out})/2. \]  \hspace{1cm} (4.5)

A trend may be observed that the flow conductance reaches a minimum at \( P_{ref} = 0.5 \) Pa \((Kn = 0.6)\) and increases at lower and higher pressures. The effect of the support structure on the flow rate is quite constant over the considered pressure range and reduces the conductance by about 10.5 \%. Apparently the simulations with inlet and outlet pressures of 1.1 Pa and 1 Pa \((P_{ref} = 1.05 \) Pa\) produce a disproportionally high conductance compared to that obtained by the other simulations. Probable reasons for that are discussed in the following chapter and here it is only noted that the value obtained by the simulation with inlet and outlet pressures of 1.5 Pa and 0.5 Pa \((P_{ref} = 1.0 \) Pa\) is considered much more reliable.
4.2.2 Pressure distribution along the receiver

The continuous vacuum chamber in the HITECO design extends over the full length of a Solar Collector Assembly (SCA) and the vacuum pump is placed in the middle to evacuate gases from both halves. Each half is composed of 6 Solar Collector Elements (SCE) with a length of 12 meters each as shown in figure 4-11, which results in a 72 meter long semi SCA.

![Figure 4-10: Conductance of a 1 meter long tube segment without and with support in the middle as a function of reference pressure.](image)

![Figure 4-11: Solar Collector Element (SCE) of the HITECO receiver.](image)
Every 6 meters two glass tube segments are joined to each other and a support structure is placed in the annular gap that centers the inner steel tube. In order to avoid uneconomical pumping costs seals with high air tightness are required and in the following calculation a maximum leak rate of $2 \times 10^{-4}$ mbar l/s is assumed for each connection. At an ambient temperature of 25 °C, this corresponds to $2.34 \times 10^{-10}$ kg/s of air entering every 6 meters and thus the mass flow purely due to leakage increases from the ends of the SCA to the middle when the vacuum pump is evacuating. The flow conductance of a semi SCE may be calculated by assuming that it is composed of five 1-m segments without support and one segment with a support structure in the middle and applying the formula for conductances connected in series,

$$\frac{1}{C} = \frac{1}{C_1} + \frac{1}{C_2} + \frac{1}{C_3} + \ldots$$  \hspace{1cm} (4.6)

The values obtained at different pressure levels are summarized in the table below.

<table>
<thead>
<tr>
<th>Outlet pressure [Pa]</th>
<th>Conductance [kg/(s*Pa)]</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.1</td>
<td>6.69e-8</td>
</tr>
<tr>
<td>0.5</td>
<td>6.59e-8</td>
</tr>
<tr>
<td>1.0</td>
<td>6.76e-8</td>
</tr>
</tbody>
</table>

Due to the high air tightness of the system the leakage flow rates and the corresponding pressure drop along the receiver are expected to be small and hence the same conductance is used for all SCEs of a semi Solar Collector Assembly corresponding to the pressure level at the outlet to the vacuum pump. The pressure distribution during gas evacuation along a semi SCA due to leaks at the equally spaced glass connections may then be calculated and is shown in figure 4-12. As the mass flow increases towards the vacuum pump the pressure does not follow a linear function in axial coordinate and the total pressure drop along 72 meters is in the range of 0.27 Pa at all three pressure levels considered.
4. Results

Figure 4-12: Pressure distribution along a semi Solar Collector Assembly for three different pressure levels at the intake of the vacuum pump.

4.2.3 Effect of axial flow on conduction heat transfer

In the figure below the conductive heat loss along the receiver tube with pressures of 0.5 Pa and 0.1 Pa at the inlet and outlet respectively is compared to the results obtained by two-dimensional DS2V calculations at the corresponding pressure levels.

Figure 4-13: Conduction heat loss through air in axial flow as a function of pressure.
The reason for the slightly declining heat conduction rate towards both ends of the receiver segment in the axial flow simulation is that uniform flow boundaries are set in the DS3V program over the entire cross-section at the inlet and outlet. Hence the correct temperature gradient and conduction heat transfer rate corresponding to the surface temperatures are only established at a certain distance from the flow entry and exit. Apart from this effect heat conduction in the annular gap is not affected by axial flow in considered pressure range between 0.15 Pa and 1.5 Pa.
5 **DISCUSSION**

In this chapter the results obtained by the Direct Simulation Monte Carlo method are verified by means of an independence study of computational parameters and by comparison to analytical solutions available for the one-dimensional problems of radial heat exchange and axial flow between coaxial cylinders.

### 5.1 Accuracy and sensitivity of simulation results

As noted in chapter 2 there are random fluctuations present in the DSMC results due to the stochastic nature of the method. Therefore this section aims at determining the statistical accuracy of the direct simulation results and assessing their sensitivity to computational parameters set in the DS2V/DS3V programs.

#### 5.1.1 Errors due to scattering

**Heat transfer rate**

The heat flux $q_{i,gas}$ is sampled for all $N$ surface intervals and triangles by the DS2V and DS3V programs respectively. In the 2-D heat transfer simulations the semi absorber and glass tubes are represented by 60 straight line segments each, i.e. $N = 120$. The total heat conduction rate $Q'_{23,gas}$ is directly calculated by the average

$$Q'_{23,gas} = \text{mean}(2\pi r_2 q'_{2,i,gas}, 2\pi r_3 q'_{3,i,gas}),$$

and according to the central limit theorem in statistics the level of scatter $\sigma$ in this quantity may be characterized by
where the function \( \text{std}(\cdot) \) denotes the standard deviation. To describe the accuracy of the simulation results the absolute error \( 2\sigma \) is used here, which yields a level of significance of 5 \% if the results of identical simulations are normally distributed with mean \( Q_{23,\text{gas}}' \) and variance \( \sigma^2 \). In other words, the probability that the result of a repeated simulation lies within the confidence interval \( Q_{23,\text{gas}}' \pm 2\sigma \) is 95\%. It is noted that the normal distribution of results obtained by equal simulations is not verified in this project and the actual probability might be different, but values within the confidence interval formulated above were reproduced successfully for several cases by repetition.

In this project simulations are only performed for eventual steady flows and hence the scattering may be reduced by time averaging. Accordingly, once a steady state is achieved the calculations are usually continued for a reasonable long time to achieve large sample sizes such that the fractional deviation \( 2\sigma/Q_{23,\text{gas}}' \) becomes smaller than 1 \%. The absolute and relative errors of some DS2V calculations are given in table 5-1.

<table>
<thead>
<tr>
<th>Pressure [Pa]</th>
<th>Krypton, VHS ( 2\sigma / Q_{23,\text{gas}}' ) [%]</th>
<th>Air, VSS Zr = f(T) ( 2\sigma / Q_{23,\text{gas}}' ) [%]</th>
<th>Air, VSS Zr = const. ( 2\sigma / Q_{23,\text{gas}}' ) [%]</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.05 [W/m] 0.24%</td>
<td>0.08 [W/m] 0.15%</td>
<td>0.13 [W/m] 0.26%</td>
</tr>
<tr>
<td>10</td>
<td>0.18 [W/m] 0.37%</td>
<td>0.53 [W/m] 0.41%</td>
<td>0.75 [W/m] 0.56%</td>
</tr>
<tr>
<td>50</td>
<td>1.15 [W/m] 2.07%</td>
<td>2.70 [W/m] 1.79%</td>
<td>5.23 [W/m] 3.23%</td>
</tr>
<tr>
<td>100</td>
<td>1.67 [W/m] 2.92%</td>
<td>2.63 [W/m] 1.69%</td>
<td>9.56 [W/m] 5.61%</td>
</tr>
</tbody>
</table>

It may be seen that the error bars are insignificant to the thermal performance of the solar receiver for pressures in the annulus up to 10 Pa. At higher pressures, however, it was not possible to achieve a relative error below 1 \% due to the limited computational resources, and 100 Pa \( (Kn = 0.0033) \) is considered as the upper limit in this application that may be simulated on a personal notebook, mainly because of the long computation time required to achieve a steady flow. Nevertheless, the continuum regime results obtained for krypton by the VHS model and for air using the VSS model with variable \( Z_r \) are considered reliable. Comparable scattering levels are produced by the VSS model for krypton and both VHS variants for air respectively, whereas the VSS model with constant \( Z_r = 5 \) shows much higher statistical deviations although the simulations are run for
a similarly long time as for the other molecular models of air. It was found that the VSS model with constant $Z_r$ delivers different values for the heat conduction rates at the absorber $Q'_{2,gas} = \text{mean}(2\pi r_2 q'_{2,i,gas})$ and at the vacuum jacket $Q'_{3,gas} = \text{mean}(2\pi r_3 q'_{3,i,gas})$, which increases the standard deviation $\sigma$ of the mean heat transfer rate $Q'_{23,gas}$ (cf. figure 5-1). This indicates that either no steady-state is achieved or energy is not conserved in the simulation, and the reason for this has not been elaborated yet. The use of the VSS model with constant $Z_r$ in the DS2V/DS3V programs is therefore not recommended.

![Figure 5-1](image_url)  

**Figure 5-1:** Deviation between heat transfer rates at absorber and glass jacket for VSS model with constant $Z_r$.

### Mass flow rate

As no record of molecules entering and leaving through specified flow entry boundaries is provided by the DS3V program, the mass flow rate $\dot{M}$ needs to be calculated by means of the density $\rho$ and the axial velocity component $u$ in the flow field, which are both subject to fluctuations. To reduce scattering the mass flow is averaged over the entire flow domain,

$$\dot{M} = \frac{1}{h} \int_0^h \dot{M}(x) dx = \frac{1}{h} \iiint_V \rho(x,y,z)u(x,y,z) dV,$$

where $h$ is the axial length of the segment and $V = Ah$ the flow volume. The DSMC method delivers a discrete description of the macroscopic properties in space and hence the integral is replaced by a sum,
Here $N_c$ is the number of sampling cells, $N$ the number of molecule simulators, $n$ the number density, $F_N = nV/N = V/\sum_{i=1}^{N_c} N_i/n_i$ the number of real molecules represented by each simulated molecule and the index $i$ denotes the properties in cell $i$. The second step in the equation above is necessary because the cell volumes $V_i$ are not given in the output file of the DS3V program. The definition of a measure of dispersion for the mass flow rate is not straightforward. One possibility is to divide the flow field into $N_x$ axial segments and to calculate the local mass flow rate $\dot{M}(x)$ according to equation (5.4) by summing up over the cells $N_{c,x}$ within the interval $(x - \Delta x/2, x + \Delta x/2)$ only and replacing $h$ by $\sum_{i=1}^{N_{c,x}} V_i/A$. The statistical error may then be defined in the same way as for the heat transfer rate,

$$\sigma = \frac{\text{std} \left( \dot{M}(x) \right)}{\sqrt{N_x}}. \tag{5.5}$$

As $\sigma$ depends on the arbitrarily chosen number of axial divisions, its significance is limited. However, it is noted that the value of $\dot{M}$ is based on the average properties of the entire flow volume and as typically millions of molecules are simulated in three-dimensional calculations, the statistical noise is usually small. For verification some results were reproduced and the relative deviation between the values was far below 1%.

Generally the scatter is higher at lower relative pressure differences $(P_{in} - P_{out})/P_{in}$ as the macroscopic flow velocity is then smaller and thus the noise caused by the thermal motion of the molecules is comparatively larger. However, it has been verified by reproduction of results that the unrealistically high conductance predicted by the simulation with $P_{in} = 1.1$ Pa and $P_{out} = 1.0$ Pa is not due to scattering. The pressure distribution along the receiver section obtained by the simulation is shown in the figure below.
Figure 5-2: Pressure distribution along solar receiver segment with air in on-sun configuration.

Apparently the gas pressure increases rapidly in a small interval starting at the inlet and likewise a sharp decrease takes place in front of the outlet, which is not observed at a higher inlet pressure of $P_{in} = 1.5$ Pa. It was assumed first that this effect is caused by the uniform flow boundary conditions although a temperature difference is applied to the inner and outer cylindrical surfaces. However, more accurate boundaries taking a radial temperature variation into account did not solve the problem and the same effect is encountered, even though to a lesser extent, in the simulation at pressures $P_{in} = 0.6$ Pa and $P_{out} = 0.5$. It is therefore concluded that the issue is due to the low relative pressure difference and $(P_{in} - P_{out})/P_{in} > 0.2$ is proposed here for axial flow simulations using the DS3V code. The high level of scatter in the results of low velocity flows produced by the DSMC method has led to the introduction of modifications such as the information preservation (IP) method described in (Shen 2005) or the molecular block (MB) model presented in (Pan, Ng et al. 2001). The applicability of these techniques to the axial flow problem at smaller pressure differences might be evaluated.

### 5.1.2 Effect of number of molecules

If the standard computational options are utilized in the DS2V/DS3V programs, which are adequate in most cases, the only parameter that needs to be specified by the user is the initial number of simulated molecules used in the calculation. As stated in the user manual this number should be
chosen large enough such that the ratio of the mean collision separation to the mean free path
\((\text{MCS}/\text{MFP})\) is smaller than 0.2 in the large part of the flow field. The sensitivities of the heat
transfer and mass flow results to this parameter have been analyzed by means of 2-D simulations
for air at 10 Pa using the VHS model along with a constant \(Z_r\) and by 3-D isothermal flow
simulations with \(P_{\text{in}} = 1.5\) Pa and \(P_{\text{out}} = 0.5\) Pa for xenon at 300 K respectively.

It is seen in figure 5-3 that for \(\text{MCS}/\text{MFP} > 0.4\) the result is somewhat out of bounds. As the number
of molecules is increased the heat transfer rate approaches a limit and convergence is achieved for
\(\text{MCS}/\text{MFP} < 0.05\). Therefore the 2-D simulations are usually performed with a sufficiently large
number of molecules such that this condition is satisfied, except for the simulations at 50 Pa and
100 Pa for which the ratio is slightly higher in order to reduce computation time.

![Figure 5-3: Heat transfer rate and MCS/MFP ratio as a function of number of simulated molecules.](image)

For the mass flow a similar behavior is observed, i.e. the flow rate increases with the number of
molecules. In this particular case, however, it was not possible to reach convergence due to the low
Knudsen number of the problem \((Kn = 0.1)\), which is right at the limit to the slip flow regime. It is
thus expected that the actual mass flow rate is somewhat higher than predicted by the simulation
with \(\text{MCS}/\text{MFP} = 0.17\).
5. Discussion

Figure 5-4: Mass flow rate and MCS/MFP ratio as a function of number of simulated molecules.

For the 3-D simulations with air in on-sun arrangement the temperature and thus the Knudsen number are higher and convergence may be achieved at less computational cost. However, the large radial temperature gradient requires a finer grid in this direction because an insufficient resolution of the flow details can lead to unphysical effects. This may be achieved either by increasing the number of molecules, which slows down the simulation, or by changing the default number of cells in the three spatial directions. In this project a combination of the two options has been chosen. As the axial flow gradients in a 1 meter long receiver section are much smaller than the radial ones, the number of cells in both spatial directions of the cross-sectional area is typically doubled while the cells along the axial coordinate are reduced.

5.2 Comparison to analytical solutions

5.2.1 Conduction heat transfer

A detailed treatment of the one-dimensional heat conduction problem between two concentric cylinders with radii $r_i$ and $r_o$ ($r_i < r_o$) may be found in (Sharipov and Bertoldo 2006). The temperature of the outer cylinder is denoted by $T_o$ and the temperature of the inner cylinder is
5. Discussion

\( T_i = T_o + \Delta T \) with \( \Delta T > 0 \). The equation of heat conduction in one dimension in a continuum may be written in cylindrical coordinates as

\[
\frac{d}{dr} \left( r \frac{dT}{dr} \right) = 0, \quad \text{(5.6)}
\]

and the heat flux is given by Fourier’s law,

\[
q'' = -K \frac{dT}{dr}, \quad \text{(5.7)}
\]

where \( K \) is the thermal conductivity.

In the continuum regime (\( Kn < 0.01 \)) the temperature boundary conditions are given by the surface temperatures, i.e.

\[
T = \begin{cases}
T_i, & \text{at } r = r_i, \\
T_o, & \text{at } r = r_o,
\end{cases} \quad \text{(5.8)}
\]

and the well-known expression for the radial heat transfer rate \( Q' = 2\pi rq'' \) in units W/m is obtained,

\[
Q'_c = \frac{2\pi K \Delta T}{\ln(r_o/r_i)} \quad \text{(5.9)}
\]

In the slip regime (\( 0.1 > Kn > 0.01 \)) Fourier’s law is still applicable, but the boundary conditions need to be modified to

\[
T = \begin{cases}
T_i + \zeta_{T_i} \frac{dT}{dr}, & \text{at } r = r_i, \\
T_o - \zeta_{T_o} \frac{dT}{dr}, & \text{at } r = r_o,
\end{cases} \quad \text{(5.10)}
\]

Here \( \lambda \) is the viscosity-based mean free path as defined in equation (1.8) and \( \zeta_{T_i} \) and \( \zeta_{T_o} \) are the temperature jump coefficients at the inner and outer cylinders respectively. The conduction heat transfer rate in slip regime may then be expressed according to (Sharipov and Bertoldo 2006) by

\[
Q'_s = 2\pi KB\Delta T, \quad \text{(5.11)}
\]

\[
B = \left[ \ln \frac{r_o}{r_i} + \frac{1}{\delta \left( \zeta_{T_i} + \zeta_{T_o} \frac{r_i}{r_o} \right)} \right]^{-1}.
\]

In this solution the rarefaction parameter \( \delta = \frac{r_i P}{(\mu c_{mp})} \) is defined using the radius of the inner cylinder as characteristic length.
It is noted that the analytical solution is derived for small temperature gradients between the cylinders and thus a constant thermal conductivity is assumed along the radius. However, the temperature difference in the HITECO receiver is significant (> 300 °C) and as the thermal conductivity $K$, viscosity $\mu$ and most probable thermal speed $c_{mp} = \sqrt{\frac{2kT}{m}}$ are functions of temperature, one difficulty in the analytical solution consists of specifying an adequate “average” temperature. Here the mean temperature of the gas in the corresponding DSMC simulation is utilized to calculate the viscosity and thermal conductivity according to the gas properties in the appendix.

The two slip solutions shown in figure 5-5 differ in the value of the temperature jump coefficient, which generally depends on the energy accommodation of gas molecules to the surface. In solution (1) the temperature jump coefficient is calculated by the following equation for polyatomic gases (Sharipov 2011),

$$\zeta_r = \frac{\gamma}{\gamma + 1} \frac{\Pr}{\alpha_d} \left( 2 - \frac{\alpha_d}{\alpha_d} + 0.17 \right),$$

(5.12)

where $\gamma$ is the specific heat ratio, $\alpha_d$ the fraction of diffuse reflection and $\Pr = \mu/(Kc_p)$ the Prandtl number. Constant values of $\gamma = 1.4$ and $c_p = 1005 \text{ J/(kg} \cdot \text{K)}$ are used for the specific heat of air, whereas the ratio of the viscosity $\mu$ to the thermal conductivity $K$ is evaluated at the surface temperatures $T_i$ and $T_g$ for the temperature jump coefficients at the outer absorber and inner glass tubes respectively. $\alpha_d$ is set to unity corresponding to completely diffuse reflection from the walls, whereas in solution (2) the jump coefficients from (Roesle and Coskun 2011) are utilized that consider partial surface accommodation effects. The corresponding values are shown in the table below.

<table>
<thead>
<tr>
<th></th>
<th>Solution (1)</th>
<th>Solution (2)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Absorber</td>
<td>1.817</td>
<td>2.193</td>
</tr>
<tr>
<td>Glass jacket</td>
<td>1.727</td>
<td>2.232</td>
</tr>
</tbody>
</table>

The difference in conduction heat loss predicted by the two analytical expressions may be regarded as a measure of influence of gas-surface interactions on heat transfer. It is seen in figure 5-5 that the effect is significant in the transitional and slip regimes whereas at pressures above 50 Pa the two curves converge to the continuum value. Towards the free molecule range the fractional deviation
keeps increasing, but the absolute value of conductive heat transfer becomes so small that it no longer affects the thermal performance of the solar receiver.

![Graph](image.png)

Figure 5-5: Conduction heat transfer through air in off-sun configuration compared to 1-D analytical solutions in slip regime.

As expected solution (2) reproduces precisely the simulation results of the ANSYS CFX model, whereas solution (1) provides a good approximation to the DSMC simulations at pressures of 5 Pa and higher. As the pressure decreases below 5 Pa the DSMC method starts to deviate from the analytical solution. This behavior is not unexpected, since the limit of $Kn = 0.1$, above which the continuum approach loses its validity, is reached at 3.2 Pa. Accordingly the DSMC results are considered more reliable in the transitional and free-molecular regions and, as diffuse boundary conditions with complete accommodation to the surface temperatures are used in the simulations, they may be regarded as an upper limit to conduction heat loss over the full pressure range.

### 5.2.2 Axial flow

The problem of a rarefied gas flowing through an annular tube is studied in (Breyiannis, Varoutis et al. 2008). Considered are again two coaxial cylinders with radii $r_i$ and $r_o$ and height $h$. The pressure boundary conditions are given by
where $x$ is the axial coordinate and $P_{in} > P_{out}$, i.e. the pressure gradient in $x$-direction is negative. The mass flow may then be defined by means of the dimensionless flow rate $G$ as

$$
M = -G \frac{Ad_h dP}{c_{mp} dx}
$$

where $A = \pi(r_o^2 - r_t^2)$ is the cross-sectional area of the flow and $d_h = 2(r_o - r_t)$ the hydraulic diameter.

In the slip regime the dimensionless flow rate $G$ may be calculated as the sum of the continuum solution $G_c$ and a slip correction term $G_s$,

$$
G = G_c + G_s = \frac{\delta}{4} \left[ r_1^2 + r_2^2 + \frac{1}{2} \ln \left( \frac{r_1}{r_2} \right) \right] + \frac{\sigma_p}{2} \left[ 1 + 2r_1 r_2 + \frac{r_1}{\ln(r_1/r_2)} + \frac{(r_1 + r_2)^2}{8r_1 r_2 \ln(r_1/r_2)} \right].
$$

Here $r_1 = r_t/d_h$ and $r_2 = r_o/d_h$ are the normalized radii, $\delta = d_h P/(\mu c_{mp})$ is the rarefaction parameter based on the hydraulic diameter and $\sigma_p$ the viscous slip coefficient, which like the temperature jump coefficient depends on the gas-surface interaction. An overview of numerical data for the viscous slip coefficient is given in (Sharipov 2011) and for completely diffuse reflection from the walls a value of $\sigma_p = 1$ is recommended. Inserting equation (5.15) into (5.14) yields an ordinary differential equation, which may be solved subject to the boundary conditions (5.13) for the mass flow rate,

$$
M_s = \frac{1}{h} \left[ \left( \frac{G_c}{\delta} \right) \frac{Ad_h^2}{\mu c_{mp}} \left( P_{in}^2 - P_{out}^2 \right) + G_s \frac{Ad_h}{c_{mp}} (P_{in} - P_{out}) \right].
$$

For the PTR 70 receiver the ratio of inner to outer radius is $r_t/r_o = 0.6$ and the purely geometric expressions amount to $G_c/\delta = 0.0418$ and $G_s/\sigma_p = 0.504$.

The mass flow rate in transitional regime may be obtained via kinetic theory by solving the kinetic equations. In (Breyiannis, Varoutis et al. 2008) the fully developed flow through concentric circular pipes due to an external pressure gradient is simulated by the BGK model using diffuse-specular boundary conditions and detailed tables are given for the dimensionless flow rate $G$ in terms of
radius ratio \( r_i/r_o \) and gas rarefaction \( \delta \), covering the whole range of Knudsen numbers. An extract for a radius ratio of 0.6 and completely diffuse reflection is shown in table 5-3.

Table 5-3: Dimensionless flow rate as a function of rarefaction for completely diffuse reflection and radius ratio of 0.6 (Breyiannis, Varoutis et al. 2008).

<table>
<thead>
<tr>
<th>( \delta )</th>
<th>0.01</th>
<th>0.1</th>
<th>0.5</th>
<th>1</th>
<th>2</th>
<th>5</th>
<th>10</th>
<th>100</th>
</tr>
</thead>
<tbody>
<tr>
<td>( G )</td>
<td>0.8560</td>
<td>0.8375</td>
<td>0.7736</td>
<td>0.7533</td>
<td>0.7537</td>
<td>0.8274</td>
<td>1.007</td>
<td>4.707</td>
</tr>
</tbody>
</table>

Here the gas rarefaction parameter is defined by the mean pressure, i.e. \( \delta = d_h (P_{in} + P_{out}) / (2\mu c_{mp}) \). The corresponding dimensionless flow rate is obtained by interpolation from the tables and the mass flow rate in transitional regime may be directly calculated by

\[
\dot{M}_t = -G \frac{A d_h (P_{in} - P_{out})}{c_{mp}} h
\]  

(5.17)

It is noted that the slip and transitional solutions both involve the viscosity \( \mu \) and the most probable molecular speed \( c_{mp} \), which are calculated here by the average temperature \( T = 1/2(T_i + T_o) \) of the outer absorber and the inner glass jacket surfaces. The resulting conductances of a 1 meter long receiver section with air in the annulus are plotted as a function of reference pressure \( P_{ref} = (P_{in} + P_{out})/2 \) in figure 5-6 and compared to the simulation results obtained by the DSMC method and the 3-D ANSYS CFX model (Coskun 2011).

The DSMC simulations cover a Knudsen number range of \( 2.2 > Kn > 0.22 \) and deliver results that are consistent with the solution of the kinetic equations in (Breyiannis, Varoutis et al. 2008), with a maximum fractional deviation of 4 % observed at \( Kn = 0.27 \). Similarly the results obtained by the 3-D CFX model are in good agreement with the slip flow solution, although different temperature boundary conditions are utilized in the ANSYS simulations. The underestimation of flow rate by the continuum approach in the considered range of the transitional regime varies between 32 % at \( Kn = 2.2 \) and 12 % at \( Kn = 0.22 \). This discrepancy may strongly affect the calculation of the pressure distribution along the solar receiver, and as the Navier-Stokes equations with slip boundary conditions are generally valid for \( Kn < 0.1 \), it is recommended to use the conductances predicted by the DSMC method in the transitional regime.
The analytical solutions are derived for a constant viscosity in the flow domain and a mean value corresponding to the average of the absorber and vacuum jacket temperatures is used in the calculation of the values shown above. In order to separate the problem of axial flow from the issue of a radial temperature gradient DSMC simulations are also performed under isothermal conditions at 300 K. For these calculations the heavy inert gas xenon is selected and the variable hard sphere model with standard parameters is applied. The results are shown in the figure below and compared to analytical solutions and values obtained by ANSYS simulations under similar conditions. As the temperature in this kind of simulations is smaller than in the irradiated case, the gas density is generally higher and DSMC simulations are only carried out up to a reference pressure of 1 Pa, covering $0.66 > Kn > 0.1$. $Kn = 0.1$ is considered as the lowest Knudsen number for which the CPU and memory requirements of a 3-D simulation of a 1 meter long receiver segment may be handled by a personal notebook and corresponds exactly to the limit between the transition and slip regimes.
Figure 5-7: Conductance of 1 meter long segment without support for isothermal xenon at 300 K compared to analytical solutions.

The continuum models coincide exactly, while the DSMC method lies between the slip solution and the BGK model at high Knudsen numbers and converges to the CFX results at $Kn = 0.1$. However, due to the effect described in section 5.1, it is probable that more simulated molecules should be used in the last two simulations at 0.75 Pa and 1 Pa to avoid the underprediction of flow rate and exact convergence between the Direct Simulation Monte Carlo method and the ANSYS CFX model is thus expected at lower Knudsen numbers.

For the problem of an annular duct with a support structure in the middle no analytical solution is available and the DSMC results may only be compared to that of the ANSYS CFX model. In the figure below the ratio of the flow rate with support to that achieved without blockage of the flow is plotted for the irradiated air and isothermal xenon problems. In both cases the continuum approach seems to overestimate the flow restriction by the support structure. As for the conductance without support discussed above it is expected to reach convergence for xenon at 300 K at pressures slightly higher than 1 Pa. The discrepancy between the microscopic and macroscopic models for air in on-sun arrangement is much larger, which is due to the higher Knudsen number and different surface boundary conditions in the simulations.
Finally it is noted that all three-dimensional DSMC simulations of axial flow are performed at pressure levels for which the influence of the molecular model utilized to calculate the collisions between molecules on the simulation results is marginal. As the analysis is extended to lower Knudsen numbers, it has to be verified whether the molecular models identified in the 2-D heat conduction problem, i.e. the variable soft sphere model with temperature dependent rotational relaxation collision number for air and the VHS model for a simple monoatomic gas, converge to the continuum solution.
6 CONCLUSION

A two-dimensional heat transfer model of a solar parabolic trough receiver has been developed using the Direct Simulation Monte Carlo method to simulate conduction heat transfer through the rarefied gas in the annular gap between the absorber and vacuum jacket tubes. The gas simulations are coupled to an overall heat transfer model that includes convection to the heat transfer fluid and the environment, conduction in the receiver tube walls and thermal radiation from the absorber and glass surfaces modeled using the gray band approximated radiosity method for semi-transparent enclosures. The non-uniform incident solar flux on the receiver is determined using a Monte Carlo ray tracing approach. The treatment of radiation at this level of detail is necessary to provide realistic temperature boundary conditions for the gas conduction problem. Two-dimensional heat transfer simulations are performed for the off-sun configuration, corresponding to lab-scale heat loss tests, and in on-sun arrangement, simulating normal operation conditions. In addition the effect of axial flow occurring during vacuum pumping is examined by three-dimensional DSMC calculations and the results are compared to a similar series of simulations accomplished using a continuum model of the rarefied gas with slip boundary conditions (Roesle and Coskun 2011).

It is found that the intermolecular collision model of gas molecules begins to affect heat conduction at pressures above 1 Pa and appropriate phenomenological models for the simulation of conductive heat transfer, which converge to the continuum solution at 100 Pa ($Kn < 0.01$), have been identified for air and krypton. For krypton highly consistent heat transfer rates are obtained by the two models over the full range of Knudsen number $27 > Kn > 0.0027$, with a maximum deviation of 0.5 W/m at 2.5 Pa. For air the DSMC method generally predicts higher conduction heat loss than the continuum approach and the largest difference of 6 W/m is observed at 1 Pa ($Kn = 0.33$). The relative deviation between the two models continues to increase at lower pressures, but the absolute value of the conduction heat loss becomes so small that it is no longer of interest from a receiver technology point of view. Because the continuum model with slip boundaries is generally accurate for $Kn < 0.1 (P > 3 \text{ Pa})$, the DSMC simulations are considered more reliable. However, it is
noted that like the results obtained by continuum models, the heat transfer rates predicted by the DSMC method depend on gas-surface interactions in the pressure range of interest between 0.1 Pa and 10 Pa. The diffuse reflection model utilized in the simulations therefore provides an upper limit of conduction heat loss at the considered pressure levels and validation through experiments is required.

The average surface temperatures calculated by the overall heat transfer model are found to be consistent with those obtained by continuum simulations and the difference in total heat loss predicted by the two models is mainly due to different gas conduction rates. The highest deviations in mean temperature of the vacuum jacket occur at 1 Pa and amount to 0.9 °C and 0.5 °C in the off-sun and on-sun cases respectively. The geometry and spectral properties used in the overall heat transfer model correspond to those specified for current state-of-the-art receivers and simulations have been performed exclusively for a HTF temperature of 400 °C. These parameters may be varied to evaluate the thermal performance of different designs.

For the 3-D simulations performed from 0.15 Pa up to 1.5 Pa (2.2 > Kn > 0.22) it is found that axial flow does not affect the heat conduction rate across the annulus. The flow conductance predicted by the DSMC method is in close agreement with a correlation for isothermal flow (Breyiannis, Varoutis et al. 2008) in the considered pressure range, whereas the continuum model yields substantially lower values. The fractional deviation between the models is in the range of 10-20 %, increasing with Knudsen number, and due to the high degree of rarefaction it is concluded that the slip flow model is outside its range of validity. Accordingly, the pressure drop along the solar receiver calculated by the DSMC results when the vacuum pump is operating is significantly lower for the same rate of leakage, thus reducing pumping requirements. Convergence between the two models is expected for Kn < 0.1, which needs to be verified through DSMC simulations at higher pressures.

It is important to note that the heat loss due to conduction through the gas is small compared to that by radiation, but conductive heat transfer may become significant in absolute terms in large-scale applications. For air in the annular gap at 1 Pa the share of gas conduction in total heat loss is evaluated at 12.5 % (47.8 W/m) in this project. Considering for instance the 50 MW<sub>e</sub> Andasol power plant located in Spain that has roughly 90 km of receivers, this sums up to 4.3 MW and the difference between the DSMC simulation and the continuum model amounts to no less than 0.5 MW. This thesis provides technical data to an economic analysis of the receiver that will determine the optimal operating pressure and vacuum system in order to minimize the cost of electricity.
ACKNOWLEDGEMENT

At the end of this thesis I want to express my thanks to all people who enabled and contributed to this project. First of all to my Professor Aldo Steinfeld, who admitted me to his research group and gave me the opportunity to perform my thesis on this exciting topic. Secondly I would like to thank Volkan Coskun for his preceding work on the subject and all the other people from the lab of Renewable Energy Carriers at ETH Zurich for the special atmosphere on the edge of research. My special thanks go to my supervisor Dr. Matt Roesle for guiding the whole project to a success while leaving me the freedom to conduct my research, and who always had an answer ready to my questions. Last but not least I want to thank the European Commission for funding the HITECO project and for their effort in promoting renewable energy technologies.
REFERENCES


APPENDIX

A Gas properties

All gas simulations in this project are performed with the representative properties summarized in the table below.

Table A-1: Gas properties under standard conditions (101,325 Pa and 0°C) and model parameters used in DSMC simulations (Bird 1994).

<table>
<thead>
<tr>
<th>Gas</th>
<th>Molecular mass $m \times 10^{27}\text{kg}$</th>
<th>Viscosity coefficient $\mu \times 10^5\text{Pa}\cdot\text{s}$</th>
<th>Viscosity index $\omega$</th>
<th>VSS parameter $\alpha$</th>
<th>VHS diameter $d \times 10^{10}\text{m}$</th>
<th>VSS diameter $d \times 10^{10}\text{m}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nitrogen (N$_2$)</td>
<td>46.5</td>
<td>1.656</td>
<td>0.74</td>
<td>1.36</td>
<td>4.17</td>
<td>4.11</td>
</tr>
<tr>
<td>Oxygen (O$_2$)</td>
<td>53.12</td>
<td>1.919</td>
<td>0.77</td>
<td>1.4</td>
<td>4.07</td>
<td>4.01</td>
</tr>
<tr>
<td>Argon (Ar)</td>
<td>66.3</td>
<td>2.117</td>
<td>0.81</td>
<td>1.4</td>
<td>4.17</td>
<td>4.11</td>
</tr>
<tr>
<td>Krypton (Kr)</td>
<td>139.1</td>
<td>2.328</td>
<td>0.8</td>
<td>1.32</td>
<td>4.76</td>
<td>4.7</td>
</tr>
<tr>
<td>Xenon (Xe)</td>
<td>218</td>
<td>2.107</td>
<td>0.85</td>
<td>1.44</td>
<td>5.74</td>
<td>5.65</td>
</tr>
</tbody>
</table>

It is noted that the reference diameters of the VHS and VSS models in the table above are defined for the mean value of $c_r^{2\omega-1}$ in an equilibrium gas at temperature $T_{ref} = 273$ K, which may be calculated by means of the Maxwell distribution function,

$$
\frac{c_r^{2\omega-1}}{c} = \sqrt{\frac{2kT_{ref}/m_r}{I(5/2 - \omega)}},
$$

(A.1)
Appendix

Here $\Gamma$ denotes the gamma function and $m_r$ is the reduced mass of two molecules. For this effective relative speed the reference diameter may be written as

$$d_{\text{ref}} = \sqrt{\frac{5(\alpha + 1)(\alpha + 2)\sqrt{m k_{\text{ref}}/\pi}}{4\alpha(5 - 2\omega)(7 - 2\omega)\mu_{\text{ref}}}}$$  \hfill (A.2)

and the total collision cross-section at relative speed $c_r$ is obtained by

$$\sigma_T = \pi d^2 = \pi d_{\text{ref}}^2 c_r^{2\omega - 1}/c_r^{2\omega - 1}.$$  \hfill (A.3)

The reference diameter of the VHS model is calculated using $\alpha = 1$, and it is noted that the same collision cross-sections are obtained as by equations (2.36) and (2.42) for the two models (Bird 1994).

The gas properties used in the analytical solutions shown in section 5.2 are calculated directly from the table above for monoatomic gases, using

$$\mu = \mu_{\text{ref}} \left(\frac{T}{T_{\text{ref}}}\right)^\omega$$  \hfill (A.4)

and the first approximation of the Chapman-Enskog solution for the thermal conductivity,

$$K = \frac{15}{4} \frac{k}{m} \mu.$$  \hfill (A.5)

As this expression is not valid for polyatomic gases with internal degrees of freedom the dilute gas correlation equations from (Lemmon and Jacobsen 2004) are utilized for the properties of air. Some values in the temperature range of interest in this project are shown in the following table.

<table>
<thead>
<tr>
<th>Temperature</th>
<th>Viscosity [Pa·s]</th>
<th>Conductivity [W/m]</th>
<th>Temperature</th>
<th>Viscosity [Pa·s]</th>
<th>Conductivity [W/m]</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>1.82E-05</td>
<td>0.0258</td>
<td>220</td>
<td>2.68E-05</td>
<td>0.0395</td>
</tr>
<tr>
<td>40</td>
<td>1.92E-05</td>
<td>0.0273</td>
<td>240</td>
<td>2.76E-05</td>
<td>0.0407</td>
</tr>
<tr>
<td>60</td>
<td>2.01E-05</td>
<td>0.0288</td>
<td>260</td>
<td>2.83E-05</td>
<td>0.0420</td>
</tr>
<tr>
<td>80</td>
<td>2.10E-05</td>
<td>0.0302</td>
<td>280</td>
<td>2.91E-05</td>
<td>0.0432</td>
</tr>
<tr>
<td>100</td>
<td>2.19E-05</td>
<td>0.0316</td>
<td>300</td>
<td>2.98E-05</td>
<td>0.0444</td>
</tr>
<tr>
<td>120</td>
<td>2.28E-05</td>
<td>0.0330</td>
<td>320</td>
<td>3.05E-05</td>
<td>0.0456</td>
</tr>
<tr>
<td>140</td>
<td>2.36E-05</td>
<td>0.0343</td>
<td>340</td>
<td>3.12E-05</td>
<td>0.0468</td>
</tr>
<tr>
<td>160</td>
<td>2.44E-05</td>
<td>0.0356</td>
<td>360</td>
<td>3.19E-05</td>
<td>0.0479</td>
</tr>
<tr>
<td>180</td>
<td>2.52E-05</td>
<td>0.0369</td>
<td>380</td>
<td>3.26E-05</td>
<td>0.0491</td>
</tr>
<tr>
<td>200</td>
<td>2.60E-05</td>
<td>0.0382</td>
<td>400</td>
<td>3.33E-05</td>
<td>0.0502</td>
</tr>
</tbody>
</table>
B Calculation of configuration factors

The configuration factors between two diffuse surface areas $A_1$ and $A_2$, i.e. the fraction of energy leaving one surface that is incident on the other surface, are calculated in general by

$$F_{1-2} = \frac{1}{A_1} \int \int \frac{\cos \theta_1 \cos \theta_2}{\pi S^2} dA_2 dA_1,$$  \hspace{1cm} (B.1)

$$F_{2-1} = \frac{A_1}{A_2} F_{1-2}. \hspace{1cm} (B.2)$$

Here the configuration factors between two circumferential segments on coaxial cylinders with radii $r_1$ and $r_2$ ($r_1 < r_2$) are considered.

![Figure B-1: Configuration factors between circumferential cylinder segments.](image)

The distance $S$ expressed in the position coordinates of the two points $P_1 = (x_1, r_1, \phi_1)$ and $P_2 = (x_2, r_2, \phi_2)$ is

$$S^2 = r_1^2 + r_2^2 - 2r_1r_2 \cos(\phi_1 - \phi_2) + (x_2 - x_1)^2 \hspace{1cm} (B.3)$$

and the angles to the normal vectors of the surfaces are
The configuration factor between an inner cylinder segment with \( a_1 \leq x_1 \leq b_1, \alpha_1 \leq \varphi_1 \leq \beta_1 \), and a segment on the outer cylinder with \( a_2 \leq x_2 \leq b_2, \alpha_2 \leq \varphi_2 \leq \beta_2 \), may then be written as

\[
F_{1-2} = \frac{1}{A_1} \int_{a_1}^{b_1} \int_{a_2}^{b_2} \int_{a_1}^{b_1} \int_{a_2}^{b_2} \frac{(r_2 \cos(\varphi_1 - \varphi_2) - r_1)(r_2 - r_1 \cos(\varphi_1 - \varphi_2))}{\pi S^4} dx_2 dx_1 r_2 d\varphi_2 r_1 d\varphi_1,
\]

where the surface area is given by \( A_1 = (b_1 - a_1)(\beta_1 - \alpha_1)r_1 \). In the above formula integration over the axial coordinates may be performed analytically, which yields

\[
f = \int_{a_1}^{b_1} \int_{a_2}^{b_2} 1 / S^4 dx_2 dx_1
\]

\[
= \frac{4}{\Delta^{3/2}} \left[ -(b_2 - b_1) \tan^{-1} \left( \frac{2(b_2 - b_1)}{\sqrt{\Delta}} \right) + (b_2 - a_1) \tan^{-1} \left( \frac{2(b_2 - a_1)}{\sqrt{\Delta}} \right) \right]
\]

\[
+ (a_2 - b_1) \tan^{-1} \left( \frac{2(a_2 - b_1)}{\sqrt{\Delta}} \right) - (a_2 - a_1) \tan^{-1} \left( \frac{2(a_2 - a_1)}{\sqrt{\Delta}} \right),
\]

with

\[
\Delta = 4(r_1^2 + r_2^2 - 2r_1 r_2 \cos(\varphi_1 - \varphi_2)).
\]

For the calculation of the configuration factors in the 2-D heat transfer model the axial dimension of the first circumferential segment has to be small compared to that of the second segment to minimize the fraction of rays leaving through the top and the bottom of the cylinders, e.g. \(-0.1 \leq x_1 \leq 0.1\) and \(-10 \leq x_2 \leq 10\). Due to the complexity of the expression integration over the circumferential coordinates needs to be achieved numerically, using for example the Matlab function "quad2d" and the configuration factors are obtained by

\[
F_{1-2} = \frac{1}{A_1} \frac{r_1 r_2}{\pi} \int_{a_1}^{b_1} \int_{a_2}^{b_2} f(r_2 \cos(\varphi_1 - \varphi_2) - r_1)(r_2 - r_1 \cos(\varphi_1 - \varphi_2)) d\varphi_2 d\varphi_1,
\]

\[
F_{2-1} = \frac{r_1}{r_2} F_{1-2}.
\]

It is noticed that the view between points \( P_1 \) and \( P_2 \) is blocked by the absorber tube if \(|\varphi_2 - \varphi_1| > \delta = \cos^{-1}(r_1/r_2)\) and hence integration is not carried out over the full surface areas if the angular
displacement between the segments permits values of $|\varphi_2 - \varphi_1| > \delta$. In these cases the upper boundary of the second integral in equation (B.8) has to be adapted as follows:

$$
\beta_2(\varphi_1) = \begin{cases} 
\min(\varphi_1 + \delta, \beta_2), & \text{if } \alpha_2 - \alpha_1 < \delta < \beta_2 - \alpha_1, \\
\max(\varphi_1 + \delta, \alpha_2), & \text{if } \alpha_2 - \alpha_1 = \beta_2 - \beta_1 > \delta.
\end{cases}
$$

(B.10)

To determine the configuration factors between two surface segments located on the outer cylinder, two points $P_1 = (x_1, r_2, \varphi_1)$ and $P_2 = (x_2, r_2, \varphi_2)$ at radius $r_2$ are considered. The distance $S$ is then given by

$$
S^2 = 2r_2^2(1 - \cos(\varphi_1 - \varphi_2)) + (x_2 - x_1)^2
$$

(B.11)

and the angles may be expressed as

$$
\cos \theta_1 = \cos \theta_2 = \frac{r_2(1 - \cos(\varphi_1 - \varphi_2))}{S}.
$$

(B.12)

Equation (B.6) for the factor $f$ is still valid, but with

$$
\Delta = 8r_2^2(1 - \cos(\varphi_1 - \varphi_2)).
$$

(B.13)

The configuration factor is then obtained by numerical integration of

$$
F_{2-2} = \frac{1}{A_1} \frac{1}{\pi} \frac{r_2^4}{\alpha_1} \int_{\alpha_1}^{\beta_1} \int_{\alpha_2}^{\beta_2} f(1 - \cos(\varphi_1 - \varphi_2))^2 \, d\varphi_2 \, d\varphi_1,
$$

(B.14)

where the surface area of the first segment is given by $A_1 = (b_1 - a_1)(\beta_1 - \alpha_1)r_2$. It is seen that the view between two points on the outer cylinder is blocked if $|\varphi_2 - \varphi_1| > 2\delta = 2 \cos^{-1}(r_1/r_2)$, and again the upper boundary of the second integral needs to be modified in these cases:

$$
\beta_2(\varphi_1) = \begin{cases} 
\min(\varphi_1 + \delta, \beta_2), & \text{if } \alpha_2 - \alpha_1 < 2\delta < \beta_2 - \alpha_1, \\
\max(\varphi_1 + \delta, \alpha_2), & \text{if } \alpha_2 - \alpha_1 = \beta_2 - \beta_1 > 2\delta.
\end{cases}
$$

(B.15)

The configuration factors obtained if each cylinder is divided into 120 circumferential elements as applied in the two-dimensional heat transfer model are given in the table below in terms of the angular displacement between the segments. The outer radii $r_2 = 0.0575$ m and $r_2 = 0.05875$ m correspond to the inner glass radius (opaque glass) and to the mean radius of the vacuum jacket (semi-transparent glass) respectively.
Table B-1: Configuration factors as a function of circumferential displacement used in the 2-D model.

<table>
<thead>
<tr>
<th>$\alpha_2 - \alpha_1$</th>
<th>$r_1 = 0.035 , m, r_2 = 0.0575 , m$</th>
<th>$r_1 = 0.035 , m, r_2 = 0.05875 , m$</th>
</tr>
</thead>
<tbody>
<tr>
<td>[deg]</td>
<td>$F_{1-2}$</td>
<td>$F_{2-1}$</td>
</tr>
<tr>
<td>0</td>
<td>6.67E-02</td>
<td>4.06E-02</td>
</tr>
<tr>
<td>3</td>
<td>6.56E-02</td>
<td>3.99E-02</td>
</tr>
<tr>
<td>6</td>
<td>6.23E-02</td>
<td>3.79E-02</td>
</tr>
<tr>
<td>9</td>
<td>5.73E-02</td>
<td>3.49E-02</td>
</tr>
<tr>
<td>12</td>
<td>5.13E-02</td>
<td>3.12E-02</td>
</tr>
<tr>
<td>15</td>
<td>4.49E-02</td>
<td>2.73E-02</td>
</tr>
<tr>
<td>18</td>
<td>3.85E-02</td>
<td>2.34E-02</td>
</tr>
<tr>
<td>21</td>
<td>3.25E-02</td>
<td>1.98E-02</td>
</tr>
<tr>
<td>24</td>
<td>2.70E-02</td>
<td>1.65E-02</td>
</tr>
<tr>
<td>27</td>
<td>2.22E-02</td>
<td>1.35E-02</td>
</tr>
<tr>
<td>30</td>
<td>1.80E-02</td>
<td>1.09E-02</td>
</tr>
<tr>
<td>33</td>
<td>1.43E-02</td>
<td>8.71E-03</td>
</tr>
<tr>
<td>36</td>
<td>1.12E-02</td>
<td>6.79E-03</td>
</tr>
<tr>
<td>39</td>
<td>8.44E-03</td>
<td>5.13E-03</td>
</tr>
<tr>
<td>42</td>
<td>6.09E-03</td>
<td>3.71E-03</td>
</tr>
<tr>
<td>45</td>
<td>4.05E-03</td>
<td>2.47E-03</td>
</tr>
<tr>
<td>48</td>
<td>2.28E-03</td>
<td>1.39E-03</td>
</tr>
<tr>
<td>51</td>
<td>7.52E-04</td>
<td>4.58E-04</td>
</tr>
<tr>
<td>54</td>
<td>2.93E-05</td>
<td>1.78E-05</td>
</tr>
<tr>
<td>57</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>60</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>63</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>66</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>69</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>72</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>75</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>78</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>81</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>84</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>87</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>90</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>93</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>96</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>99</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>102</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>105</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>108</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

Appendix
C Geometry of support structure

The geometry of the support structure used in the simulations is shown in the figure below. As the DSMC codes used in this project do not support curved surfaces the circular edges have to be approximated by straight lines.

![Geometry of the support structure.](image)

The support structure has a thickness of 8 mm and reduces the flow cross-section to 27.6 cm², which corresponds to 42.2 % of the total annular cross-section between the absorber and the vacuum jacket.