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PROYECTO FIN DE CARRERA

INGENIERO INDUSTRIAL

Numerical-Stochastic Modeling, Simulation and
Design Optimization of Small Particle Solar Receivers
for Concentrated Solar Power Plants

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Abstract

While most commercial Concentrated Solar Power plants rely on surface absorption of solar irradiation to drive a steam turbine (Rankine cycle), there exist several advantages in employing gas turbines (Brayton cycle). First, it requires less water to generate electricity; second, it leads to higher thermodynamic efficiency (due to the higher temperatures required); and third, the air is a non-problematic heat transfer fluid owing to its inert nature within the temperature range of interest.

This *Proyecto Fin de Carrera* aims to first develop a robust multi-physics numerical model for a Small Particle Solar Receiver, one such receiver to drive a gas turbine in Concentrated Solar Power plants. This concept is based on employing carbon nanoparticles in an air stream to *volumetrically* absorb highly concentrated solar irradiation and drive a gas turbine at temperatures in excess of 1300 K, with the corresponding three advantages previously mentioned. The thermo-fluid dynamic modeling of the Small Particle Solar Receiver requires solving a system of eight coupled, non-linear integro-partial differential equations in six independent variables (three spatial variables, two directional variables and wavelength). The solution procedure relies on the coupling of the CFD solver ANSYS Fluent to an in-house Monte Carlo Ray Trace software developed in this *Proyecto Fin de Carrera*. On the one hand, ANSYS Fluent is utilized as the mass-, momentum- and energy-equation solver and requires the divergence of the radiative heat flux, which constitutes a source term of the energy equation. On the other hand, the MCRT solver calculates the radiation heat transfer in the solar receiver and needs the temperature field to do so. By virtue of the coupled nature of the problem, both codes should provide feed-back to each other and iterate until convergence. The coupling between ANSYS Fluent and our in-house MCRT code is done via User-Defined Functions (UDFs). Both the UDFs and the MCRT

were programmed specifically for this *Proyecto Final de Carrera* and consist of over 12,500 lines of code. Moreover, they can be used interchangeably for either the two-dimensional (axisymmetric) or the three-dimensional version of the CFD solver.

After developing the mathematical model, setting up the code, validating the software and optimizing the coupled solution procedure, the receiver was simulated under fifteen different solar irradiation and mass flow rate cross combinations in an effort to assess the potential of this new technology to generate electricity. Among other results, the behavior of the receiver at different times of the day and the optimum mass flow rate as a function of the solar thermal input are presented. On an average day, the thermal efficiency of the receiver is found to be over 89% and the outlet temperature over 1250 K at all times from 7:30 AM to 4:00 PM (Albuquerque, USA) by properly adapting the mass flow rate. The origin of the losses and how to improve the efficiency of the Small Particle Solar Receiver are discussed as well.

A multidisciplinary design optimization is finally conducted in order to maximize the efficiency, reduce the initial and operating costs, increase the lifespan of the different components and, in turn, minimize the generation cost of the electricity. The design space consists of the geometry of the receiver, the geometry of the window, the radiative properties of the walls and the direction of the fluid flow with respect to the concentrated solar irradiation. The constraints are based on material limits (stresses and temperatures), the space available on the top of the tower and other technical issues; though some of them are imposed via a penalty method. The design space is explored via parametric study and a multidisciplinary approach is adopted. The cocurrent flow direction, aluminum oxide walls, a 45° spherical-cap window and the so-called *Design 2* showed the best compromise between thermal efficiency and wall temperature. Moreover, the particles were proved to be fully oxidized prior to exiting the solar receiver and the outlet air ready to drive a gas turbine at high temperature, which is the ultimate goal of the Small Particle Solar Receiver. Finally, several ideas and considerations to further improve the design are presented and discussed as well.

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“Do not go where the path may lead; go instead
where there is no path and leave a trail”,

Ralph Waldo Emerson

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Nomenclature

Latin Letters

A	= Area, m^2 . = Surface area of the carbon particles, $m^2/\text{particle}$. = Absorptivity of the window.
a	= Radius of the carbon particles, m. = Heating rate, K/s. = Radius of the spherical cap window.
Arr	= Arrhenius coefficient.
C	= Correction factor for the drag force at high Knudsen number.
c_p	= Specific heat at constant pressure, $J\cdot kg^{-1}\cdot K^{-1}$.
c_r	= Size parameter of an ellipsoidal window ($x^2 + y^2 + \alpha^2 z^2 = c_r^2$), m.
$c_{r,E}$	= Size parameter of the ellipsoid that limits some fluid cells of Type 3 on the z^+ face, m.
$c_{r,W}$	= Size parameter of the ellipsoid that limits some fluid cells of Type 3 on the z^- face, m.
D	= Diameter, m.
D_h	= Hydraulic diameter, m.
D_ω^+	= Positive portion of the cross-diffusion term.
d	= Carbon particle diameter, μm . = Thickness of the window, m.
E	= Emissive power, W/m^2 . = Activation energy, J. = Expected value of a random variable.
E_b	= Blackbody emissive power, W/m^2 .
E_n	= Exponential integral of order n ($E_n(z) = \int_1^\infty e^{-zt} t^{-n} dt$)
$\hat{e}$	= Unit vector.
e_i	= Energy of the ray number i , W.
F	= Test statistic in a hypothesis testing.
F_1, F_2	= Blending functions.
F_c	= Critical value of the test statistic in a hypothesis testing.
f	= Probability Density Function. = Equation of surface.

f_s	= Specular fraction.
G	= Dual objective function or dual objective functional.
g	= Objective function or objective functional.
H_l	= Performance function of the objective value l .
$\mathbf{h}$	= Additional restrictions of the design optimization problem (in vector form.)
h	= Specific enthalpy, J·kg ⁻¹ .
h_{ext}	= Exterior convective heat transfer coefficient (from the outer surface of the receiver to the ambient), W·m ⁻² ·K ⁻¹ .
$\hat{h}_{ext}$	= Effective exterior convective heat transfer coefficient (for modeling purposes), W·m ⁻² ·K ⁻¹ .
h_{int}	= Interior convective heat transfer coefficient (from the inner surface of the walls to the air-particle mixture), W·m ⁻² ·K ⁻¹ .
I	= First fundamental form.
II	= Second fundamental form.
	= Total interpolated radiative source term, W.
I	= Turbulence intensity.
IT	= Inlet temperature, K.
i	= Radiative intensity, W·m ⁻² ·sr ⁻¹ .
	= Axial index of the MCRT mesh.
i_b	= Blackbody intensity, W·m ⁻² ·sr ⁻¹ .
i_{win}	= Intensity on the inner surface of the window coming from the heliostat field, W·m ⁻² ·sr ⁻¹ .
j	= Radial index of the MCRT mesh.
K	= Gaussian curvature.
K_i	= Mathematical domain of the Monte Carlo cell i .
k	= Turbulence kinetic energy, m ² ·s ⁻² .
	= Thermal conductivity, W·m ⁻¹ ·K ⁻¹ .
	= Low-scale thermal conductivity (Kinetic Theory value), W·m ⁻¹ ·K ⁻¹ .
	= Imaginary part of the complex index of refraction (absorptive index).
	= Azimuthal index of the MCRT mesh.
k_B	= Boltzmann constant, J/K.
Kn	= Knudsen number.
L	= Length, m.
	= Thickness of the layer of the walls in which the source term is supposed to be uniformly distributed (Eq. 4-2 and Appendix H), m.
	= Integro-differential operator of the Radiative Transfer Equation.

L_e	= Entrance length, m.
$L^p(\Omega)$	= L^p functions in $\Omega \in \mathbb{R}^d$, $d \in \mathbb{N}$, i.e. p -integrable functions in Ω .
L^*	= Adjoint operator of the Radiative Transfer Equation.
l	= Number of levels of a parametric study. = Macroscale of turbulence, m. = Objective value in a Monte Carlo simulation. = Arc-length parameter, m.
$\hat{l}$	= Estimator of the objective value l in a Monte Carlo simulation.
l_f	= Distance to the closest face of the Monte Carlo cell through the prolongation of the ray.
l_κ	= Distance to absorption, m.
l_{σ_s}	= Distance to scattering, m.
m	= Mass per carbon particle, kg/particle. = Number of strata when applying stratified sampling in a Monte Carlo simulation.
$\dot{m}$	= Mass flow rate, kg/s.
$\dot{m}''$	= Rate of oxidation of carbon particles per unit time and unit particle surface area, $\text{kg}\cdot\text{s}^{-1}\cdot\text{m}^{-2}$.
M	= Molecular weight, $\text{kg}\cdot\text{m}^{-3}$. = Number of cells of the Monte Carlo mesh.
N	= Number of rays traced. = Number of parallel threads. = Carbon particles per unit volume, $\text{particles}/\text{m}^3$. = Normal distribution.
N_i	= Number of elements in the sample of the stratum i in a stratified Monte Carlo simulation.
n	= Real part of the complex index of refraction. = Number of factors (variables) of a parametric study.
$\hat{n}$	= Outward unit normal vector to the boundary of the solar receiver.
P	= Portion of code susceptible to parallelization (measured as the fraction of CPU time before the parallelization.)
P_k	= Generation of turbulence kinetic energy due to mean velocity gradients, $\text{kg}\cdot\text{m}^{-1}\cdot\text{s}^{-3}$.
$\mathbf{p}$	= Restrictions of the design optimization problem due to material limits (in vector form.)
p	= Thermodynamic pressure, Pa.
p_i	= Probability that an element belongs to the stratum i in a stratified Monte Carlo simulation.

- p_{op} = Operating thermodynamic pressure, Pa.
 p_γ = Partial pressure of the specie γ , Pa.
 Q_i^{rad} = Net radiative energy absorbed by the Monte Carlo cell number i , W.
 Q_{sol}^{input} = Solar thermal input, W.
 q_i = Orthogonal coordinates ($i = 1,2,3$)
 q_i^r = Radiative heat flux vector, $W \cdot m^{-2}$.
 q_v = Radiative source term on the walls when distributing the energy over a thickness L ($q_v = \frac{q_w}{L}$), W/m^3 .
 q_w = Radiative heat flux on the wall, $W \cdot m^{-2}$.
 R = Universal gas constant, $J \cdot mol^{-1} \cdot K^{-1}$.
 = Radius, m.
 = Reflectivity of the window.
 = Cumulative Distribution Function (CDF).
 R_E = Radial coordinate of the maximum axial position of a conical Monte Carlo cell (E from *East*).
 R_N = Maximum radial coordinate of a spherical/ellipsoidal Monte Carlo cell (N from *North*).
 = Maximum radial coordinate of a fluid of Type 3 Monte Carlo cell (N from *North*).
 R_{NE} = Radial coordinate of the edge with the maximum radial and maximum axial position of a three-dimensional Monte Carlo cell (N from *North*, E from *East*).
 R_{NW} = Radial coordinate of the edge with the maximum radial and minimum axial position of a three-dimensional Monte Carlo cell (N from *North*, W from *West*).
 R_S = Minimum radial coordinate of a spherical/ellipsoidal Monte Carlo cell (S from *South*).
 = Minimum radial coordinate of a fluid of Type 3 Monte Carlo cell (S from *South*).
 R_{SE} = Radial coordinate of the edge with the minimum radial and maximum axial position of a three-dimensional Monte Carlo cell (S from *South*, E from *East*).
 R_{SW} = Radial coordinate of the edge with the minimum radial and minimum axial position of a three-dimensional Monte Carlo cell (S from *South*, W from *West*).
 R_W = Radial coordinate of the minimum axial position of a conical Monte Carlo cell (W from *West*).
 R_φ = Random number for the variable φ .
 r = Radial coordinate of a cylindrical or spherical coordinate system, m.
 = Ratio between principal axes of the ellipsoidal window.
 = Ratio between the average temperature of the walls using a thickness L when distributing the radiative source term and the actual temperature of the inner surface of the wall, $r(L) = T(L)/\lim_{L \rightarrow 0} T(L)$.

r_N	= Maximum radial coordinate of a Monte Carlo cell (N from <i>North</i> , $r_N = r_N(z)$).
r_S	= Minimum radial coordinate of a Monte Carlo cell (S from <i>South</i> , $r_S = r_S(z)$).
Re_D	= Reynolds number based on the diameter.
S	= Modulus of the mean rate-of-strain tensor. = Expected speedup of the parallelization. = Divergence of the radiative heat flux ($S = \nabla \cdot \mathbf{q}^{rad}$). Only for the three-dimensional cells in Eq. 5-2 and Appendix I), W/m. = Radiative heat flux through the walls ($S = -\mathbf{q}^{rad} \cdot \hat{\mathbf{n}}$). Only for the two-dimensional cells in Eq. 5-2), W.
s	= Path length, m.
s^2	= Sample variance.
$\hat{\mathbf{s}}$	= Direction vector.
$\hat{\mathbf{s}}'$	= In-scattering direction vector.
T	= Thermodynamic temperature, K. = Transmissivity of the window.
$\mathbf{T}$	= Transformation matrix.
T_{inlet}^*	= Corrected inlet temperature (considering the radiative source term on the inlet surface) before the possible clipping.
t	= Time, s. = Parameter of the equation of a line, m.
t_0	= Initial time, s.
t_w	= Actual wall thickness, m.
$\hat{t}_w$	= Wall thickness of the CFD model, m.
TM	= CPU time of a Monte Carlo simulation.
U	= Bulk velocity, m/s.
$\mathbf{U}$	= Set of random numbers required to trace a ray using the Monte Carlo method.
u	= Velocity, m/s.
$\mathbf{u}$	= Fluid flow and radiative solution (in compact form.)
u_i	= Velocity vector, m/s.
u_η	= Kolmogorov velocity scale, m/s.
V	= Volume, m ³ .
$\check{V}_i$	= Volume of the i^{th} eighth part of a three-dimensional Monte Carlo cell (used in Appendix I).
$\mathbf{v}$	= Arbitrary vector. = Unit vector in the direction in which the ray is travelling.

$\mathbf{x}_o$	= Current location of the ray ($\mathbf{x}_o \in \mathbb{R}^3$).
x	= First Cartesian coordinate.
x_i	= Cartesian coordinates, m.
$\mathbf{Y}$	= Set of variables necessary to trace a ray using the Monte Carlo method and determined statistically using random numbers and CDFs.
y	= Distance from a flow field point to the nearest wall, m. = Second Cartesian coordinate, m.
Z_0	= Distance between the center of the spherical cap window and the origin of the global Cartesian coordinate system.
Z_E	= Maximum axial coordinate of a two-dimensional Monte Carlo cell (E from <i>East</i>). = Maximum axial coordinate of a fluid of Type 2 Monte Carlo cell (E from <i>East</i>).
Z_N	= Axial coordinate of the maximum radial position of a spherical/ellipsoidal Monte Carlo cell (N from <i>North</i>).
Z_{NE}	= Axial coordinate of the edge with the maximum radial and maximum axial position of a three-dimensional Monte Carlo cell (N from <i>North</i> , E from <i>East</i>).
Z_{NW}	= Axial coordinate of the edge with the maximum radial and minimum axial position of a three-dimensional Monte Carlo cell (N from <i>North</i> , W from <i>West</i>).
Z_S	= Axial coordinate of the minimum radial position of a spherical/ellipsoidal Monte Carlo cell (S from <i>South</i>).
Z_{SE}	= Axial coordinate of the edge with the minimum radial and maximum axial position of a three-dimensional Monte Carlo cell (S from <i>South</i> , E from <i>East</i>).
Z_{SW}	= Axial coordinate of the edge with the minimum radial and minimum axial position of a three-dimensional Monte Carlo cell (S from <i>South</i> , W from <i>West</i>).
Z_W	= Minimum axial coordinate of a two-dimensional Monte Carlo cell (W from <i>West</i>). = Minimum axial coordinate of a fluid of Type 2 Monte Carlo cell (W from <i>West</i>).
z	= Third Cartesian coordinate or axial coordinate of a cylindrical coordinate system.
z_E	= Maximum axial coordinate of a Monte Carlo cell (E from <i>East</i> , $z_E = z_E(r)$).
z_W	= Minimum axial coordinate of a Monte Carlo cell (W from <i>West</i> , $z_W = z_W(r)$).

Greek Letters

α	= Vector of design variables.
α	= Absorptivity. = Accommodation coefficient. = Level of significance in a hypothesis testing. = Angle between the generatrix and the axis of symmetry. = Shape parameter of an ellipsoidal window ($x^2 + y^2 + \alpha^2 z^2 = c_r^2$).
α_E	= Shape parameter of the ellipsoid that limits some fluid cells of Type 3 on the z^+ side.

α_W	= Shape parameter of the ellipsoid that limits some fluid cells of Type 3 on the z^- side.
Γ	= Lipschitz boundary of the air-particle mixture domain ($\Gamma = \partial\Omega$).
$\Delta\gamma$	= Difference between the maximum and the minimum γ coordinate in a Monte Carlo cell ($\gamma = z, r, \varphi$).
δ_{ij}	= Kronecker delta.
ε	= Hemispherical emissivity. = Dissipation rate of turbulent kinetic energy, m^2/s^3 .
ε'	= Directional emissivity.
ζ	= Mean free path, m.
η	= Kolmogorov length scale, m.
θ	= Zenithal coordinate of a spherical coordinate system, rad.
θ_{cap}	= Cap angle, rad.
θ_N	= Zenith angle of the maximum radial position of a spherical Monte Carlo cell (N from <i>North</i> . The origin of the spherical coordinate system is located in the center of the sphere), rad.
θ_S	= Zenith angle of the minimum radial position of a spherical Monte Carlo cell (S from <i>South</i> . The origin of the spherical coordinate system is located in the center of the sphere), rad.
κ	= Planck-mean absorption coefficient, m^{-1} .
λ	= Wavelength, μm .
μ	= Molecular dynamic viscosity, $\text{kg}\cdot\text{s}^{-1}\cdot\text{m}^{-1}$. = Mean.
μ_t	= Turbulent eddy viscosity, $\text{kg}\cdot\text{s}^{-1}\cdot\text{m}^{-1}$.
μ_3	= Three-dimension Lebesgue measure of a set.
ν	= Kinematic viscosity, $\text{m}^2\cdot\text{s}^{-1}$.
ν_t	= Kinematic turbulent viscosity, $\text{m}^2\cdot\text{s}^{-1}$.
ξ	= Particle size parameter.
ρ	= Density, $\text{kg}\cdot\text{m}^{-3}$. = Reflectivity of an interface.
ρ_p	= Reflectivity of the parallel component of an electromagnetic wave when it reaches an interface.
ρ_s	= Reflectivity of the perpendicular component of an electromagnetic wave when it reaches an interface.
ρ''	= Bidirectional reflection function, sr^{-1} .
σ	= Stefan-Boltzmann constant, $\text{W}/\text{m}^2\cdot\text{K}^4$.

	= Variance.
	= Covariance.
σ_k	= Turbulent Prandtl number for k .
σ_p	= Particle hard shell diameter, m.
σ_s	= Scattering coefficient, m^{-1} .
σ_ω	= Turbulent Prandtl number for ω .
τ	= Transmissivity of an interface.
	= Optical thickness.
	= Time constant, s.
τ_{ji}	= Viscous stress tensor, Pa.
τ_p	= Transmissivity of the parallel component of an electromagnetic wave.
τ_s	= Transmissivity of the perpendicular component of an electromagnetic wave.
τ_η	= Kolmogorov time scale, s.
Φ	= Scattering phase function.
Φ_b	= Dimensionless emissive power.
	$\Phi_b = (T^4 - T_1^4)/(T_2^4 - T_1^4)$, where T_1 and T_2 are the temperature of the first and second plate, respectively.
φ	= Mass loading, kg/m^3 .
	= Fluid flow variable.
	= Azimuthal coordinate of a cylindrical or spherical coordinate system, rad.
ϕ	= Volume fraction.
ϕ	= Adjoint variables.
Ψ	= Interpolation function of the radiative source term, W/m^3 .
ψ	= Stream function, m^2/s .
Ω	= Solid angle, sr.
	= Air-particle mixture domain (with Lipschitz boundary.)
ω	= Specific dissipation rate, s^{-1} .
	= Parameter related to the way the emitted rays are distributed throughout the Monte Carlo mesh, $\omega \in [1, \infty)$.

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$\mathcal{C}^n(\Omega)$	= n -times differentiable functions in $\Omega \in \mathbb{R}^d$, $d \in \mathbb{N}$.
$\mathcal{F}$	= System of governing equations of the fluid flow and radiative heat transfer (in vector form.)
σ	= Order of magnitude.
	= Average case performance.

- $\wp$ = Performance figure of merit of the MCRT method.
- $\Re$ = Combined convection-conduction thermal resistance per unit area of the walls of the solar receiver, $\text{K}\cdot\text{m}^2\cdot\text{W}^{-1}$.

Subscripts

- 0 = Inlet conditions of the particles.
 = Conditions of the air at the outlet of the recuperator or the compressor (for recuperated and non-recuperated cycles, respectively).
 = Current location of a ray.
- 1 = Incident ray.
 = Minimum axial position of a conical Monte Carlo cell (in Appendix E).
 = Left plate or inner cylinder in the Monte Carlo method validation (Appendix F).
 = φ^- , r^- , z^- vertex of a three-dimensional Monte Carlo cell.
- 11 = r^- , z^- position of a three-dimensional Monte Carlo cell.
- 12 = r^- , z^+ position of a three-dimensional Monte Carlo cell.
- 2 = Refracted ray.
 = Maximum axial position of a conical Monte Carlo cell (in Appendix E).
 = Right plate or outer cylinder in the Monte Carlo method validation (Appendix F).
 = φ^- , r^- , z^+ vertex of a three-dimensional Monte Carlo cell.
- 21 = r^+ , z^- position of a three-dimensional Monte Carlo cell.
- 22 = r^+ , z^+ position of a three-dimensional Monte Carlo cell.
- 3 = φ^- , r^+ , z^- vertex of a three-dimensional Monte Carlo cell.
- 4 = φ^- , r^+ , z^+ vertex of a three-dimensional Monte Carlo cell.
- 5 = φ^+ , r^- , z^- vertex of a three-dimensional Monte Carlo cell.
- 6 = φ^+ , r^- , z^+ vertex of a three-dimensional Monte Carlo cell.
- 7 = φ^+ , r^+ , z^- vertex of a three-dimensional Monte Carlo cell.
- 8 = φ^+ , r^+ , z^+ vertex of a three-dimensional Monte Carlo cell.
- air = Air-particle mixture.
- amb = Ambient.
- CO_2 = Carbon dioxide (CO_2).
- cr = Critical value for which the particles are assumed to be fully oxidized.
- e = Emission.
- eff = Effective.
- g = Global coordinate system.
- $hist$ = Historical value.
- i = Cell number i of the Monte Carlo mesh.

	= i -th component of a vector.
	= Incident.
<i>inlet</i>	= Inlet surface of the air-particle mixture.
<i>l</i>	= Local coordinate system.
<i>max</i>	= Maximum.
<i>min</i>	= Minimum.
<i>new</i>	= New cell of the Monte Carlo mesh in which the ray is entering.
<i>old</i>	= Current cell of the Monte Carlo mesh in which the ray is located.
<i>ot</i>	= Outlet tube.
<i>outlet</i>	= Outlet surface of the air-particle mixture.
<i>ox</i>	= Conditions at which the particles fully oxidize.
<i>p</i>	= Particle.
<i>r</i>	= Reflected.
<i>rec</i>	= Receiver.
<i>ref</i>	= Reference.
<i>rel</i>	= Relative.
<i>w</i>	= Wall.
<i>win</i>	= Window.
α	= Minimum z - and mid r - position of a three-dimensional Monte Carlo cell.
β	= Mid z - and mid r - position of a three-dimensional Monte Carlo cell.
γ	= Maximum z - and mid r - position of a three-dimensional Monte Carlo cell.
δ	= Mid z - and minimum r - position of a three-dimensional Monte Carlo cell.
ε	= Mid z - and maximum r - position of a three-dimensional Monte Carlo cell.
λ	= Spectral.
∞	= Environment.

Superscripts

"	= Bidirectional.
*	= Numerical value that take the different components of $\mathbf{Y}$ after picking the corresponding random number (i.e., φ^* is the value of φ chosen after picking the random number R_φ).
	= Adjoint operator.
γ^+	= Most positive γ -face of a Monte Carlo cell ($\gamma = z, r, \varphi$)
γ^-	= Least positive γ -face of a Monte Carlo cell ($\gamma = z, r, \varphi$)

- (i) = Iteration number i .
 = Ray number i of a Monte Carlo iteration.
 T = Transpose.

Accents and other symbols

- $INF(\cdot)$ = Largest integer smaller than $\cdot$.
 $SUP(\cdot)$ = Smallest integer greater than $\cdot$.
 $\overline{\quad}$ = Reynolds time average.
 $\overline{\quad}$ = Reynolds-averaged part.
 $\overline{\quad}$ = Closure of a region.
 $\sim$ = Dimensionless variable for the interpolation scheme of the radiative source term.
 $\dot{\quad}$ = Time derivative.
 ∇ = Del operator acting as gradient.
 $\nabla \cdot$ = Del operator acting as divergence.
 $\langle \quad \rangle$ = Arithmetic mean.
 $| \quad |$ = Determinant.
 $\| \quad \|_2$ = Euclidean norm.
 $\frac{\partial \mathbf{q}}{\partial \mathbf{v}}$ = Jacobian of the transformation $\mathbf{q} = \mathbf{q}(\mathbf{v})$.

Acronyms

- CDF = Cumulative Distribution Function
 CFD = Computational Fluid Dynamics
 DNS = Direct Numerical Simulation
 GPU = Graphics Processing Unit
 HTF = Heat Transfer Fluid
 LES = Large Eddy Simulation
 LTE = Local Thermodynamic Equilibrium
 MCRT = Monte Carlo Ray Trace
 MDO = Multidisciplinary Design Optimization
 N-S = Navier-Stokes
 ODE = Ordinary Differential Equation
 OTFA = Optically Thin Fluctuation Approximation
 PDE = Partial Differential Equation
 RANS = Reynolds-Averaged Navier Stokes

RNS	= Random Number Generator
RTE	= Radiative Transfer Equation
SST	= Shear Stress Transport
TRI	= Turbulence-Radiation Interactions
UDF	= User-Defined Function
URF	= Under-Relaxation Factor

Chapter 1

Introduction

This first chapter introduces the context in which this *Proyecto Fin de Carrera* is developed by gradually approaching the topic under research. First, we present a brief introduction to solar energy and its importance for the mankind's future. Then we focus on Concentrated Solar Power (CSP), probably the most promising way of producing electricity from solar energy. Finally, the Small Particle Solar Receiver concept is presented, as well as a brief description of its advantages and the interest of the project.

1.1. Solar Energy as a solution towards sustainable development

For many years human beings have utilized the resources that nature has put at their disposal to satisfy their energy requirements without worrying about the impact that behaviour could cause to the planet's future. However, since a group of scientists warned for the first time of the possible effects of human activity on the climate a few decades ago, many studies have been conducted to assess and predict global warming [1-5]. Unfortunately, a number of these scientific predictions have come true with alarming accuracy during recent years. For example, David Frame –from the Victoria University of Wellington– and Dáithí Stone –from the Lawrence Berkeley National Laboratory– have recently confirmed [6] that the predictions made by a team of scientists in December 1990 about the temperature rising due to CO₂ emissions [7,8] were right. The accuracy of these estimations is even more sensational if we take into account that many recent events were unknown in 1990, such as the Mont Pinatubo Eruption, the sudden reduction of greenhouse gases emissions in Russia or the emergence of China as an industrial giant.

Besides global warming, it is a reality that fossil fuels are non-renewable energy resources and their reserves will run out in a more or less near future. Therefore, the dire need to find a solution for the future of sustainable energy is apparent. We must act in advance and spare no effort to avoid a traumatic transition towards sustainable energy sources, which, for the time being, are still far from being widely applied.

To solve these two problems, it is necessary to reduce reliance on fossil fuels and introduce new, more efficient sustainable forms of energy in order to diminish the emissions, preserve the environment and guarantee the planet's future. Facing and giving a solution to this problem constitutes one of the mankind's most urgent and important challenges, and requires mutual cooperation between political institutions and scientific community. From the technological point of view, there exist several fields in which we must make an urgent effort: solar energy, wind power, new generation biofuels,

thermoelectric technologies, energy storage, ocean energy, and so on. Among them, solar energy stands out on its own due to its *unlimited*, free and non-polluting character.

1.2. Concentrated Solar Power

Concentrated Solar Power (CSP) is one of two primary technologies to produce electricity from solar energy. Roughly speaking, it consists of employing a vast field of mirrors to concentrate solar irradiation and heat up a fluid. Then, once the fluid is at high temperature, the thermal energy is transformed into electricity through a thermodynamic power cycle (heat engine), as in a conventional thermal power plant.

Among these CSP technologies, there exist several categories:

- Parabolic Trough
- Solar Power Tower
- Dish Stirling
- Fresnel Reflectors

While most current commercial CSP plants employ the parabolic trough technology, the Solar Power Tower possesses several advantages and is the technology to be employed in most of the largest CSP plants in the world (Ivanpah Solar Power Facility [9], Crescent Dunes Solar Energy Project in Tonopah [10], etc.), currently under construction. In this Solar Power Tower technology the mirrors (called heliostats and numbered in the thousands) concentrate the solar irradiation onto the top of a large tower, where the *solar receiver* is located. This solar receiver is the device where the heat transfer fluid (HTF) is heated. For a better understanding of this CSP technology, Figure 1 shows an image of the PS10 Solar Power Plant, the world's first commercial Solar Power Tower plant located in Sanlúcar la Mayor (Spain).



Figure 1 – PS10 Solar Power Plant (Sanlúcar la Mayor, Spain).

An independent study promoted by the World Bank [11] confirms Concentrated Solar Power technologies as the most economical way of producing large scale electricity from solar energy. Its diagnosis reveals, nevertheless, the CSP plant's direct capital cost is between 2.5 and 3.5 greater than a conventional thermal power plant, and the cost of the electricity produced from 2 to 4 times greater. Therefore, it is necessary to make an effort in R&D in CSP as it will constitute one of the main future energy sources in the medium- and long-term. Indeed, CSP could meet up to 7% of the world's power needs by 2030 and fully one quarter by 2050 [12], upstaging nuclear power and approaching our current global usage of coal and gas [13].

1.3. Small Particle Solar Receiver

To date, all central receivers utilized in commercial CSP plants are based on surface absorption of solar irradiation on the exterior surface of pipes, which transfer the heat to the heat transfer fluid (HTF) flowing inside them. This way the pipes are hotter than the HTF, which increases the thermal losses and limits the maximum achievable temperature due to materials limits. Moreover, the HTFs employed so far (oils, molten salts) degrade at temperatures over 800 K. These two facts limit current CSP plants to operate Rankine cycles at temperatures below 800 K, which reduces the overall efficiency of CSP plants. Of course, this limitation could be overcome and higher overall efficiencies could be achieved if new receivers capable of operating at higher temperature were developed.

Another challenge faced by current CSP plants is the large amount of cooling water required for Rankine cycle operation [14], which is a major concern for new solar power plants because the locations with greatest solar potential are often located in dry regions already subjected to water shortages. Some current central receiver power plants are forced to use dry cooling methods, which add to the overall cost and decrease the efficiency of the system. Again, this limitation could be fixed if new technology solar receivers were developed.

One such receiver able to overcome the two previous limitations (produce higher outlet temperature and very significantly reduce the water requirements), first proposed by Hunt in 1979 [15,16], is the Small Particle Solar Receiver. This concept is based on employing a mixture of air and carbon nanoparticles to *volumetrically* absorb concentrated solar irradiation. It is essentially a large, pressurized vessel with a window (through which the concentrated solar irradiation enters) and an air-particle mixture flowing inside, as schematically depicted in Figure 2. Since solar irradiation is absorbed volumetrically by the air-particle mixture, the walls are at lower temperature and do not limit the operating conditions anymore. Moreover, the air is a non-problematic heat transfer fluid owing to its inert nature within the temperature range of interest. Therefore, it is possible to produce outlet temperatures in excess of 1300 K, with the corresponding increase in thermodynamic efficiency. On account of the high temperature, the carbon particles oxidize prior to exiting

the solar receiver [17] and the outlet air flow is fully ready (no particles, high temperature) to drive a gas turbine (Brayton cycle). In addition, gas turbines are generally easier to operate than steam turbines, and are expected to withstand more stops and starts. As such, they are better suited to the intermittent nature of solar energy, which can require nightly shutdown. The Small Particle Solar Receiver, in turn, would lead to more flexible operation, would exceedingly reduce the water requirements and would produce higher thermodynamic efficiency compared to lower temperature liquid cooled receivers.

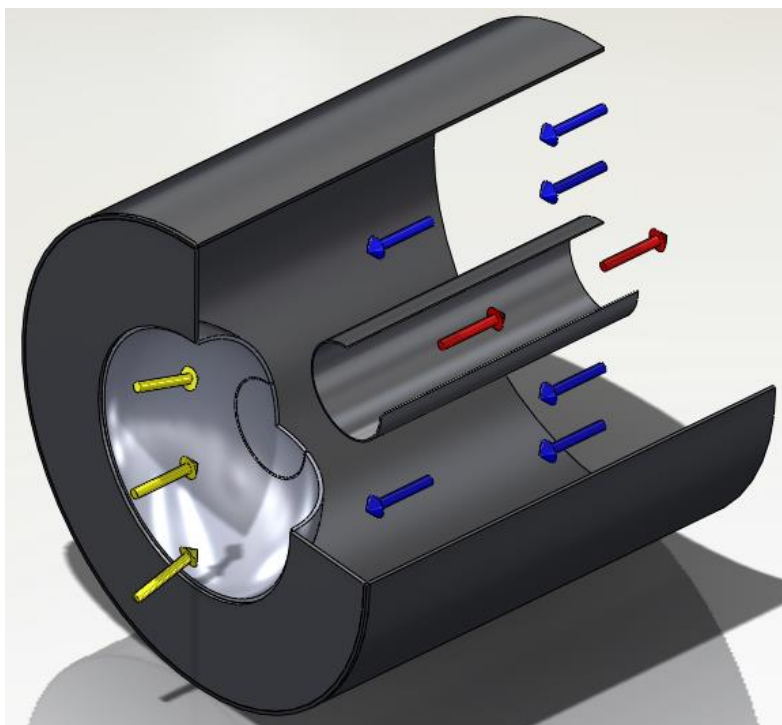


Figure 2 – Schematic representation of the Small Particle Solar Receiver (yellow arrows: solar irradiation; blue arrows: air-particle mixture inlet; red arrows: air-particle mixture outlet).

The Small Particle Solar Receiver can also accommodate higher incident flux levels than any existing technology, which reduces the size of the solar receiver with the corresponding cost and thermal losses reduction. Furthermore, the Small Particle Solar Receiver concept is not limited only to electricity generation. The high incident flux levels and the intimate mixing between gas and particles offer many possibilities for solar chemistry as well [18].

1.4. Scope and Objective of this *Proyecto Fin de Carrera*

Previous work conducted by our group [19,20] was concerned about developing a preliminary numerical model for the Small Particle Solar Receiver with the unique purpose of analyzing general trends, such as how efficiency varies when modifying the air-particle mixture inlet conditions, the mass flow rate, etc. However, these previous models have several limitations:

1. They were two-dimensional (axisymmetric) models and three important effects couldn't be modeled. First, incoming solar irradiation is actually non-axisymmetric¹; second, gravity forces –which are non-negligible– are non-axisymmetric either; and third, the fluid flow is highly turbulent and three-dimensional turbulent flow effects do occur, especially in the recirculation zone prior to entering the outlet tube.
2. A simplified model for the incoming intensity from the heliostat field was employed: The directional dependence was supposed to be uniformly distributed over a certain solid angle, and the radial distribution of intensity was assumed uniform (or Gaussian) over the window.
3. Only cylindrical receivers could be simulated. This didn't allow optimizing the design of the receiver, since curved geometries are expected to increase the efficiency and reduce the wall temperature (see Section 7.2).
4. The window was radiatively non-participating (i.e., it was a simple transparent aperture without glazing) and flat (which is non-realistic since a curved geometry is required to withstand the mechanical loading due to the pressurized air inside the receiver.)
5. The outlet tube of the air-particle mixture was either not present [19] or transparent as for the radiation heat transfer [20].
6. The simulation time was extremely high even though it was only a two-dimensional model.

Recent funding was provided to our group by the U.S. Department of Energy through the SunShot Initiative under the Award #DE-EE0005800 to design (by March 2014), build and test in the National Solar Thermal Test Facility (Albuquerque, NM, USA) a 5 MW_{th} Small Particle Solar Receiver. In order to design the receiver, a new, accurate and flexible multi-physics solver is required. The development and validation of such software is the first objective of this *Proyecto Fin de Carrera*. While the main features of the new code are thoroughly discussed in Chapters 3 (Radiation Heat Transfer), 4 (Fluid Dynamics) and 5 (coupling between both solvers), it is convenient to briefly introduce them at this point:

1. The model is three-dimensional so that, for the first time, it is possible to model and analyze the three previously mentioned effects.
2. Any axisymmetric geometry for the solar receiver can be modeled (rather than only right-cylindrical receivers).

¹ Among other things, this implies that wall temperatures cannot be accurately predicted in a 2-D model, a significant design constraint.

3. The software is coupled to a 3-D heliostat field and window model developed by Mecit [21,22], which provides the actual spatial, directional and wavelength dependence of the concentrated solar intensity. Hence, it is possible to simulate the receiver at different times and days.
4. The outlet tube participates in the radiation heat transfer, i.e., it is not transparent anymore.
5. The window participates in the radiation heat transfer as well by emitting radiation and by absorbing/reflecting/transmitting the incident irradiation. Three different window geometries can be simulated: flat, ellipsoidal, or a spherical cap.
6. Non-uniform meshes are utilized to improve the accuracy of the radiative solution.
7. The CPU time has been dramatically diminished thanks to a combination of different strategies: Variance reduction techniques (stratified sample, antithetic random numbers), efficient programming, and the availability of different Monte Carlo Ray Trace methods (collision-based and pathlength-based). See Sections 3.7.1, 3.7.3 and 3.7.2, respectively, for further discussion.
8. Others: Several effects that used to contribute to the energy imbalance in the previous model [20] have been fixed, different optical properties are allowed for each wall, additional post-processing information is provided and the code was programmed to facilitate an eventual parallelization and coupling it to an oxidation model.

In order to achieve the improvements described above, over 12,500 lines of code in FORTRAN and C are required. This software is flexible, accurate and comprehensive enough to be employed not only as a general purpose simulation tool, but also as a design and optimization tool. The latter is of the upmost importance in the highly competitive energy market to maximize the efficiency, reduce the initial and operating costs and, in turn, reduce the generation cost of the electricity. Hence, the second and third objectives of this *Proyecto Fin de Carrera* are to perform a parametric study of the operating conditions (mass flow rate and time of the day) and a multidisciplinary design optimization of the Small Particle Solar Receiver, respectively.

Main Objectives of this *Proyecto Fin de Carrera*

1. Develop and validate an accurate and flexible multi-physics solver for a 5MW Small Particle Solar Receiver to be built under the U.S. DOE's SunShot Initiative's Award #DE-EE0005800.
 2. Perform a parametric study of the operating conditions (time of the day and mass flow rate) in order to assess the electric generation possibilities of the Small Particle Solar Receiver.
 3. Conduct a multidisciplinary design optimization of the Small Particle Solar Receiver with the ultimate goal of increasing the efficiency, reducing the initial and operating costs and, in turn, reducing the generation cost of the electricity.
-

Table 1 – Main objectives of this *Proyecto Fin de Carrera*.

Chapter 2

Problem Statement and Model Overview

The purpose of this Chapter is to illustrate the exceedingly complicated nature of the problem to be addressed, namely the fluid flow and radiative heat transfer modeling of the Small Particle Solar Receiver. First, the mathematical formulation of the problem is presented. It involves a system of six coupled, nonlinear, integro-partial differential equations with eight unknowns and six independent variables (three spatial, two directional and wavelength). Moreover, two additional equations are employed for the turbulence modeling and several constitutive relations are required to close the problem as well. Of course, such a formidable problem does not admit an analytical solution and must be solved numerically. Then, a general overview of the model developed is presented, which will be extensively discussed in Chapters 3 (Radiation Heat Transfer), 4 (Fluid Dynamics) and 5 (coupling between the previous two sub-models). The chapter ends introducing, discussing and justifying the two main simplifying hypotheses of the model, namely that the particles move as part of the air flow and that they are at local thermodynamic equilibrium with their surroundings.

2.1. Mathematical Formulation of the Problem

With the only purpose of showing the exceedingly complicated mathematical nature of the problem, the system of governing equations, boundary conditions and constitutive relations necessary to close the problem are presented. First, the motion of fluids is governed by the Navier-Stokes equations², Equations 2-1.a-c. At the high Reynolds numbers present in parts of the Small Particle Solar Receiver ($Re_D \sim 10^5$ in the outlet tube, for instance), turbulent flow occurs. The approach to handle this turbulence that will be employed here is to utilize Reynolds decomposition³ and Reynolds averaging of the Navier-Stokes equations to obtain the Reynolds-Averaged Navier Stokes (RANS) equations. This averaging process introduces the so-called Reynolds stresses, $\overline{u'_i u'_j}$, which are –in some way– nothing but extra variables that require extra equations to close the problem. To do so, turbulence models, which relate

² Even though Claude-Louis Navier and George Gabriel Stokes only derived the momentum equation, it is sometimes customary to apply the term *Navier-Stokes equations* to the whole mass-, momentum- and energy-system of equations. This is the nomenclature to be employed throughout this *Proyecto Fin de Carrera*.

³ A mathematical technique to separate the average ($\bar{\phi}$) and fluctuating (ϕ') part of a scalar variable (ϕ):

$$\phi = \bar{\phi} + \phi'$$

Where, for steady-state flows, $\bar{\phi} \equiv \lim_{T \rightarrow \infty} \frac{1}{T} \int_{t_0}^{t_0+T} \phi(t) dt$ and $\phi' \equiv \phi - \bar{\phi}$. Note that $\bar{\phi}$ is independent of the initial time t_0 if the flow field is *ergodic*, which in general is a good assumption for most turbulent flow fields.

the fluctuation terms to mean flow properties and their gradients, are required. In particular, the two equation SST $\kappa - \omega$ turbulence model (in its modified version published in 2003 [23], Equations 2-1.d-e) is employed for the Small Particle Solar Receiver modeling, as more deeply discussed in Section 4.4 of Chapter 4.

The radiation heat transfer within a participating medium is governed by the Radiative Transfer Equation (RTE), Eq. 2-1.f. For the Small Particle Solar Receiver, as for the vast majority of engineering applications, the speed of light is much greater than the time and length scales of interest so that the Lagrangian derivative in the general RTE may be replaced just by the spatial derivative⁴, leading to the *quasi-steady* form of the Radiative Transfer Equation [24]. While all quantities in the RTE may vary in space and wavelength, only the directional dependence has been explicitly indicated in Eq. 2-1.f to simplify notation. Note also that Turbulence-Radiation Interactions (TRI) [25-31] have been neglected, i.e. $\overline{\kappa_\lambda i_{b\lambda}} \approx \kappa_\lambda(\bar{T}) i_{b\lambda}(\bar{T})$ and $\overline{(\kappa_\lambda + \sigma_{s,\lambda}) i_\lambda} \approx [\kappa_\lambda(\bar{T}) + \sigma_{s,\lambda}(\bar{T})] \bar{i}_\lambda$. The former can be applied invoking the Optically Thin Fluctuation Approximation (OTFA) since the optical thickness of the radiating media, based on the macroscale of turbulence l , is small, i.e. $\overline{(\kappa_\lambda + \sigma_{s,\lambda})} l \ll 1$ [32].

The strong formulation of the problem, expressed in tensor notation, is presented in Eq. 2-1. The first three equations are the RANS equations (mass-, momentum- and energy-, respectively), the fourth and fifth are the SST $\kappa - \omega$ equations and the sixth is the Radiative Transfer Equation. The seventh equation relates the N-S equations and the RTE, while the last nine equations are simply boundary conditions for the previous integro-partial differential equations.

$$\begin{aligned}
 & \frac{\partial \rho \bar{u}_i}{\partial x_i} = 0 \quad \text{in } \Omega \\
 & \frac{\partial}{\partial x_j} (\rho \bar{u}_i \bar{u}_j) + \frac{\partial}{\partial x_j} (\rho \bar{u}'_i \bar{u}'_j) + \frac{\partial \bar{p}}{\partial x_i} - \frac{\partial \bar{\tau}_{ij}}{\partial x_j} = 0 \quad i = 1, 2, 3 \quad \text{in } \Omega \\
 & \quad \text{for } i = 1, 2, 3 \\
 & \frac{\partial}{\partial x_j} \left(\rho \bar{u}_j \left(\bar{h}(\bar{T}) - \frac{\bar{p}}{\rho} \right) \right) - \frac{\partial}{\partial x_j} \left(k_{eff} \frac{\partial \bar{T}}{\partial x_j} \right) + \frac{\partial \bar{q}_j^r}{\partial x_j} = 0 \quad \text{in } \Omega \\
 & \frac{\partial (\rho \bar{u}_j k)}{\partial x_j} = \tilde{P}_k - \beta^* \rho k \omega + \frac{\partial}{\partial x_j} \left[(\mu + \sigma_k \mu_t) \frac{\partial k}{\partial x_j} \right] \quad \text{in } \Omega \\
 & \frac{\partial (\rho \bar{u}_j \omega)}{\partial x_j} = \frac{\alpha}{\nu_t} \tilde{P}_k - \beta \rho \omega^2 + \frac{\partial}{\partial x_j} \left[(\mu + \sigma_\omega \mu_t) \frac{\partial \omega}{\partial x_j} \right] + 2(1 - F_1) \frac{\rho \sigma_{\omega 2}}{\omega} \frac{\partial k}{\partial x_j} \frac{\partial \omega}{\partial x_j} \quad \text{in } \Omega \\
 & \hat{\mathbf{s}} \cdot \nabla i_\lambda(\hat{\mathbf{s}}) = \kappa_\lambda i_{b\lambda} - [\kappa_\lambda + \sigma_{s,\lambda}] i_\lambda(\hat{\mathbf{s}}) + \frac{\sigma_{s,\lambda}}{4\pi} \int_{4\pi} i_\lambda(\hat{\mathbf{s}}') \Phi_\lambda(\hat{\mathbf{s}}, \hat{\mathbf{s}}') d\Omega' \quad \text{in } \Omega \\
 & \frac{\partial \bar{q}_j^r}{\partial x_j} = \int_0^\infty \kappa_\lambda \left(4\pi i_{b\lambda} - \int_{4\pi} i_\lambda d\Omega \right) d\lambda \quad \text{in } \Omega \\
 & u_i = 0 \quad \text{in } \bar{\Gamma}_w \cup \bar{\Gamma}_{window}
 \end{aligned} \tag{2-1}$$

⁴ For example, the time-constant for radiative transport in an enclosure of characteristic dimension of a meter is in the order of few tens of nanoseconds.

$$\begin{aligned}
u_i &= u_{i,inlet} && \text{in } \bar{\Gamma}_{inlet} \\
p &= p_{inlet} && \text{in } \bar{\Gamma}_{inlet} \\
T &= T_{inlet} && \text{in } \bar{\Gamma}_{inlet} \\
n_i q_i + \int_0^\infty d\lambda \int_{2\pi} i_\lambda(\hat{s}) (\hat{n} \cdot \hat{s}) d\Omega &= (T - T_{amb})/\mathfrak{R} && \text{in } \bar{\Gamma}_w \\
&&& \text{and } \forall \hat{s} \cdot \hat{n} > 0 \\
T &= T_{win} && \text{in } \bar{\Gamma}_{window} \\
i_\lambda(\hat{s}) &= \varepsilon'_\lambda i_{b\lambda}(\hat{s}) + \int_{2\pi} \rho''_\lambda(\hat{s}', \hat{s}) i_\lambda(\hat{s}') \cos \theta' d\Omega' && \text{in } \Gamma_w \cup \Gamma_{inlet} \cup \Gamma_{outlet} \\
&&& \text{for } \hat{s} \cdot \hat{n} > 0 \\
&&& \text{and } \forall \hat{s}' \cdot \hat{n} < 0 \\
i_\lambda(\hat{s}) &= i_{win,\lambda}(\hat{s}) && \text{in } \Gamma_{window} \\
&&& \text{for } \hat{s} \cdot \hat{n} > 0 \\
\sqrt{2k/3 \sum_{i=1}^3 \bar{u}_i^2} &= I_{inlet} && \text{in } \bar{\Gamma}_{inlet}
\end{aligned} \tag{2-1}$$

Where $\Omega \in \mathbb{R}^3$ is the bounded domain that represents the air-particle mixture domain with Lipschitz boundary $\partial\Omega = \Gamma$. This boundary has been split by convenience into Γ_w , Γ_{win} , Γ_{inlet} and Γ_{outlet} , where $\bigcup_{i=1}^4 \bar{\Gamma}_i = \Omega$ and $\mu_3(\Gamma_i \cap \Gamma_j) = \delta_{ij}$. It should be noted that the body forces have not been included in the momentum equation, Eq. 2-1.b, since they are not considered in this *Proyecto Fin de Carrera* (i.e., buoyancy forces are neglected). This is convenient at this point of the design process as will be discussed in Chapter 7. Similarly, the pressure work, kinetic energy, viscous dissipation and chemical reaction terms are negligible compared to the divergence of the radiative heat transfer and are not included in the energy equation, Eq. 2-1.c. The air-particle mixture is modeled as a single phase for modeling purposes (see Section 2.3 for a proof) so that no extra equations are required (e.g., species transport equations are not needed.) The regularity conditions required are shown in Eq. 2-2 (the ones of the boundary condition functions, such as $u_{i,inlet}$, are not shown for simplicity.)

$$p, \rho, i_\lambda \in \mathcal{C}^1(\Omega) \qquad u_i, T, k, \omega \in \mathcal{C}^2(\Omega) \tag{2-2}$$

Finally, the constitutive relations in Eq. 2-3 are necessary to close the problem: The Fourier Law for conduction heat transfer (already included in Eq. 2-1.c in its turbulent version), the Navier-Poisson Law with the Stokes hypothesis for the strain rate–stress relation (Eq. 2-3.c) and the Perfect Gas Law for thermodynamic relations (Eq. 2-3.b). Further closure coefficients and auxiliary relations are required for the turbulence modeling [23]⁵ and are shown in Appendix G.

⁵ Note that a typographical error exists in [23], which was subsequently corrected by the authors [33]. Namely, the production term in the ω -equation was incorrectly given as $\alpha \rho S^2$, while it should actually be $\frac{\alpha \beta_k}{\nu_t}$.

$$\bar{\rho} = \frac{pM_{air}}{R\bar{T}}$$

$$\bar{h}(\bar{T}) = \bar{h}(T_{ref}) + \int_{T_{ref}}^{\bar{T}} c_p(T')dT' \quad (2-3)$$

$$\bar{\tau}_{ji} = \mu \left[\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} - \frac{2}{3} \frac{\partial \bar{u}_k}{\partial x_k} \delta_{ij} \right]$$

The mathematical formulation presented above is the one in which only the air-particle mixture is modeled. For higher accuracy, one can also solve also the conduction heat transfer in the walls, which makes the formulation of the problem even more involved. The latter case is the one solved by the multiphysics numerical model developed in this *Proyecto Fin de Carrera*, as will be explained in Chapters 3, 4 and 5.

2.2. Model Overview

Two different sub-models are employed for the fluid flow and for the radiation heat transfer in order to overcome the difficulties associated with this problem. For the fluid dynamics, the commercial CFD software ANSYS Fluent is employed; while for the radiative heat transfer an in-house Monte Carlo Ray Tracing code has been developed and programmed in FORTRAN for this *Proyecto Fin de Carrera*. This Monte Carlo code consists of around 10,000 lines and contains many features to allow high flexibility and solution accuracy. Both codes are coupled via User Define Functions (UDFs) programmed in C and iterate alternatively until convergence (see Figure 3). These two models are extensively discussed in Chapters 3 (Monte Carlo Ray Tracing model) and 4 (CFD model), while Chapter 5 deals with the way they are coupled together and the solution procedure.

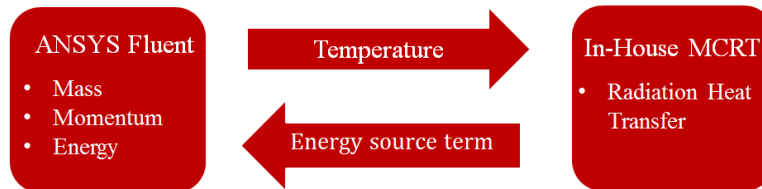


Figure 3 – Schematic diagram of the solution procedure [20].

2.3. Main hypotheses of the model

Two basic hypotheses are assumed in order to simplify the complexity of the problem: First, the particles are at local thermodynamic equilibrium with their surroundings; and second, they move as part of the fluid flow (i.e., they follow the entire turbulence spectrum, even the Kolmogorov scale). By virtue of these two hypotheses, the mixture of air and carbon nanoparticles can be treated as a single phase for modeling purposes. Note, finally, that these two hypotheses were implicitly imposed in the formulation of the problem, Eq. 2-1.

2.3.1. Local Thermodynamic Equilibrium

While Local Thermodynamic Equilibrium (LTE) is easily guaranteed in most homogeneous fluid flows⁶, this basic assumption is not as trivial in the Small Particle Solar Receiver: Since essentially only the carbon nanoparticles absorb solar irradiation (the CO₂ contribution is neglected, see Section 3.5), they need to *instantaneously* transfer this heat to the air by convection and conduction in order to be in thermal equilibrium with their surroundings. From kinetic theory, the heat transfer rate from a particle with radius a to its surroundings is given by [34]:

$$Q = \frac{4\alpha k a \Phi (T_p - T_\infty)}{Kn + \frac{\Phi \alpha}{(2Kn + 1)\pi}} \quad (2-4)$$

Where $Kn = \zeta/2a$ is the Knudsen number, α is the accommodation coefficient, k is the low-scale thermal conductivity of the air (the kinetic theory value) and $\Phi = 48/95$ for diatomic gases.

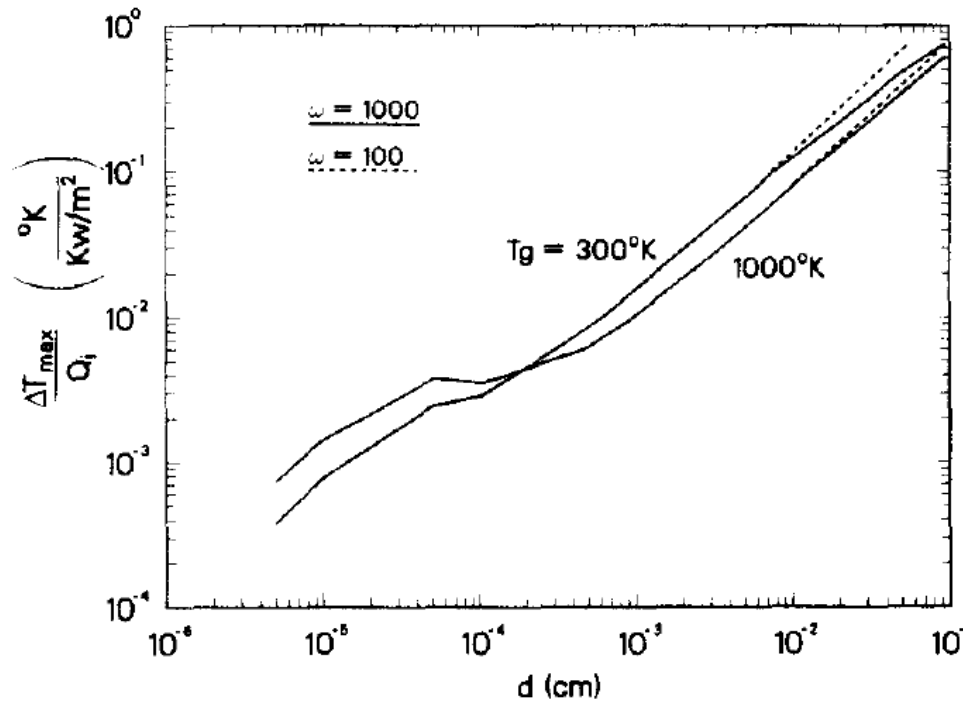


Figure 4 – Normalized Temperature Difference vs. Particle Size [34]. Perfect accommodation ($\alpha = 1$) and no adsorption are assumed. The solar irradiation is 1 kW/m² and ω denotes the concentration factor.

⁶ For the vast majority of engineering applications the characteristic length is much greater than the mean free path, and the characteristic time is much greater than the mean free time. Exceptions are chemically reacting flows and very sudden state changes, as in a strong shock wave.

It can be also demonstrated that there exists a theoretical maximum temperature difference between the particles and the gas, whose value is plotted in Figure 4 [34] for different particle sizes and irradiation levels. Based on this model, and for the incident radiative fluxes and particles sizes present in the Small Particle Solar Receiver, the maximum temperature difference between air and particles is below 4 K, which is consistent with experimental observations [17].

Note that Local Thermodynamics Equilibrium is of the utmost importance since otherwise (1) another equation would be needed to be added to Eq. 2-1 to handle this non-equilibrium, (2) properties wouldn't be related by ordinary equilibrium thermodynamics and (3) the form of the Radiative Transfer Equation presented in Eq. 2-1.f wouldn't be valid (for example, Kirchhoff's law wouldn't apply.)

2.3.2. Particles move with the air flow as a unique phase

The following paragraphs aim to illustrate the ability of the carbon nanoparticles to move as part of the air flow as a single phase. The model presented here is only a rough approximation to reality, but provides a nice intuitive idea of their extraordinary ability to follow the turbulence spectrum. It will be assumed that the particles are spherical, which is approximately true according to experimental results [35]. If the particles are not single spheres but agglomerated spheres, then they would follow the flow even better as they would have larger drag force per unit mass.

The Knudsen number of the flow past a carbon nanoparticle is $Kn = \zeta/2a = k_B T / 2\sqrt{2}\pi\sigma_p^2 p a \approx 0.031 \mu m / 0.2 \mu m = \sigma(0.1)$ ($p = 5 \text{ bar}$, $T = 700 \text{ K}$) so that the mean free path of a molecule is only one order of magnitude smaller than the length scale of the problem. Therefore, the continuum hypothesis is no longer valid and statistical mechanics needs to be invoked. Fortunately, it is possible to relate the drag force at high Knudsen number to the force predicted by continuum mechanics employing the correction factor proposed by Cunningham [36].

$$C = 1 + \frac{\lambda}{a} \left(A_1 + A_2 e^{-\frac{2A_3 a}{\lambda}} \right) = 1.393 \quad (2-5)$$

Where $A_1 = 1.257$, $A_2 = 0.400$ and $A_3 = 0.55$ for particles immersed in air [37].

Under the continuum hypothesis and the assumption of incompressible, steady-state flow, the velocity field derives from a stream function $\mathbf{v} = \nabla \times \boldsymbol{\psi}$. Additionally, $Re_a \ll 1$ for any value of the velocity and kinematic viscosity present in the Small Particle Solar Receiver so that the convective acceleration terms are negligible in the momentum equations, i.e. it is a creeping or Stokes flow. Thus, the stream function is biharmonic and, in spherical coordinates, the problem can be written as in Eq. 2-6.

$$\left(\frac{\partial^2}{\partial r^2} + \frac{1}{r^2} \frac{\partial^2}{\partial \theta^2} - \frac{\cot \theta}{r^2} \frac{\partial}{\partial \theta}\right)^2 \psi = 0$$

$$\frac{\partial \psi}{\partial r} = \frac{\partial \psi}{\partial \theta} = 0 \text{ at } r = a$$

$$\lim_{r \rightarrow \infty} \psi = \frac{1}{2} U_{rel} a^2 \sin^2 \theta$$

Whose solution is:

$$\psi = \frac{1}{4} U_{rel} a^2 \sin^2 \theta \left(\frac{a}{r} - \frac{3r}{a} + \frac{2r^2}{a^2} \right) \quad (2-7)$$

The velocity, pressure and shear-stress fields, which can be readily computed from ψ , are:

$$u_r = U_{rel} \cos \theta \left(1 - \frac{3a}{2r} + \frac{a^3}{2r^3} \right) \quad u_\theta = U_{rel} \sin \theta \left(-1 + \frac{3a}{4r} + \frac{a^3}{4r^3} \right) \quad (2-8)$$

$$p = p_\infty - \frac{3\mu a U_{rel}}{2r^2} \cos \theta \quad \tau_{r\theta} = -\frac{\mu U_{rel} \sin \theta}{r} \frac{3a^3}{2r^3}$$

The total drag force predicted by continuum mechanics is obtained integrating the shear stress and pressure fields over the particles' surface, which leads to the celebrated Stokes' law for the drag over spheres moving at low Reynolds number:

$$F = - \int_0^\pi \tau_{r\theta}|_{r=a} \sin \theta dA - \int_0^\pi p|_{r=a} \cos \theta dA = \dots = 6\pi\mu U_{rel} a \quad (2-9)$$

The actual drag force is finally obtained utilizing the correction factor by Cunningham (Eq. 2-5):

$$F = \frac{6\pi\mu U_{rel} a}{C} \quad (2-10)$$

Hence, the one-dimensional governing equation of the particle motion⁷ is:

$$\frac{2Ca^2\rho_p}{9\mu} \ddot{u} + u = U_\infty \quad (2-11)$$

First, let's analyze the step response of the particles, i.e. their response to the Heaviside function; which is expressed in Eq. 2-12 and plotted in Figure 5 for a particle radius $a = 100 \text{ nm}$.

⁷ The projection of the inertial, gravity and buoyancy forces in the direction of motion are not included in this simple one-dimensional model.

$$\frac{u}{U_{\infty}} = 1 - e^{-\frac{9\mu}{2ca^2\rho_p}t} \quad (2-12)$$

Therefore, the time constant is $\tau \sim 0.1 \mu s$ and the particles will easily follow the bulk velocity field. The scales of turbulence the particles are able to follow can be estimated from their frequency response, which for linear ODEs with constant coefficients can be illustrated through the Bode plot (Figure 6).

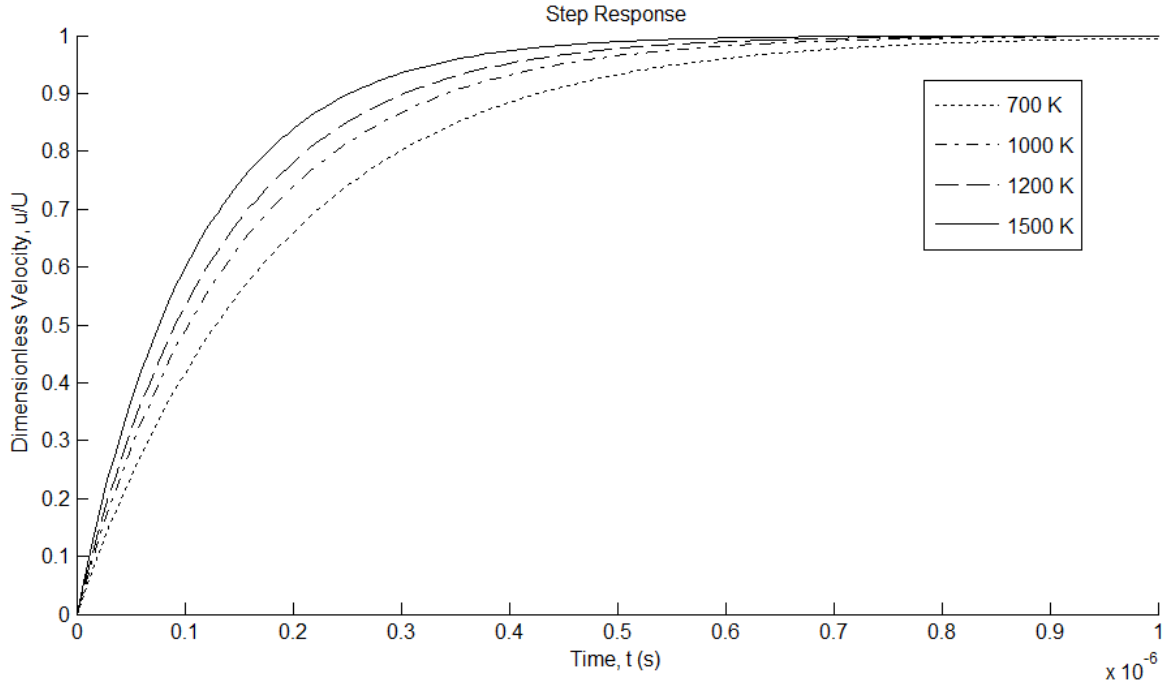


Figure 5 – Dimensionless step response of the carbon particles for different air temperatures (particle radius $a = 100 \text{ nm}$).

The spectrum of turbulence needs to be determined as well. From dimensional analysis, the Kolmogorov scales can be estimated as follows:

$$\text{Kolmogorov Length Scale: } \eta \sim \left(\frac{\mu^3}{\rho_{air}^3 \varepsilon} \right)^{1/4} = \left(\frac{(6.6046 \cdot 10^{-6} \text{ m}^2/\text{s})^3}{500 \text{ m}^2/\text{s}^3} \right)^{1/4} = 27.55 \mu\text{m}$$

$$\text{Kolmogorov Time Scale: } \tau_{\eta} \sim \left(\frac{\mu}{\rho_{air} \varepsilon} \right)^{1/2} = \left(\frac{6.6046 \cdot 10^{-6} \text{ m}^2/\text{s}}{500 \text{ m}^2/\text{s}^3} \right)^{1/2} = 2.26 \cdot 10^{-4} \text{ s} \rightarrow 4,400 \text{ Hz}$$

$$\text{Kolmogorov Velocity Scale: } u_{\eta} \sim \left(\frac{\mu \varepsilon}{\rho_{air}} \right)^{1/4} = \left(6.6046 \times 10^{-6} \text{ m}^2/\text{s} \cdot 500 \text{ m}^2/\text{s}^3 \right)^{1/4} = 0.240 \text{ m/s}$$

Where the kinematic viscosity present in the Small Particle Solar Receiver that leads to the faster Kolmogorov eddies (i.e., $\nu = 6.6 \times 10^{-6} \text{ m}^2/\text{s}$ at $T = 700 \text{ K}$) has been used.

Based on this simplified one-dimensional model, the particles could follow velocity fluctuations of, at least, 10,000 Hz; which corresponds with the entire turbulence spectrum, including the Kolmogorov scale. In reality, particles follow three-dimensional eddies and the inertial *force* due to rotation inside the eddies needs to be included in the equation of the particle motion. Moreover, the transient term in the Navier-Stokes equations may actually be non-negligible and might need to be included as well. Therefore, the previous results are only a rough estimate of the extraordinary ability of the particles to follow high-frequency signals and as such should be interpreted. Note, however, that for our hypothesis to be valid (the particles move with the air flow as a single phase for modeling purposes) it is only necessary that the particles can follow the turbulence scales that are resolved by the CFD solver (grid scales) but not those that are modeled (sub-grid scales), which is definitely true for the particle sizes (200 nm) and mesh sizes (around 5 mm in the smallest cell) employed.

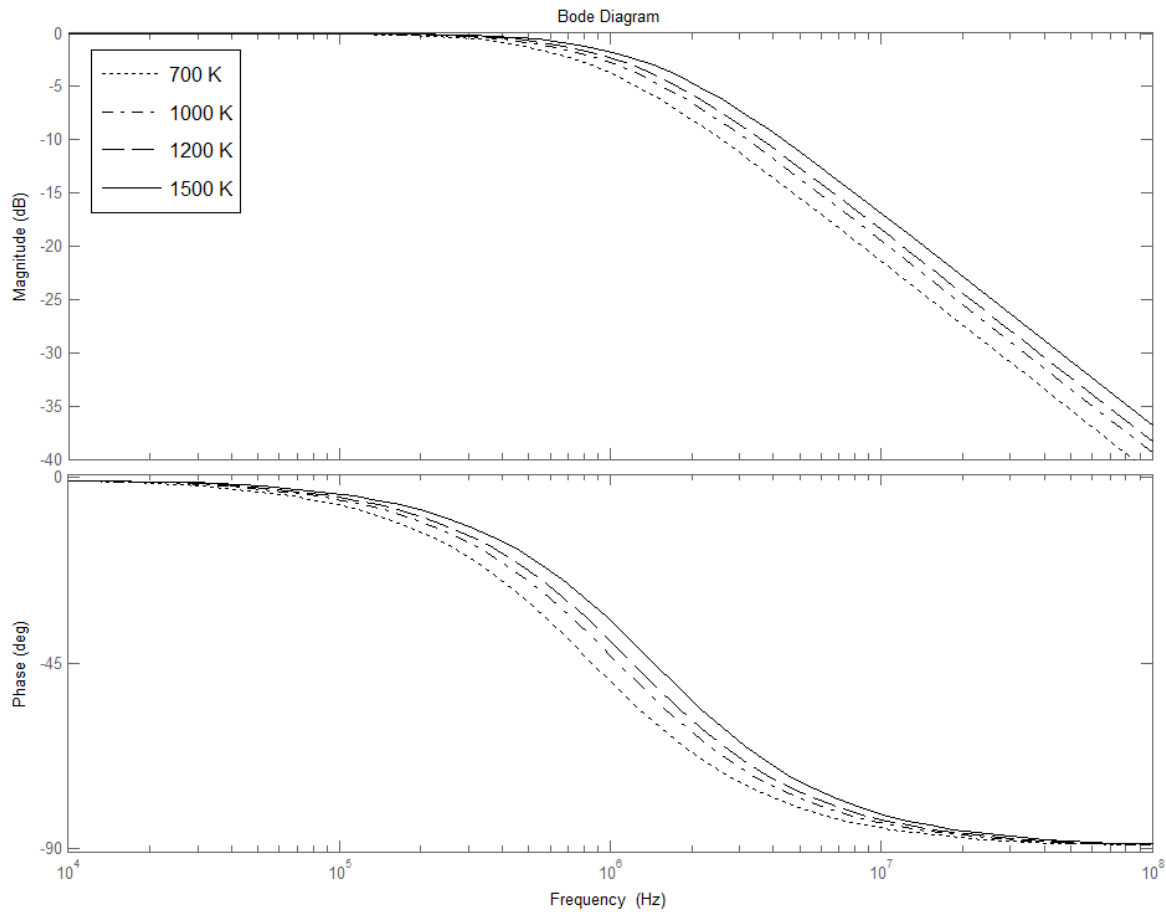


Figure 6 – Bode plot of the particles response under air velocity fluctuations at different air temperatures (particle radius $a = 100 \text{ nm}$).

Chapter 3

The Monte Carlo Ray Tracing Method for Radiation Heat Transfer

Radiative heat transfer within participating media is one of the most mathematically challenging engineering problems. In fact, except for a few simple geometries and radiative properties, very few closed-form solutions to radiation heat transfer problems do exist. Therefore, in most situations it is necessary to rely on numerical techniques to find a solution to thermal radiation problems. Of course, classical numerical methods for Partial Differential Equations –such as finite difference, finite element or finite volume methods– can be applied to thermal radiation whenever the governing integro-partial differential equation (the Radiative Transfer Equation, Eq. 2-1.f) can be transformed into a set of partial differential equations, which can be accomplished via Spherical Harmonics [38-42] or Discrete Ordinates [43-48] methods⁸. Another possibility is to tackle the integral equations directly employing numerical quadrature for the integrals [24]. However, if the thermal radiation problem is involved, as occurs in the Small Particle Solar Receiver⁹, a solution by conventional numerical techniques becomes extremely complicated, if not impossible. For these situations, only the Monte Carlo Ray Tracing (MCRT) method is well suited [49-55]. Figure 7 schematically shows the CPU time required to solve a radiative heat transfer problem as a function of its complexity [24]. For simple problems, conventional methods show the best performance; while when the problem becomes involved the MCRT method is the best, and maybe only, option to obtain a solution.

Therefore, the Monte Carlo Ray Tracing method is employed for the radiative heat transfer modeling of the Small Particle Solar Receiver due to its unique capacity to exactly model the physics of the radiation in complex geometries with spatial, spectral and temperature-dependent radiative properties; all of them features present in the Small Particle Solar Receiver. The MCRT methods use a statistical approach to probabilistically model the underlying physics of the radiation heat transfer, rather than numerically solving the Radiative Transfer Equation (Eq. 2-1.f). In particular, Monte Carlo Ray Tracing methods simulate radiative heat transfer by tracking a statistically significant number of rays that

⁸ These methods replace the directional dependence of a continuous function, namely intensity, by a set of functions that does not depend on direction (but still depend on position and maybe wavelength) and represent an *average* of the intensity over the corresponding range of solid angles. This way, derivatives and integrals over directional variables are replaced by simple algebraic operations.

⁹ The radiative properties of the carbon particles have a strong spectral dependence. Moreover, it is necessary to accurately model the directional dependence of the concentrated solar irradiation from the heliostat field to predict the temperature of the receiver's walls.

represent energy bundles or photons. These photon bundles are traced throughout the receiver domain, Ω , and interact with the air-particle mixture (scattering, absorption), the walls (reflection, absorption) and the window of the receiver (reflection, absorption, transmission). This way, Monte Carlo simulations produce statistical estimates of parameters describing the radiation heat transfer, such as the radiative heat flux or the divergence of the radiation heat flux. However, Monte Carlo methods suffer from the statistical nature of their results, which sometimes demands a large computation time to obtain the precision and accuracy required in engineering applications.

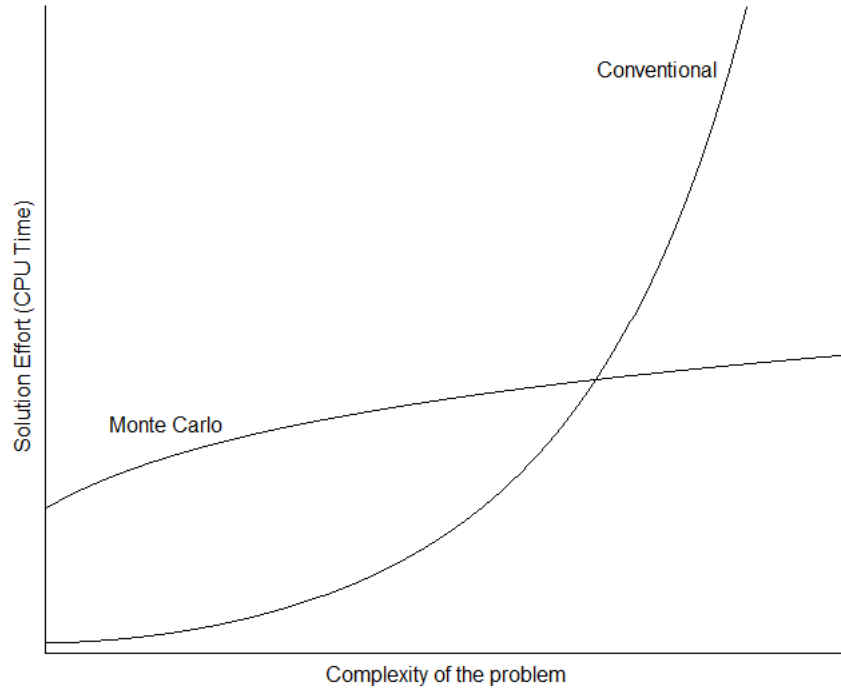


Figure 7 – Comparison between conventional solution techniques and the Monte Carlo method for radiation heat transfer.

3.1. Intuitive Idea of the Monte Carlo Ray Tracing Method

One can think of the Monte Carlo Ray Tracing method from a quite abstract point of view in which a set of random numbers ($\mathbf{U}$) –generated in a Random Number Generator (RNG)– is employed to produce a set of variables ($\mathbf{Y}$) –by inverting proper Cumulative Distribution Functions (CDF)– that characterize how a photon is emitted (location, direction, wavelength) and how it interacts with the boundaries and the participating medium. Of course, the information obtained after tracing only one ray is insignificant, but repeating the process over and over (thousands or maybe millions of times) it is possible to reproduce the features of the radiation heat transfer and obtain an accurate estimate of the objective function (I), such as the view factor, the radiative heat flux, the divergence of the radiative heat flux, and the like. Figure 8 shows a schematic representation of such intuitive idea. $\mathbf{U}^{(i)}$ is the d -dimensional random vector based on a $[0,1]^d$ uniform distribution for the ray i , $\mathbf{Y}^{(i)}$

is the d -dimensional vector containing the variables that describe the ray i and how it interacts with the boundaries and the participating medium (position, direction and wavelength of emission; whether a ray is absorbed or reflected when hitting a boundary, etc.), H_l is the performance function, $\hat{l}^{(i)}$ is the estimator of the objective value (radiative heat flux, divergence of the radiative heat flux, etc.) obtained for the ray i and $\hat{l} = \langle \hat{l}^{(i)} \rangle$ is the estimator of the objective value after tracing N rays. Note that the only randomness of the MCRT method lies on the generation of $\mathbf{U}^{(i)}$ and all the rest of the process is purely deterministic¹⁰.

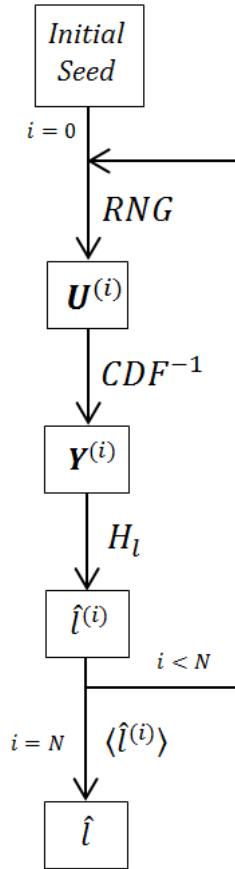


Figure 8 – Schematic representation of a Monte Carlo Ray Tracing simulation.

3.2. Cumulative Distribution Functions

In order to follow the histories of radiative energy bundles in a statistically meaningful way, the position, direction and wavelength of emission, the behavior of the surfaces and the

¹⁰ In reality, some random numbers need to be picked during the ray tracing when using the collision-based MCRT (one of the two MCRT strategies to be discussed in Section 3.7.2) and the dimension of $\mathbf{U}^{(i)}$ is ray-dependent. Nevertheless, the same intuitive reasoning applies for the collision-based method as well.

participating media, etc. must be chosen according to proper Cumulative Distribution Functions (CDF). For example, if a given property γ (position of emission, wavelength, etc.) has a probability density function $f(\gamma)$, it is possible to reproduce its behavior by picking a random number from a $[0,1)$ uniform distribution and inverting Eq. 3-1. Of course, only one random number does not mimic the actual behavior of γ , but in the limit of an infinite number of random numbers the actual behavior is reproduced.

$$R(\gamma) = \int_0^{\gamma} f(\gamma') d\gamma' \quad (3-1)$$

Although the expression of the CDFs can become much more involved when dealing with coupled, multidimensional probability density functions (it could involve multiple integrals), this concept also applies to such situations and constitutes the basic underlying concept of any Monte Carlo simulation.

3.3. Random Number Generator

In order to probabilistically solve a radiation heat transfer problem via Monte Carlo simulation, thousands or maybe millions of random numbers need to be utilized. Externally generating such a large set of random numbers and storing them in the computer would require a prohibitive amount of memory. Hence, the only feasible way to do so is by generating the random numbers within the computer itself. This appears to be a contradiction since digital computers are the incarnation of a logic system (i.e., deterministic) [24], but there exist several techniques to generate pseudorandom numbers (which are actually deterministic but behave as truly random numbers.) After making the choice of a starting point (an initial seed), these methods deterministically generate a new pseudorandom number from the previous one.

In our Monte Carlo code, a prime modulus multiplicative linear congruential generator based on Schrage's method with proper parameters [56] is employed to generate a virtually infinite sequence of statistically independent, uniformly distribute numbers between 0 and 1. This is done by the algorithm of Park and Miller [57] and the initial seed is obtained from the local time through the `localtime` function from the `time.h` header file of the C Standard Library [20], i.e. it varies between Monte Carlo iterations.

3.4. Monte Carlo Mesh Generation

Prior to perform a Monte Carlo Ray Tracing simulation, the mathematical domain $\bar{\Omega}$ must be discretized into a finite number of cells K_i so that $\bar{\Omega} = \cup_{i=1}^M K_i$ and $\mu_3(K_i \cap K_j) = \delta_{ij}$, where M is the number of Monte Carlo cells. Note that $\bar{\Omega}$ is used instead of Ω since both fluid zone (three-dimensional cells) and boundaries (two-dimensional cells) participate in thermal radiation and need to be included in the Monte Carlo Ray Trace mesh.

As stated in Chapter 2, the in-house Monte Carlo code developed in this *Proyecto Fin de Carrera* is able to simulate arbitrarily complex axisymmetric receivers, which is of utmost importance for the design and optimization of the solar receiver as non-cylindrical geometries will most likely increase the thermal efficiency and reduce the wall temperature. Therefore, the mesh generator must be able to generate meshes for any axisymmetric geometry. Moreover, on account of the high temperature and radiative-heat-transfer-divergence gradients present in the Small Particle Solar Receiver, non-uniform MCRT meshes would produce more accurate results [55]. Hence, the MCRT model utilizes structured (to speed up the ray tracing), non-uniform (to improve accuracy) meshes. Additionally, the size of the cells in different regions is a user-dependent input of the mesh generator (see Figure 9 for greater clarity). The procedure employed by the mesh generator to generate structured, non-uniform meshes in arbitrary axisymmetric geometries is described in the subsequent paragraphs.

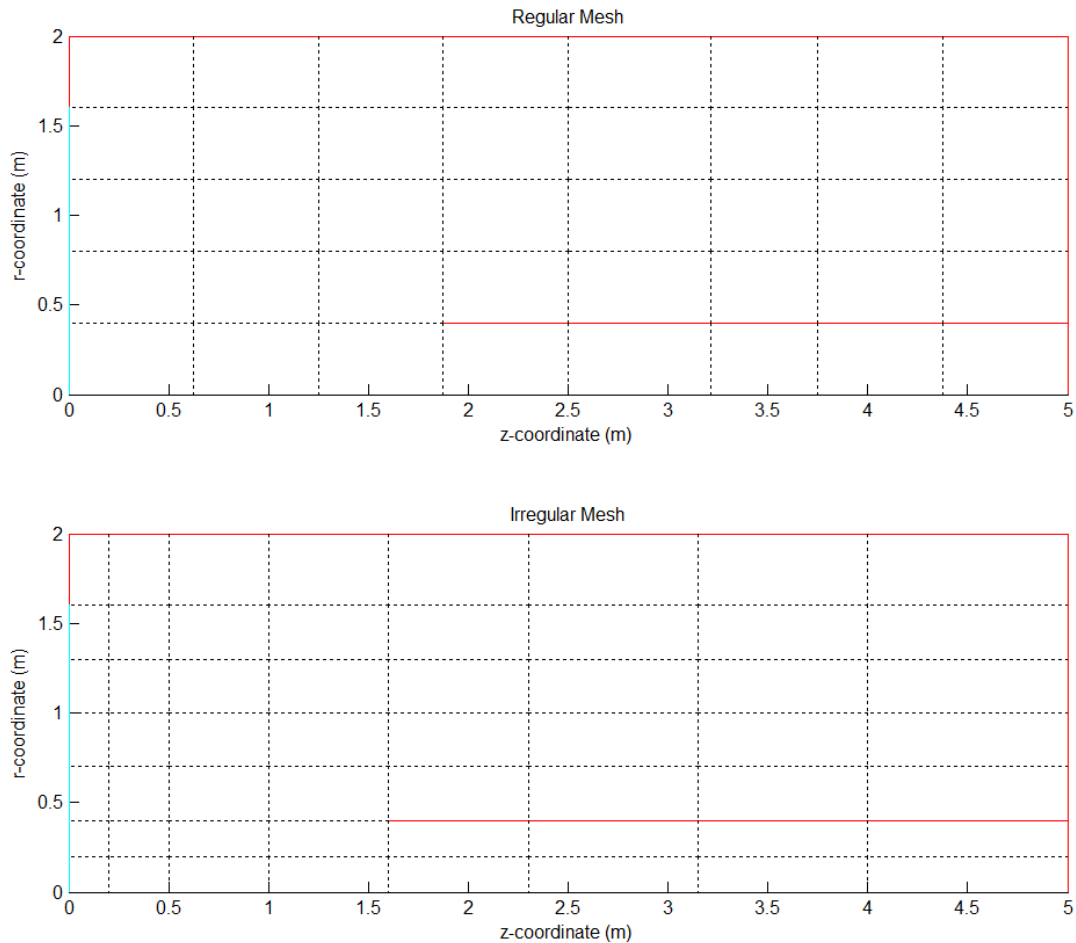


Figure 9 – Regular Monte Carlo mesh (top) vs. irregular Monte Carlo mesh to improve the accuracy of the radiative heat transfer solution (bottom). A ϕ -section is shown. The red lines represent the walls, outlet tube, inlet surface and outlet surface; while the light blue line represents the (flat) window.

First, the two-dimensional position of the nodes¹¹ (in a φ -plane) will be generated and stored in cylindrical coordinates (r, z) . They are calculated as summarized in Algorithm 1 and stored in a two-dimensional matrix, which implicitly takes into account the connectivity of the cells.

Algorithm 1

1. Generate the mesh as if the window was flat (Figure 10.a).
 2. If the window is curved (elliptical, spherical cap), reconstruct the mesh to include it: The fluid cells near the window are displaced and compressed towards the right to accommodate the presence of the curved window (Figure 10.b).
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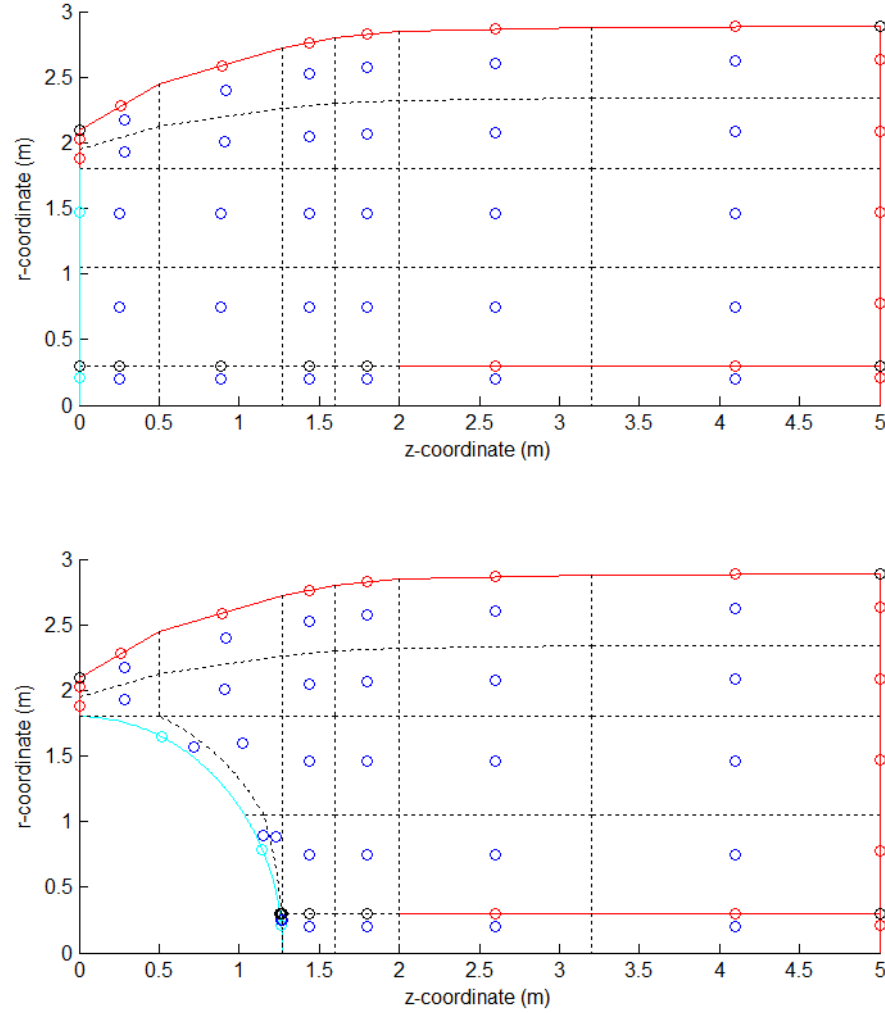


Figure 10 – Example of a φ -section of the Monte Carlo mesh with a flat window (top) and an ellipsoidal window (bottom). The figure on the top is also the intermediate step to generate the mesh with curved windows (the so-called Step 1 in Algorithm 1). The red lines represent the walls, outlet tube, inlet surface and outlet surface; while the light blue line represents the window. For completeness, the centroids of the Monte Carlo cells are shown in circles as well (dark blue: fluid cells; red: wall, outlet tube, inlet and outlet cells; light blue: window cells; black: fictitious cells, necessary to maintain the structured character of the mesh.)

¹¹ Hereinafter, *node* will denote the vertexes of the cells.

Once the (r, z) coordinates of the nodes are generated, the position of the cells' centroids are calculated and stored in a two-dimensional matrix as well. For the sake of simplicity, the equations to calculate the centroids of the different kind of MCRT cells are not presented here. Finally, the three-dimensional Cartesian coordinates of both the nodes and the centroids of the cells are generated (by proper rotation of the (r, z) coordinates around the Z axis, Eq. 3-2) and stored in three-dimensional matrices:

$$\begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} \cos \varphi & -\sin \varphi & 0 \\ \sin \varphi & \cos \varphi & 0 \\ 0 & 0 & 1 \end{pmatrix} \cdot \begin{pmatrix} r \\ 0 \\ z \end{pmatrix} \quad (3-2)$$

On account of the structured character of the Monte Carlo mesh, any cell (fluid cell, wall cell or window cell) can be identified by three indexes (i, j, k) ; which denote the axial, radial and angular position, respectively, and make the connectivity between cells trivial. Thus, memory and CPU time requirements are reduced compared to unstructured referencing.

It is convenient to introduce the following nomenclature for the air-particle mixture cells of the Monte Carlo mesh, for which Figure 10.b may be useful:

- Cells Type 1: Cells whose centroid verifies $r < R_{win}$ and $z > z_{win}|_{r=0}$. The common feature of cells Type 1 is that the z^- and z^+ faces are always planes and the r^- and r^+ faces are always cylinders, i.e. $\partial z_{max}/\partial r = \partial z_{min}/\partial r = \partial r_{max}/\partial z = \partial r_{min}/\partial z = 0$.
- Cells Type 2: Cells whose centroid is such that $r > R_{win}$. In these cells, the z^- and z^+ faces are planes and the r^- and r^+ faces are cones (of which cylinders are a particular case), i.e. $\partial z_{max}/\partial r = \partial z_{min}/\partial r = 0$ but $\partial r_{max}/\partial z, \partial r_{min}/\partial z \neq 0$.
- Cells Type 3: Cells whose centroid verifies $r < R_{win}$ and $z < z_{win}|_{r=0}$. In cells Type 3 the r^- and r^+ faces are always cylinders, while the z^- and z^+ faces can be a portion of a sphere or an ellipsoid, i.e. $\partial r_{max}/\partial z = \partial r_{min}/\partial z = 0$ but $\partial z_{max}/\partial r, \partial z_{min}/\partial r \neq 0$.

Regardless the type of air-particle mixture cell, the φ^- and φ^+ faces are always planes. Note also that with the mesh generation algorithm employed, either the minimum and maximum radial positions or the minimum and maximum axial positions of every Monte Carlo cell are always constant across the cell (they do not depend on the axial or radial coordinate, respectively.) This is of great importance to simplify the computation of the volume and the Cumulative Distribution Functions of the location of emission¹².

Finally, it should be pointed out that the geometries of the window that the MCRT mesh generator can generate are:

1. Flat windows with one degree of freedom, namely the size (e.g., the diameter.)

¹² This way, only the dependence of one coordinate cannot be inverted analytically and needs to be tabulated.

2. Ellipsoidal windows with two degrees of freedom: Size and shape (only one degree of freedom is required to characterized the shape of an axisymmetric oblate spheroid. In particular the ratio between principal axes is employed.)
3. Spherical cap windows with two degrees of freedom: Size and shape (the shape is characterized through the cap angle.)

3.5. Steps of the Ray Tracing

The main steps to perform a Monte Carlo Ray Tracing simulation are outlined in Figure 11. For the sake of simplicity, only the analytical expression of the Monte Carlo cells' volume and the Cumulative Distribution Functions (instead of their mathematical proof) will be presented. Hence, the goal of this section is to illustrate the procedure rather than delving deeper into the rigorous mathematical formulation.

1. Calculate the area (two-dimensional cells) or the volume (three-dimensional cells) of all the cells of the Monte Carlo mesh

The area (two-dimensional cells) and the volume (three-dimensional cells) of the Monte Carlo cells needs to be computed to (1) calculate the emissive power of every cell (Step #2) and (2) calculate the source term per unit volume or per unit area (Step #8), which is the variable to be passed to the CFD solver ANSYS Fluent. When the MCRT code is not coupled to ANSYS Fluent, e.g., to validate the code or to perform statistical analyses of different MCRT strategies (see Section 3.7.2 in this chapter), the *mathematical* volume/area of the Monte Carlo cells is calculated by integration over their geometrical domain. The analytical expressions of the area of the different types of two-dimensional cells are reported in Appendix A. Using, without loss of generality, a cylindrical coordinate system such that $\varphi = z = 0$ in the intersection of the r^- , φ^- and z^- faces of the cell i , the volume of the three-dimensional cells can be readily computed as:

- Cells Type 2:

$$V_i = \int_0^{\Delta\varphi} \int_0^{\Delta z} \int_{r_S(z)}^{r_N(z)} dV = \dots = \Delta\varphi \int_0^{\Delta z} \frac{1}{2} [r_N^2(z) - r_S^2(z)] dz \quad (3-3)$$

- Cells Type 3:

$$V_i = \int_0^{\Delta\varphi} \int_{R_S}^{R_N} \int_{z_W(r)}^{z_E(r)} r dr dz d\varphi = \dots = \Delta\varphi \int_{R_S}^{R_N} r [z_E(r) - z_W(r)] dr \quad (3-4)$$

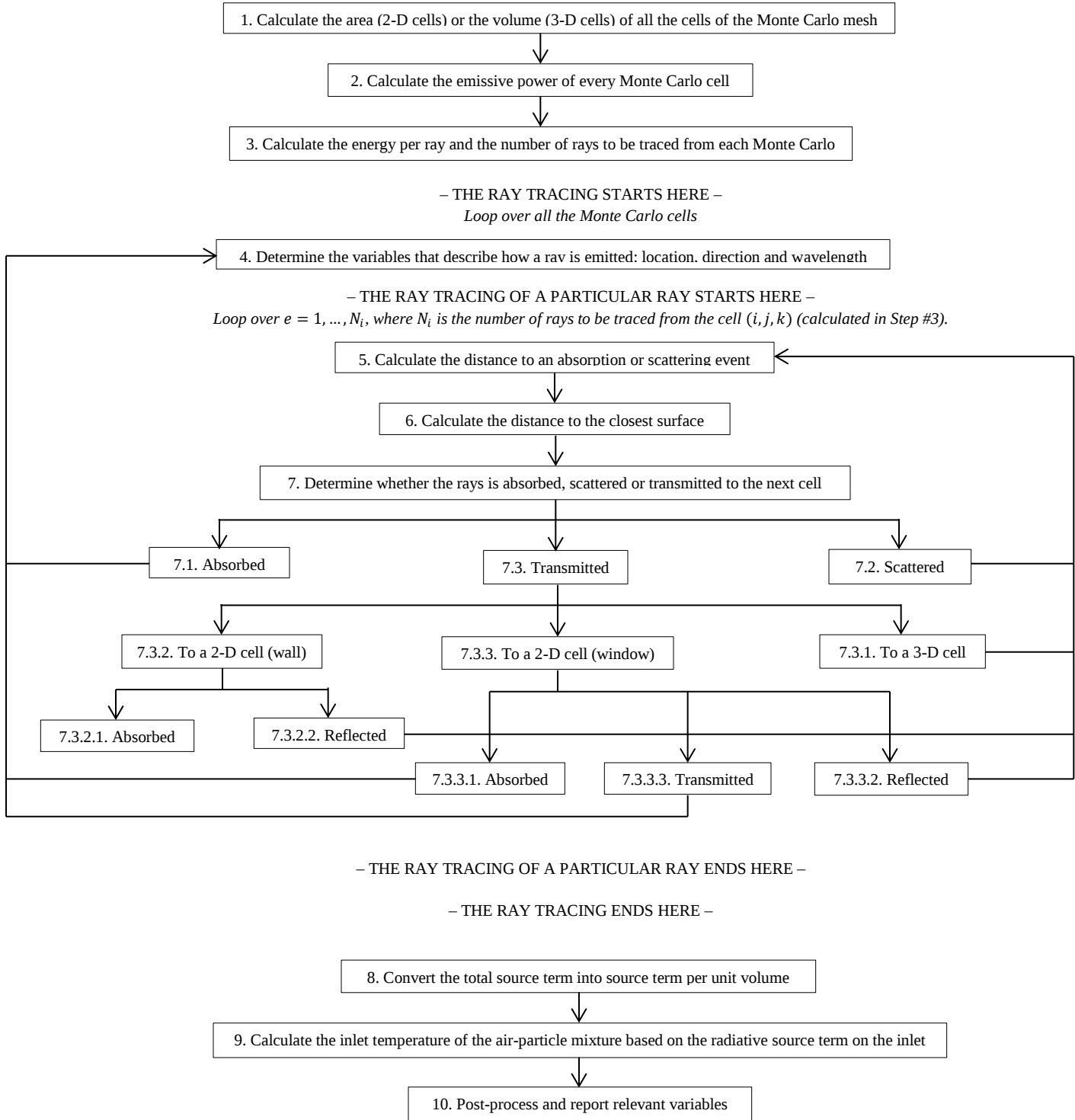


Figure 11 – Flow chart with the main steps to perform a Monte Carlo Ray Tracing simulation.

Since cells Type 1 are just a particular case of both cells Type 2 and cells Type 3, either equation leads to the same result $V = \frac{1}{2}(R_N^2 - R_S^2)\Delta z\Delta\phi$. The integrals in Eq. 3-3 and 3-4

for all the cell geometries present in the Monte Carlo mesh have been calculated and are reported in Appendix B.

When the MCRT is coupled to the CFD solver, the previous strategy may lead to an energy imbalance: The mathematical domain of the fluid, walls and window is discretized into a finite number of CFD cells, and the total volume/area of the CFD model does not exactly match the area/volume provided in Appendices A and B. Since the way the source term is passed from the MCRT code to ANSYS Fluent is per unit area/volume, the total source term in the receiver (energy per unit time) that is plugged into the energy equation of the CFD solver wouldn't be exact. Moreover, as the error in the thermal efficiency of the receiver or the useful power –two of the main outputs of the model– is of the same order as the energy imbalance, this error cannot be tolerated. Thus, the area/volume of all the CFD cells that are inside a Monte Carlo cell are added up (via User-Defined Functions, see Section 5.1) and this is the area/volume employed in the MCRT code.

2. Calculate the emissive power of every Monte Carlo cell

Once the area/volume (calculated in Step #1), temperature (passed from ANSYS Fluent via UDF, see Section 5.1) and spectral emissive properties are known (the latter two assumed constant in each Monte Carlo cell), the emissive power of the cells can be readily obtained.

- Emissive Power of 2-D cells:

$$E_i = A_i \varepsilon_i(T_i) \sigma T_i^4$$

$$\varepsilon_i(T_i) = \frac{\int_0^\infty \varepsilon_{\lambda,i}(T_i) E_{b,\lambda}(T_i) d\lambda}{\int_0^\infty E_{b,\lambda}(T_i) d\lambda} \approx \frac{\int_0^{\lambda_{\uparrow\uparrow}} \varepsilon_{\lambda,i}(T_i) E_{b,\lambda}(T_i) d\lambda}{\int_0^{\lambda_{\uparrow\uparrow}} E_{b,\lambda}(T_i) d\lambda} \quad (3-5)$$

Where integrals are computed numerically in the Monte Carlo code using $\lambda_{\uparrow\uparrow} = 50\mu m$. While obviously $\varepsilon_\lambda(T) = 1$ for a blackbody, the spectral emissivity of different materials and surface conditions needs to be measured experimentally. For example, the spectral emissivity of aluminum oxide, one of the main alternatives for the material to be employed on the walls, is plotted in Figure 12.

- Emissive Power of 3-D cells:

$$E_i = 4V_i \kappa_i(T_i) \sigma T_i^4$$

$$\kappa_i(T_i) = \frac{\int_0^\infty \kappa_{\lambda,i}(T_i) E_{b,\lambda}(T_i) d\lambda}{\int_0^\infty E_{b,\lambda}(T_i) d\lambda} \approx \frac{\int_0^{\lambda_{\uparrow\uparrow}} \kappa_{\lambda,i}(T_i) E_{b,\lambda}(T_i) d\lambda}{\int_0^{\lambda_{\uparrow\uparrow}} E_{b,\lambda}(T_i) d\lambda} \quad (3-6)$$

Where the spectral absorption coefficient κ_λ of the particles is calculated via Mie theory [58] and the gas phase is modeled as radiatively non-participating due to the negligible

amount of CO₂ generated in the receiver. In particular, the partial pressure of CO₂ after the complete oxidation of the carbon particles when a mass loading of 0.5 g/m³ is employed is:

$$p_{CO_2} = \phi_{CO_2} \cdot p \approx 5.12 \cdot 10^{-4} \cdot 5 \text{ bar} = 2.5578 \cdot 10^{-3} \text{ bar}$$

which leads to $\alpha_{CO_2} \approx 0$ vs. $\alpha_P = 0.99$ for the solar spectrum and the axial path length.

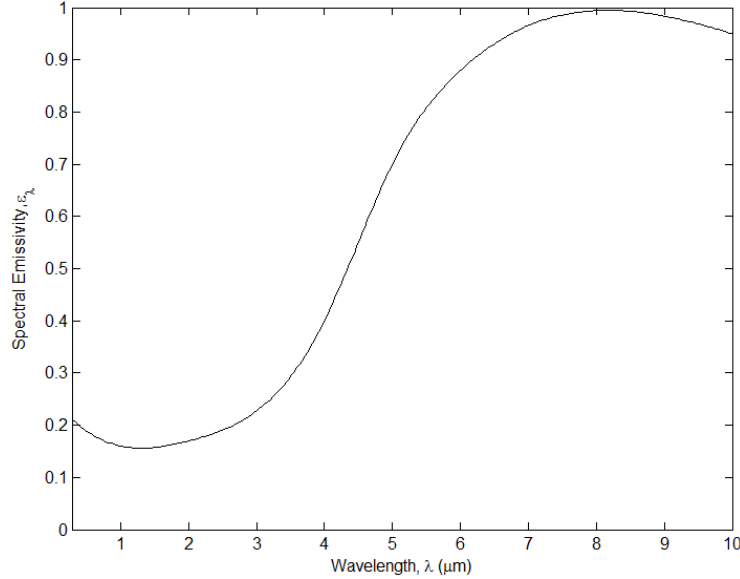


Figure 12 – Spectral emissivity of aluminum oxide (Al₂O₃). Note that, under local thermodynamic equilibrium, the spectral emissivity equals the spectral absorptivity in diffuse surfaces such as Al₂O₃.

3. Calculate the energy per ray and the number of rays to be traced from each Monte Carlo cell

As discussed in Section 3.7.1.3, the optimum strategy consists on tracing a number of rays from each cell so that the energy per ray is constant, as long as a minimum number of rays are emitted from each ray (Eq. 3-7). The maximum number of rays traced from every Monte Carlo cell is limited as well.

$$N_i = \min \left\{ \max \left[N_{TOTAL} \cdot SUP \left(\frac{E_i}{E_{TOTAL}} \right), N_{min} \right], N_{max} \right\} \quad (3-7)$$

Where N_i is the number of rays traced from the cell i , N_{TOTAL} is the total number of rays to be traced (see Section 5.4), E_i is the emissive power of the cell i , $E_{TOTAL} = \sum_i E_i$ is the total emissive power of the Small Particle Solar Receiver (including the air-particle mixture, the walls and the window), and $SUP(\cdot)$ denotes the smallest integer greater than $\cdot$. N_{min} and N_{max} are the minimum and maximum number of rays to be traced from every cell, respectively, and will be defined in Eq. 3-40.

Finally, the energy per ray is simply $e_i = \frac{E_i}{N_i}$.

4. Determine the variables that describe how a ray is emitted

4.1. Location of emission

To determine the location of emission from a three-dimensional cell, three random numbers need to be picked (one per spatial dimension). For convenience's sake, cylindrical coordinates are employed, i.e., one random number is utilized for the axial coordinate, another for the radial coordinate and one more for the azimuthal coordinate. Since both emissivity and temperature are constant over each Monte Carlo cell, the position of emission can be calculated based on the Cumulative Distribution Function of the volume. Employing a general orthogonal coordinate system (q_1, q_2, q_3) this is expressed as in Equations 3-8.

$$\begin{aligned}
 R_{q_1} &= \frac{\int_{q_{1,min}}^{q_1} \int_{q_{3,min}(q'_1)}^{q_{3,max}(q'_1)} \int_{q_{2,min}(q'_1, q'_3)}^{q_{2,max}(q'_1, q'_3)} dV(q'_1, q'_2, q'_3)}{\int_{q_{1,min}}^{q_{1,max}} \int_{q_{3,min}(q'_1)}^{q_{3,max}(q'_1)} \int_{q_{2,min}(q'_1, q'_3)}^{q_{2,max}(q'_1, q'_3)} dV(q'_1, q'_2, q'_3)} \Rightarrow q_1^* = q_1^*(R_{q_1}) \\
 R_{q_2} &= \frac{\int_{q_{2,min}(q_1^*)}^{q_2} \int_{q_{3,min}(q_1^*, q'_2)}^{q_{3,max}(q_1^*, q'_2)} dA(q'_2, q'_3)}{\int_{q_{2,min}(q_1^*)}^{q_{2,max}(q_1^*)} \int_{q_{3,min}(q_1^*, q'_2)}^{q_{3,max}(q_1^*, q'_2)} dA(q'_2, q'_3)} \Rightarrow q_2^* = q_2^*(R_{q_2}, q_1^*) \\
 R_{q_3} &= \frac{\int_{q_{3,min}(q_1^*, q_2^*)}^{q_3} dl(q'_3)}{\int_{q_{3,min}(q_1^*, q_2^*)}^{q_{3,max}(q_1^*, q_2^*)} dl(q'_3)} \Rightarrow q_3^* = q_3^*(R_{q_2}, q_1^*, q_2^*)
 \end{aligned} \tag{3-8}$$

Where it is now obvious the coupling between the coordinates of emission. These equations can be considerably simplified by cleverly choosing the order of integration:

- Cells Type 2: Axial position – Radial position – Azimuthal position, i.e., $(q_1, q_2, q_3) = (z, r, \varphi)$
- Cells Type 3: Radial position – Axial position – Azimuthal position, i.e., $(q_1, q_2, q_3) = (r, z, \varphi)$

Since cells Type 1 are just a particular case of both cells Type 2 and cells Type 3, either order simplifies Equations 3-8. Note that the possibility of simplifying Equations 3-8 arises from the fact that for such order (1) $q_{2,min}(q_1, q_3)$ and $q_{2,max}(q_1, q_3)$ are not piecewise functions –while $q_{1,min}(q_2, q_3)$ and $q_{1,max}(q_2, q_3)$ are– and, moreover, (2) $\frac{\partial q_{3,min}}{\partial q_1} = \frac{\partial q_{3,min}}{\partial q_2} = \frac{\partial q_{3,max}}{\partial q_1} = \frac{\partial q_{3,max}}{\partial q_2} = 0 \forall q_1, q_2$.

In particular, the expressions to calculate the location of emission from cells Type 2 are given in Equations 3-9.

$$\begin{aligned}
R_z &= \frac{\int_{z_W}^z \int_{r_S(z')}^{r_N(z')} \int_0^{\Delta\varphi} dV}{\int_{z_W}^{z_E} \int_{r_S(z')}^{r_N(z')} \int_0^{\Delta\varphi} dV} = \frac{\int_{z_W}^z \left[\frac{r_N(z')^2}{2} - \frac{r_S(z')^2}{2} \right] dz'}{\int_{z_W}^{z_E} \left[\frac{r_N(z')^2}{2} - \frac{r_S(z')^2}{2} \right] dz'} \\
R_r &= \frac{\int_{r_S(z)}^r r' dr'}{\int_{r_S(z)}^{r_N(z)} r' dr'} = \frac{r^2 - r_S^2}{r_N^2 - r_S^2} \Rightarrow r = \sqrt{r_S(z)^2 + R_r[r_N(z)^2 - r_S(z)^2]} \\
R_\varphi &= \frac{\int_{\varphi_1}^\varphi d\alpha}{\int_{\varphi_1}^{\varphi_2} d\alpha} = \frac{\varphi - \varphi_1}{\varphi_2 - \varphi_1} \Rightarrow \varphi = \varphi_1 + R_\varphi(\varphi_2 - \varphi_1)
\end{aligned} \tag{3-9}$$

While for cells Type 3:

$$\begin{aligned}
R_r &= \frac{\int_{R_S}^r \int_{z_W(r')}^{z_E(r')} \int_0^{\Delta\varphi} dV}{\int_{R_S}^{R_N} \int_{z_W(r')}^{z_E(r')} \int_0^{\Delta\varphi} dV} = \frac{\int_{R_S}^r r' [z_E(r') - z_W(r')] dr'}{\int_{R_S}^{R_N} r' [z_E(r') - z_W(r')] dr'} \\
R_z &= \frac{\int_{z_W(r)}^z dz}{\int_{z_W(r)}^{z_E(r)} dz} = \frac{z - z_W(r)}{z_E(r) - z_W(r)} \Rightarrow z = z_W(r) + R_z[z_E(r) - z_W(r)] \\
R_\varphi &= \frac{\int_{\varphi_1}^\varphi d\alpha}{\int_{\varphi_1}^{\varphi_2} d\alpha} = \frac{\varphi - \varphi_1}{\varphi_2 - \varphi_1} \Rightarrow \varphi = \varphi_1 + R_\varphi(\varphi_2 - \varphi_1)
\end{aligned} \tag{3-10}$$

Equations 3-9.a-b and 3-10.a-b depend on the particular shape of the Monte Carlo cell through $r_S(z)$ & $r_N(z)$ and $z_W(r)$ & $z_E(r)$, respectively. The CDF obtained after integration for all the cell geometries present in the Monte Carlo mesh have been calculated and are reported in Appendix D.

For two-dimensional cells, similar arguments apply but only two equations –namely Equations 3-8.a-b– and two coordinates $-(q_1, q_2)$ – are required. The expressions to determine the location of emission from the different kinds of two-dimensional cells are provided in Appendix C.

4.2. Wavelength of emission

- From a surface (two-dimensional cells):

Under Local Thermodynamic Equilibrium (see Section 2.3.1 for a proof of LTE) the spectral absorptance equals the spectral emittance, as expressed by Kirchhoff's law, and the CDF for the wavelength of emission can be readily obtained as:

$$R_\lambda = \frac{\int_0^\lambda \varepsilon_\lambda i_{b\lambda}(T) d\lambda}{\int_0^\infty \varepsilon_\lambda i_{b\lambda}(T) d\lambda} = \frac{\pi}{\varepsilon_\sigma T^4} \int_0^\lambda \varepsilon_\lambda i_{b\lambda}(T) d\lambda \Rightarrow \lambda^* = \lambda^*(R_\lambda) \quad (3-11)$$

- From the air-particle mixture (three-dimensional cells):

By similar arguments as for the emission from a surface:

$$R_\lambda = \frac{\pi}{\kappa_\sigma T^4} \int_0^\lambda \kappa_\lambda i_{b\lambda}(T) d\lambda \Rightarrow \lambda^* = \lambda^*(R_\lambda) \quad (3-12)$$

Where κ_λ is obtained via Mie theory [58] and κ is the Planck-mean absorption coefficient computed by weighted-average of κ_λ (based on the blackbody emissive power at temperature T).

4.3. Direction of emission

- From a surface (two-dimensional cells):

$$R_\varphi = \frac{1}{\pi} \int_0^\varphi d\varphi' \int_0^{\pi/2} \frac{\varepsilon'_\lambda(\theta', \varphi')}{\varepsilon_\lambda} \cos \theta' \sin \theta' d\theta' \Rightarrow \varphi^* = \varphi^*(R_\varphi, \lambda^*) \quad (3-13)$$

$$R_\theta = \frac{\int_0^\theta \varepsilon'_\lambda(\theta', \varphi^*) \cos \theta' \sin \theta' d\theta'}{\int_0^{\pi/2} \varepsilon'_\lambda(\theta', \varphi^*) \cos \theta' \sin \theta' d\theta'} \Rightarrow \theta^* = \theta^*(R_\theta, \lambda^*, \varphi^*)$$

For an isotropic surface $\varepsilon'_\lambda(\theta, \varphi) = \varepsilon'_\lambda(\theta) \Rightarrow \varphi^* = 2\pi R_\varphi$. If, additionally, the surface is diffuse $\varepsilon'_\lambda(\theta, \varphi) = \varepsilon_\lambda \Rightarrow \theta^* = \sin^{-1} \sqrt{R_\theta}$. Both are, in general, good approximations to the radiative behavior of a surface and will be always employed except stated otherwise.

- From the air-particle mixture (three-dimensional cells):

Under Local Thermodynamic Equilibrium and assuming the particles –which are not perfect spheres [35]– are randomly oriented, emission within the air-particle mixture is isotropic and, therefore:

$$\varphi^* = 2\pi R_\varphi \quad \theta^* = \cos^{-1}(1 - 2R_\theta) \quad (3-14)$$

5. Calculate the distance to an absorption or scattering event

When radiation travels through a participating medium, the energy is attenuated by absorption and scattering. On account of the mathematical analogy between both phenomena, they can be treated in a similar fashion with the only difference of the parameter involved (absorption coefficient vs. scattering coefficient.)

The fraction of radiation absorbed through a path length l_κ is:

$$R_\kappa = e^{-\int_0^{l_\kappa} \kappa_\lambda ds} \quad (3-15)$$

Neither the spectral absorption coefficient nor the spectral scattering coefficient are constant throughout the Small Particle Solar Receiver, both due to temperature gradient and particle oxidation (recall the latter is not included in the model yet, as it is currently being developed by Trent Martin, a graduate student in our group.) However, all properties are assumed constant in each Monte Carlo cell and Eq. 3-15 can be inverted analytically. In particular, the distance to absorption is the average of the distance calculated for all the cells through which the ray has previously travelled (the same random number, R_κ , is employed in all the cells):

$$l_\kappa = \left(\frac{\sum_i l_i}{\sum_i l_i \kappa_{\lambda,i}} \right) \ln R_\kappa \quad (3-16)$$

Where i refers to all those cells through which the energy bundle has previously traveled from emission, l_i is the distance that the ray has traveled through the cell i , and $\kappa_{\lambda,i}$ is the spectral absorption coefficient of the cell i .

All the previous concepts are valid for scattering just by replacing κ_λ for $\sigma_{s,\lambda}$. Hence, the distance to scattering event can be computed as in Eq. 3-17.

$$l_{\sigma_s} = \left(\frac{\sum_i l_i}{\sum_i l_i \sigma_{s,\lambda,i}} \right) \ln R_{\sigma_s} \quad (3-17)$$

Both spectral absorption and scattering coefficients are computed in the MCRT code right after the wavelength of emission is determined (Step #4.2). This calculation is conducted for the pressure and temperature conditions at the inlet, i.e., referring the mass loading to the air density at the inlet. Therefore, the spectral absorption and scattering coefficients of each cell need to be modified to consider the volumetric expansion due to temperature increase ($\kappa_{\lambda,i} = \kappa_{\lambda,ref} T_{ref}/T_i$). This way the CPU time is reduced around 40% compared to calculating the spectral absorption and scattering coefficient every time a ray enters into a new cell. Of course, the strategy presented in this paragraph is only valid since particle oxidation is not included in the model and the radiative properties of particulate media are linear in the mass loading (but not in the particle size.)

6. Calculate the distance to the closest face

The calculation of the distance to the closest face is split up into two steps:

1. Calculate the distance to the six faces¹³: $\{l_i\}_{i=1,\dots,6}$
2. Pick the smallest one¹⁴: $l_f = \min_i \{l_i\}$

For the first step, the kind of surface the six faces are (planes, cylinders, cones, ellipsoids and/or spheres) is determined first and the distance itself is calculated later. While for flat and cylindrical faces the algorithm to calculate the distance was already implemented in the 2-D model [19], they have been simplified and optimized to reduce the CPU time. Moreover, the algorithms to calculate the distance to conical, ellipsoidal and spherical faces have been developed for this 3-D model. The equations to calculate the distance to the different kind of faces present in the MCRT mesh are shown in Appendix E.

Special care need to be taken when employing only one or two angular divisions. With one angular division, the MCRT reduces to a 2-D model and only four (or three¹³) intersections are to be calculated. With two angular divisions, the mathematical surface of the φ^- and φ^+ faces is the same. Hence, only one of both distances needs to be computed and it is necessary to identify with which of them the ray actually intersects.

7. Determine whether the rays is absorbed, scattered or transmitted to the next cell

7.1. If the ray is absorbed ($l_\kappa \leq l_f, l_{\sigma_s}$)

The energy of the ray is added to the corresponding Monte Carlo cell.

7.2. If the ray is scattered ($l_{\sigma_s} \leq l_f$ and $l_{\sigma_s} < l_\kappa$)

The new direction of the ray needs to be determined. The zenith and azimuthal angles respect to the initial direction of propagation can be obtained from proper CDFs for the scattering phase function. Assuming the particles are randomly oriented, the phase function of the air-particle mixture is the same as the one of an individual, spherical particle, which is derived from Mie theory [58].

$$\begin{aligned}
 R_\theta &= \frac{1}{2} \int_0^\theta \Phi_\lambda(\theta') \sin \theta' d\theta' \Rightarrow \theta^* = \theta^*(R_\theta) \\
 R_\varphi &= \frac{1}{4\pi} \int_0^\varphi \int_0^\pi \Phi_\lambda(\theta) \sin \theta d\theta d\psi' = \dots = \frac{\varphi}{2\pi} \Rightarrow \varphi^* = 2\pi R_\varphi
 \end{aligned} \tag{3-18}$$

¹³ Some cells only have five boundary faces (the cells next to the axis of symmetry and the cells next to the left wall for some geometries.) These cases need to be identified and the computation of the distance to the nonexistent face, avoided.

¹⁴ If the smallest distance is the same for two faces, the ray intersects with an edge and two indexes need to be changed simultaneously. Since double precision is employed (the probability of this to happen is less than 10^{-7}), the tracing of such rays is stopped without noticeable loss of accuracy in the numerical solution.

7.3. If the ray is transmitted ($l_f < l_{\kappa}, l_{\sigma_s}$)

7.3.1. Transmitted to a three-dimensional cell (air-particle mixture cell)

The indexes (i, j, k) that report the current Monte Carlo cell (recall the MCRT mesh is structured) need to be updated. While in general only one unit need to be added (or subtracted) to the proper index (e.g., $i_{new} = i_{old} \pm 1$), in some situations two units must be changed at once, such as when the ray crosses the extension of the outlet tube. The code is able to determine this particular case and properly modify the indexes based on that.

7.3.2. Transmitted to a two-dimensional cell (Case I: Wall)

In this situation, the ray is not actually *transmitted*. Rather, a random number is generated to determine whether the ray is absorbed or reflected by the wall: If $R \leq \alpha'_\lambda$ the ray is absorbed, while it is reflected otherwise. The directional, spectral absorptivity α'_λ is a material property (Kirchhoff's Law under LTE) and equals the directional, spectral emissivity ϵ'_λ .

7.3.2.1. If the ray is absorbed

The energy of the ray is added to the corresponding Monte Carlo cell.

7.3.2.2. If the ray is reflected

The reflective behavior of the walls is idealized as a combination of a pure diffuse and a pure specular component, i.e., the spectral, bidirectional reflection function can be expressed as in Eq. 3-19.

$$\rho''_\lambda(\theta_i, \theta_r, \varphi_i, \varphi_r) = \begin{cases} \frac{\rho_\lambda(1-f_s)}{\pi} & \text{for } \theta_r \neq \theta_i \text{ and } \varphi_r \neq \varphi_i + \pi \\ \frac{\rho_\lambda f_s}{\cos \theta_r \sin \theta_r} \delta(\theta_i - \theta_r, \varphi_i - \varphi_r) & \text{for } \theta_r = \theta_i \text{ and } \varphi_r = \varphi_i + \pi \end{cases} \quad (3-19)$$

A random number is employed to determine whether the ray is reflected specularly ($R \leq f_s$) or diffusely ($R > f_s$), and the direction of reflection is computed using Equations 3-20 or Equations 3-21, respectively [19,24]:

- Specular Reflection:

$$\theta_r = \theta_i \quad \varphi_r = \varphi_i + 2\pi \quad (3-20)$$

- Diffuse Reflection:

$$\theta_r = \sin^{-1} \sqrt{R_\theta} \quad \varphi_r = 2\pi R_\varphi \quad (3-21)$$

Where the z-axis of the spherical coordinate system (used to define θ and φ) is the inward normal vector to the wall. The orientation of the x- and y-axes on isotropic surfaces is completely arbitrary.

7.3.3. Transmitted to a two-dimensional cell (Case II: Window)

Once again, a random number is used to determine whether the ray is reflected, transmitted or absorbed by the window. The directional, spectral absorptivity (A'_λ), transmissivity (T'_λ) and reflectivity (R'_λ) of the window are calculated using electromagnetic theory¹⁵ (Equations 3-22). Note that the electromagnetic theory can be applied since the interfaces between glass and air (1) are optically smooth at the scale of the wavelength and (2) are of precisely the same (homogeneous) material as the bulk material [24].

$$\begin{aligned}
 T'_\lambda &= \frac{(1 - \rho'_\lambda)^2 e^{-k_{\lambda,2}d/\cos\theta_2}}{1 - \rho'^2_\lambda e^{-2k_{\lambda,2}d/\cos\theta_2}} \\
 R'_\lambda &= \rho'_\lambda \left[1 + \frac{(1 - \rho'_\lambda)^2 e^{-2k_{\lambda,2}d/\cos\theta_2}}{1 - \rho'^2_\lambda e^{-2k_{\lambda,2}d/\cos\theta_2}} \right] & A'_\lambda &= \frac{(1 - \rho'_\lambda)(1 - e^{-k_{\lambda,2}d/\cos\theta_2})}{1 - \rho'_\lambda e^{-k_{\lambda,2}d/\cos\theta_2}} \\
 \rho'_\lambda &= \frac{1}{2}(\rho'_{p,\lambda} + \rho'_{s,\lambda}) & n_{\lambda,1} \cos\theta_1 &= n_{\lambda,2} \cos\theta_2 \\
 \rho'_{p,\lambda} &= \left(\frac{n_{\lambda,1} \cos\theta_2 - n_{\lambda,2} \cos\theta_1}{n_{\lambda,1} \cos\theta_2 + n_{\lambda,2} \cos\theta_1} \right)^2 & \rho'_{s,\lambda} &= \left(\frac{n_{\lambda,1} \cos\theta_1 - n_{\lambda,2} \cos\theta_2}{n_{\lambda,1} \cos\theta_1 + n_{\lambda,2} \cos\theta_2} \right)^2
 \end{aligned} \tag{3-22}$$

7.3.3.1. If the ray is absorbed

The energy of the ray is added to the corresponding Monte Carlo cell.

7.3.3.2. If the ray is reflected

As electromagnetic theory applies, the reflection on the window is purely specular so that Equations 3-20 is used.

7.3.3.3. If the ray is transmitted

The ray is lost and its energy is stored in proper variables so that the following information is available when post-processing the results:

- Origin of the losses: The energy emitted from each cell (and coming from the heliostat field) that is eventually lost is stored and a complete description of the origin of the losses is obtained.
- The way the energy coming from the heliostat field is lost: just due to scattering, due to reflection on the exterior wall, etc.

¹⁵ It is also assumed that $k_{\lambda,2}$ is small enough so that Fresnel equations apply.

This information is useful to reduce the radiative losses in the design optimization process.

8. Convert the total source term into source term per unit volume

The total radiative source term calculated by the Monte Carlo method is converted into source term per unit volume, as this is the value to be used by the CFD solver in the energy equation.

$$\nabla \cdot \mathbf{q}_i^r = Q_i^{rad} / V_i \quad [W/m^3] \quad (3-23)$$

Recall that when the MCRT method and the CFD solver are coupled, the volume of all the CFD cells inside a Monte Carlo cell –instead of the *mathematical* volume– is employed to exactly match the energy balance as will be explained in Section 5.1. Finally, if the walls were modeled as boundary surfaces in ANSYS Fluent, instead of as volumetric media, the source term per unit area would be to be used.

$$\mathbf{q}_i^r \cdot \hat{\mathbf{n}} = Q_i^{rad} / A_i \quad [W/m^2] \quad (3-24)$$

9. Calculate the inlet temperature of the air-particle mixture based on the radiative source term on the inlet surface

The inlet surface participates in the radiation heat transfer and a net radiative heat flux does exist on it; so that the inlet temperature of the air-particle mixture in the receiver needs to be modified based on such a radiative source term:

$$Q_{inlet}^{rad} = \int_{T_0}^{T_{inlet}^*} \dot{m} c_p(T') dT' \quad (3-25)$$

Assuming a linear variation of the specific heat capacity at constant pressure $c_p = c_{p,ref} + \frac{\partial c_p}{\partial T} \cdot (T' - T_{ref})$ the previous integral can be explicitly inverted in terms of T_{inlet}^* :

$$T_{inlet}^* = \frac{-B \pm \sqrt{B^2 - 4AC}}{2A} \quad (3-26)$$

Where:

$$A = \frac{1}{2} \frac{\partial c_p}{\partial T} \quad B = c_{p,ref} - \frac{\partial c_p}{\partial T} T_{ref} \quad C = \frac{\partial c_p}{\partial T} T_0 T_{ref} - c_{p,ref} T_0 - \frac{1}{2} \frac{\partial c_p}{\partial T} T_0^2 - \frac{Q_{inlet}^{rad}}{\dot{m}}$$

The subscript 0 denotes the conditions at the outlet of the recuperator or the compressor (for recuperated and non-recuperated cycles, respectively). In our model $T_0 = 700K$

(recuperated cycled) is employed [60] in an effort to evaluate the solar receiver itself. Note, however, that the inlet temperature in a recuperated gas turbine engine actually varies with a number of factors [61] (e.g., solar thermal input, guide vane angle or recuperator performance).

A minimum and maximum inlet temperature (the former usually 700 K and the latter 800-1100 K depending on the ratio *mass flow rate vs. solar thermal input*) is employed to improve convergence, so that:

$$T_{inlet} = \max \left\{ T_{inlet}^{min}, \min(T_{inlet}^{max}, T_{inlet}^*) \right\} \quad (3-27)$$

10. Post-process and report relevant variables

The following variables are reported and stored in `.txt` and `.dat` files:

- Monte Carlo mesh information: Position of the cell centroids and cell nodes, as well as the volume/area of each cell.
- Energy per ray field and rays per Monte Carlo cell field. Only the file of the last iteration is kept.
- Radiative source term field. The files of all the iterations are kept.
- Temperature field. The files of all the iterations are kept.
- Summary file with the number of rays traced (both coming from the heliostat field and emitted from inside the solar receiver), the solar thermal input, the radiative losses, the total radiative source term, and some other relevant variables. The residual term of the radiative energy balance is reported as well. The data of all the iterations are kept.
- Total radiative source term per zone (air-particle mixture, left wall, right wall, exterior wall, outlet tube and window). The data of all the iterations are kept.
- Detailed description of the origin of the losses. Only the file of the last iteration is kept.

The availability of this information allows improving the understanding of the operating conditions of the receiver and, more importantly, facilitates the design optimization process to be performed later.

3.6. Coordinate Systems

Throughout the previous sections the local zenith and azimuthal angles have been used to describe the directional dependence of the radiation reaching and leaving a surface, while the ray tracing is performed in a global Cartesian coordinate system. Therefore, the local spherical coordinate system associated to a surface and the global Cartesian coordinate

system need to be related mathematically. First, the z-axis unit vector of the local Cartesian coordinate system associated to a point of the surface is:

$$\hat{\mathbf{k}}_l(x_g, y_g, z_g) = \pm \frac{\nabla f(x_g, y_g, z_g)}{\|\nabla f(x_g, y_g, z_g)\|_2} \quad (3-28)$$

Where f denotes the equation of the surface and the sign $\pm$ is chosen so that $\hat{\mathbf{k}}_l$ points to the inside of the receiver. The previous calculation is performed in different ways for flat, cylindrical, conical, spherical and ellipsoidal surfaces so that the number of computer operations is minimized.

On account of the axisymmetry of the solar receiver, a second unit vector of the local Cartesian coordinate system, let's say $\hat{\mathbf{i}}_l$ –although the election is arbitrary–, can be readily computed as:

$$\hat{\mathbf{i}}_l = -\sin \varphi_g \hat{\mathbf{i}}_g + \cos \varphi_g \hat{\mathbf{j}}_g = -\frac{y_g}{\sqrt{x_g^2 + y_g^2}} \hat{\mathbf{i}}_g + \frac{x_g}{\sqrt{x_g^2 + y_g^2}} \hat{\mathbf{j}}_g \quad (3-29)$$

And finally, $\hat{\mathbf{j}}_l = \hat{\mathbf{k}}_l \times \hat{\mathbf{i}}_l$. This way, the transformation matrices to relate the components of a vector in the global and local Cartesian coordinate systems, $\mathbf{T}_g^l$ and $\mathbf{T}_l^g$, are:

$$\{\mathbf{T}_g^l\}_{ij} = \hat{\mathbf{e}}_{l,j} \cdot \hat{\mathbf{e}}_{g,i} \quad \{\mathbf{T}_l^g\}_{ij} = \hat{\mathbf{e}}_{g,j} \cdot \hat{\mathbf{e}}_{l,i} \quad (3-30)$$

So that:

$$\mathbf{v}_g = \{\mathbf{T}_g^l\} \cdot \mathbf{v}_l \quad \mathbf{v}_l = \{\mathbf{T}_l^g\} \cdot \mathbf{v}_g \quad (3-31)$$

Of course, this expression also applies for the position vector, i.e., $\mathbf{q}_g = \{\mathbf{T}_g^l\} \cdot \mathbf{q}_l$ and $\mathbf{q}_l = \{\mathbf{T}_l^g\} \cdot \mathbf{q}_g$, where $\mathbf{q}_g = (x_g, y_g, z_g)^t$ and $\mathbf{q}_l = (x_l, y_l, z_l)^t$.

Equations 3-31 are the general expressions to relate the components of a vector in the local and global Cartesian coordinate systems. However, these expressions can be significantly simplified in some cases (e.g., on flat or cylindrical surfaces) so that it is possible to accomplish the change of basis with fewer operations. This has been taken into account in the MCRT code in order to prevent unnecessary computations.

Finally, the relation between the local Cartesian coordinate system and the local spherical coordinate system (characterized by θ and φ) is trivial and given by:

$$\theta_i = \tan^{-1}(-\hat{\mathbf{v}} \cdot \hat{\mathbf{k}}_l) = \tan^{-1}\left(\frac{\sqrt{v_{x,loc}^2 + v_{y,loc}^2}}{-v_{z,loc}}\right) \quad \varphi_i = \tan^{-1}\left(\frac{-v_{y,loc}}{-v_{x,loc}}\right) \quad (3-32)$$

Note that the minus signs in the equation of φ_i are kept to show that the inverse tangent is a multivalued function and the `atan2` function from C and FORTRAN must be used.

On the contrary, to pass from the local spherical to the local Cartesian coordinate system the equations to be used are:

$$\begin{aligned}v_{x,loc} &= \sin \theta_r \cos \varphi_r \\v_{y,loc} &= \sin \theta_r \sin \varphi_r \\v_{z,loc} &= \cos \theta_r\end{aligned}\tag{3-33}$$

While the subscript r in Eq. 3-33 denotes *reflection*, these expressions are also valid for emission by simply substituting $\theta_r \rightarrow \theta_e$ and $\varphi_r \rightarrow \varphi_e$.

3.7. Efficiency Considerations

3.7.1. Variance Reduction Techniques

As stated at the beginning of the chapter, Monte Carlo simulations try to estimate a numerical quantity l of a real system as:

$$l = E(H(\mathbf{Y}))\tag{3-34}$$

Where $\mathbf{Y}$ is an input vector with probability distribution $f(\mathbf{y})$ (e.g. the direction, location and wavelength of emission), H is the performance function (the result of the ray tracing when using the input vector $\mathbf{Y}$), and l is the quantity to be evaluated (the radiative heat flux, the divergence of the radiative heat flux, etc.) To estimate l through simulation, Monte Carlo methods generate a random sample $\mathbf{Y}_i$ ($i = 1, 2, \dots, N$) based on $f(\mathbf{y})$, compute the sample function $H(\mathbf{Y}_i)$, and use the sample-average estimator:

$$\hat{l}_N = \frac{1}{N} \sum_{i=1}^N \hat{l}^{(i)} = \frac{1}{N} \sum_{i=1}^N H(\mathbf{Y}_i)\tag{3-35}$$

which is unbiased for l and, by invoking the law of large numbers (assuming single conditions), converges to the actual quantity to be estimated as N gets large. It is easy to prove that $\sigma(\hat{l}_N) \propto N^{-1/2}$ [62] and, thus, the efficiency of the estimator is proportional to $N^{-1/2}$.

Variance reduction techniques are intended to produce another unbiased estimator, $\hat{l}_N^*$, statistically more efficient, i.e., $\sigma(\hat{l}_N^*) < \sigma(\hat{l}_N)$. However, different estimators, or even different performance functions, may not consume the same CPU time. Hence, the efficiency—understood as a measurement of the variance reduction—is not a good way of comparing estimators and performance functions. A more fair comparison is based on their

performance, which we define as the product of the variance and the CPU time for consistency with [55]:

$$\wp = \sigma(\hat{l}_N) \cdot TM(\hat{l}_N) \quad (3-36)$$

This performance happen to be independent on the sample size if $TM \propto N$ (which is quite true for most Monte Carlo simulations), and is then the parameter employed here to compare different estimator and performance functions.

3.7.1.1. Antithetic Random Numbers

Let's consider again the problem of estimating $l = E(H(\mathbf{Y}))$. Now, let $\mathbf{Y}_1$ and $\mathbf{Y}_2$ be two input vector generated from $f(\mathbf{y})$. Then $\hat{l} = [H(\mathbf{Y}_1) + H(\mathbf{Y}_2)]/2$ is an unbiased estimator of l with variance:

$$\sigma(\hat{l}) = \frac{\sigma(H(\mathbf{Y}_1)) + \sigma(H(\mathbf{Y}_2)) + 2\sigma(H(\mathbf{Y}_1), H(\mathbf{Y}_2))}{4} \quad (3-37)$$

For the crude Monte Carlo (Eq. 3-35), $\mathbf{Y}_1$ and $\mathbf{Y}_2$ are independent and then $\sigma(H(\mathbf{Y}_1), H(\mathbf{Y}_2)) = 0$. Obviously, variance reduction is obtained if $\sigma(H(\mathbf{Y}_1), H(\mathbf{Y}_2)) < 0$. The most obvious way to make the covariance negative is as follows: Whenever the uniform random number R_φ is used for a particular purpose (e.g., determine the wavelength of emission), the antithetic number $1 - R_\varphi$ is used for the same purpose the next time it is required (i.e. for the wavelength of emission of the next ray.) Since $\sigma(R_\varphi, 1 - R_\varphi) < 0$ it is expected that $\sigma(H(\mathbf{Y}_1), H(\mathbf{Y}_2)) < 0$. A formal proof of this is provided in [62] under the assumption that the performance function is monotone and the components of the input vector are independent¹⁶. Therefore, the Antithetic Random Numbers technique is employed whenever possible, i.e., for the position, direction and wavelength of emission. Especial care must be taken when synchronizing the antithetic numbers if the Monte Carlo Ray Trace was parallelized via GPU computing in the future.

3.7.1.2. Stratified Sampling

Stratification is the process of dividing members of a population into different subgroups (or strata) and applying an independent sampling within each stratum. The stratified sampling estimator of l is:

$$\hat{l}_N^* = \sum_{i=1}^m p_i \frac{1}{N_i} \sum_{j=1}^{N_i} H(\mathbf{Y}_{ij}) \quad (3-38)$$

¹⁶ When employing non-flat windows or non-cylindrical receivers, the r - and z - location of emission (in cylindrical coordinates) from some cells are actually not independent. However, albeit a formal proof for this case has not been found, variance reduction is obtained as well.

where m is the number of strata, p_i the probability that the element belongs to the stratum i , and N_i is the number of elements in the sample of the stratum i . The values Y_{ij} are generated from the conditional distribution of Y given that the element belongs to the stratum i .

While the most simple approach would be to employ a sample size for each stratum proportional to its probability (i.e., $N_i = p_i N$), greater variance reduction is achieved if more elements are taken from those strata with higher variance. In particular, it can be shown [62] that the strata sizes N_i that minimize the variance are:

$$N_i = N \frac{p_i \sigma_i}{\sum_{j=1}^m p_j \sigma_j} \quad (3-39)$$

where σ_i is the variance of $H(Y)$ conditioned to the stratum i . In our Monte Carlo Ray Tracing software, stratified sample is applied to distinguish between those rays coming from the heliostat field and those emitted from inside of the receiver. The nature of this distinction arises from the different wavelength of the rays associated with each one and the extremely different radiative behavior of the carbon particles between them, as predicted by Mie theory. While the exact values depend on the radiative properties of the walls, the Monte Carlo technique employed (see Section 3.7.2) and the particular variable analyzed, it was found that the variance of the radiative source term due to the rays coming from the heliostat field is slightly lower than the one due to the rays emitted from inside of the receiver. Hence, in general, it is advisable to use around 30-40% more rays from the receiver than from the heliostat field.

3.7.1.3. Number of emissions from each cell

In previous models developed by Ruther [19] and Crocker [20] the number of rays emitted from each cell was constant throughout the Monte Carlo grid regardless the emissive power of the cells. This is a very inefficient way to perform and should be optimized to increase the performance (product of the variance and the CPU time) of the Monte Carlo method. Actually, the ratio of emissive power between cells was proved to be as high as 3500:1, i.e., a large computational effort is done tracing rays with negligible energy, whereas others rays carry too much energy and its contribution should be split up into different rays. In reality, this strategy is nothing but a stratified sampling technique (see Section 3.7.1.2 above).

One alternative is to distribute the total number of rays to be traced, N_{TOTAL} , throughout the grid as expressed in Eq. 3-40, where $\omega \in [1, \infty)$ is the parameter to be optimized and M is the number of cells of the Monte Carlo mesh. The particular case $\omega = 1$ is simply the strategy employed by Ruther and Crocker of emitting the same number of rays from each Monte Carlo cell, while $\omega \rightarrow \infty$ implies that the number of emissions is directly proportional to the emissive power, without any lower and upper limit for the number of emissions from

each cell. In particular, ω was optimized through discrete optimization for the cases $\omega = 1$, $\omega = 2$, $\omega = 5$, $\omega = 10$, $\omega = 25$ and $\omega \rightarrow \infty$ (say $\omega = 10,000$).

$$N_i = \min \left\{ \max \left[N_{TOTAL} \cdot SUP \left(\frac{E_i}{E_{TOTAL}} \right), N_{min} \right], N_{max} \right\}$$

$$N_{min} = \frac{N_{TOTAL}}{M \cdot \omega} \quad (3-40)$$

$$N_{max} = \frac{N_{TOTAL}}{M} \cdot \omega$$

An initial study to draw a conclusion about a possible optimum of the parameter ω was conducted first. The evolution of several relevant radiative variables as a function of the number of rays traced showed $\omega = 25$ as the strategy with lower error. Thus, we would like to determine whether we can –statistically– conclude that the population standard deviation of the case $\omega = 25$ is, or is not, significantly lower than the ones of the other values of ω . For that, a hypothesis test for the difference between two population standard deviations is required. The test statistic for this type of hypothesis testing is $F = s_1^2/s_2^2$ and the critical value F_c is to be found from the F-distribution tables. The null hypothesis, levels of significance and decision rule of the hypothesis test conducted are:

- *Null Hypothesis:* The population standard deviation of the case $\omega = 25$ is not significantly smaller than the standard deviations for the other cases ($\omega = 1, 2, 5, 10$ and ∞).
- *Levels of Significance:* $\alpha = 0.01$, $\alpha = 0.05$ and $\alpha = 0.10$.
- *Decision Rule:* For $d.f.N. = 120$, $d.f.D. = 120$ and one-tailed test, we will accept the Null Hypothesis if $F < F_c$. The value of F_c for different levels of significance can be found in the F-Distribution tables and are shown in Table 2 for the three values of α employed here.

Level of Significance (α)	F_c
0.01	1.53
0.05	1.35
0.10	1.26

Table 2 – Value of F_c for different levels of significance α (from the F-Distribution with 120 degrees of freedom in both numerator and denominator.)

The variance of both the “radiative losses through the window” and the radiative source term field in the Monte Carlo mesh were analyzed. The procedure employed was the following:

1. For each value of ω , the MCRT code was employed 121 times¹⁷ to solve the radiation heat transfer problem using different initial seeds in the Random Number Generator.
2. A FORTRAN code was programmed to post-process this large amount of data, calculate the sample variance and the sample mean, and perform the Hypothesis Test for the random variable “radiative losses through the window” and for the radiative source term in all the cells. For simplicity, only one division in the azimuthal coordinate was employed in the Monte Carlo grid.

Table 3 collects the sample variances and the test statistics of the radiative losses for the six values of ω previously mentioned. Since the CPU time does not depend on ω , the performance is simply proportional to the variance and the speedup is proportional to the test statistic. As for the radiative source term field in the Monte Carlo grid, only the final results of the hypothesis test are presented for simplicity. Figures 13, 14, 15, 16 and 17 show in what cells we can (green) or we cannot (red) reject the Null Hypothesis for the levels of significance $\alpha = 0.01$, $\alpha = 0.05$ and $\alpha = 0.10$. The ratio of the sample variance (i.e., the test statistic) is shown as well (labeled as *Ratio* and colored in green if $F_{i,j} > 1$ or in red if $F_{i,j} \leq 1$.) The grey cells represent virtual cells, i.e. cells that need to be included to keep the Monte Carlo grid structured but actually do not exist physically.

ω	$s^2 (W^2)$	$F_{i,j} = s_i^2/s_j^2 (j = 5)$
1	22,355,443	13.88
2	9,298,349	5.77
5	2,977,458	1.85
10	2,118,995	1.32
25	1,610,808	1.00
∞	1,755,763	1.09

Table 3 – Sample variances and test statistics of the random variable “radiative losses through the window” for different values of the parameter ω .

Based on the previous results, the population standard deviation of the radiative losses for $\omega = 25$ is significantly smaller than the cases $\omega = 1, 2$ and 5 with a level of significance $\alpha = 0.01$ and than the case $\omega = 10$ with a level of significance $\alpha = 0.10$. However, there is not statistical evidence to state that it is significantly smaller than the case $\omega \rightarrow \infty$ for any of the levels of confidence considered here. Similar conclusions, although more involved, can be reached for the radiative source term field. Again, since the CPU time does not depend on the value of ω , the performance is proportional to the variance and the previous conclusions are also valid for the performance and the speedup. It is noteworthy that the high- ω strategies are especially well-suited to improve convergence near the window (due to the high emissive power of such cells), while the differences between different values of ω are

¹⁷ To have an F-Distribution with 120 degrees of freedom and match conventional F-Distribution tables (note that the number of degrees of freedom in the F-Distribution is the sample size minus one.)

much smaller in the back of the receiver. Note also that the front of the receiver is a more critical part due to the, at least without oxidation model, greater radiative source term. Moreover, high values of the parameter ω increase the percentage of rays coming from the heliostat field, which require less CPU time due to the higher absorptivity of the carbon nanoparticles in the solar spectrum and the fact that no CDFs are required to determine the wavelength, position and direction of emission. Therefore, $\omega = 25$ is even better compared to $\omega = 1$ than what is shown in Table 3 and Figures 13, 14, 15, 16 and 17. Finally, an estimation of the reduction of the CPU time to maintain the same uncertainty level in the radiative source term field from the case $\omega = 1$ (initial, non-optimized strategy) to $\omega = 25$ (new, optimized strategy) is shown in Table 4.

For big N_{TOTAL} and invoking the central limit theorem, the random variables follow approximately a normal distribution $N(\mu, \sigma)$, where the mean μ is the exact solution of the Radiative Transfer Equation and the standard deviation $\sqrt{\sigma}$ is proportional to $N^{-0.5}$ (i.e., $\sigma \propto N^{-1}$). Therefore, the values in Table 4 also show how many fewer rays are necessary to obtain the same level of convergence with $\omega = 25$ compared to $\omega = 1$ in each cell of the Monte Carlo grid. From that, and since the CPU time does not depend on ω , we can conclude that the reduction of CPU time achieved with an optimized distribution of the emitted rays is, on average, of one order of magnitude.

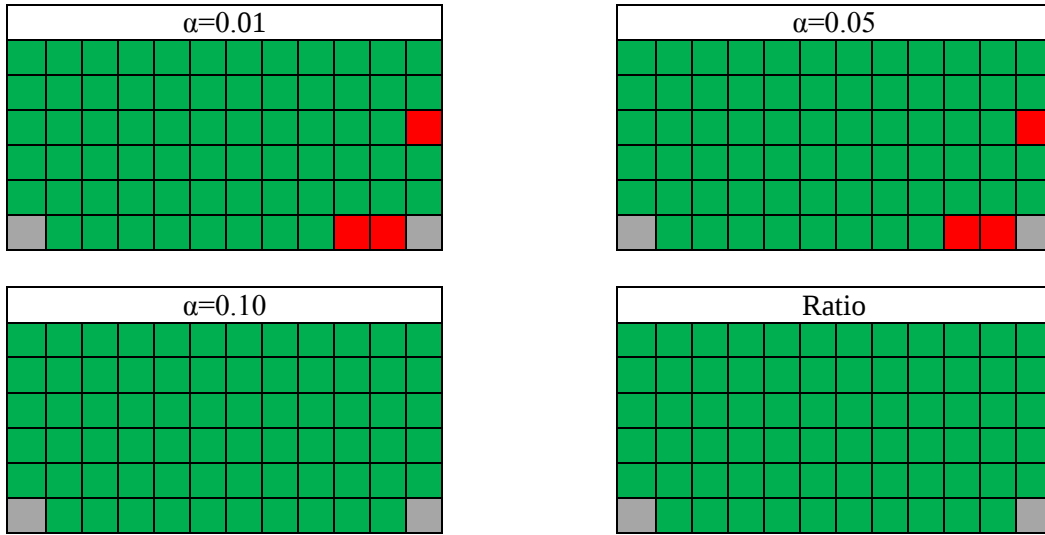


Figure 13 – Comparison $\omega = 1$ vs. $\omega = 25$. Cells in which we can reject the Null Hypothesis in green, cells in which we cannot in red and virtual cells in gray (i.e. cells that actually do not exist physically.) α denotes the level of significance. The *Ratio* table shows whether $F_{i,j} > 1$ (green) or $F_{i,j} \leq 1$ (red). Columns are different z -indices and rows are different r -indices (the azimuthal dependence has been averaged.) The window zone is on the left and the exterior wall is at the bottom (last row).

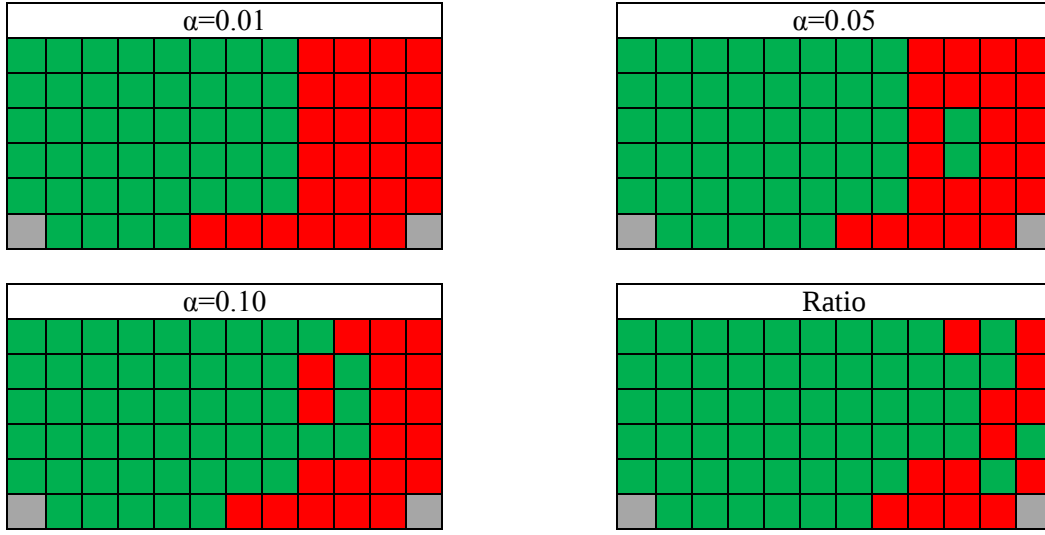


Figure 14 – Comparison $\omega = 2$ vs. $\omega = 25$. Cells in which we can reject the Null Hypothesis in green, cells in which we cannot in red and virtual cells in gray (i.e. cells that actually do not exist physically.) α denotes the level of significance. The *Ratio* table shows whether $F_{i,j} > 1$ (green) or $F_{i,j} \leq 1$ (red). Columns are different z -indices and rows are different r -indices (the azimuthal dependence has been averaged.) The window zone is on the left and the exterior wall is at the bottom (last row).

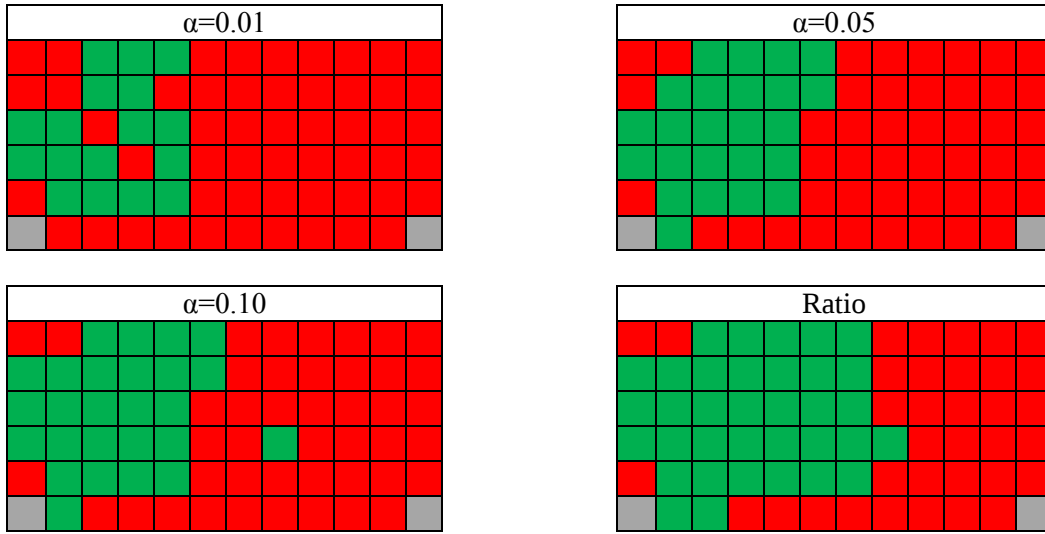


Figure 15 – Comparison $\omega = 5$ vs. $\omega = 25$. Cells in which we can reject the Null Hypothesis in green, cells in which we cannot in red and virtual cells in gray (i.e. cells that actually do not exist physically.) α denotes the level of significance. The *Ratio* table shows whether $F_{i,j} > 1$ (green) or $F_{i,j} \leq 1$ (red). Columns are different z -indices and rows are different r -indices (the azimuthal dependence has been averaged.) The window zone is on the left and the exterior wall is at the bottom (last row).

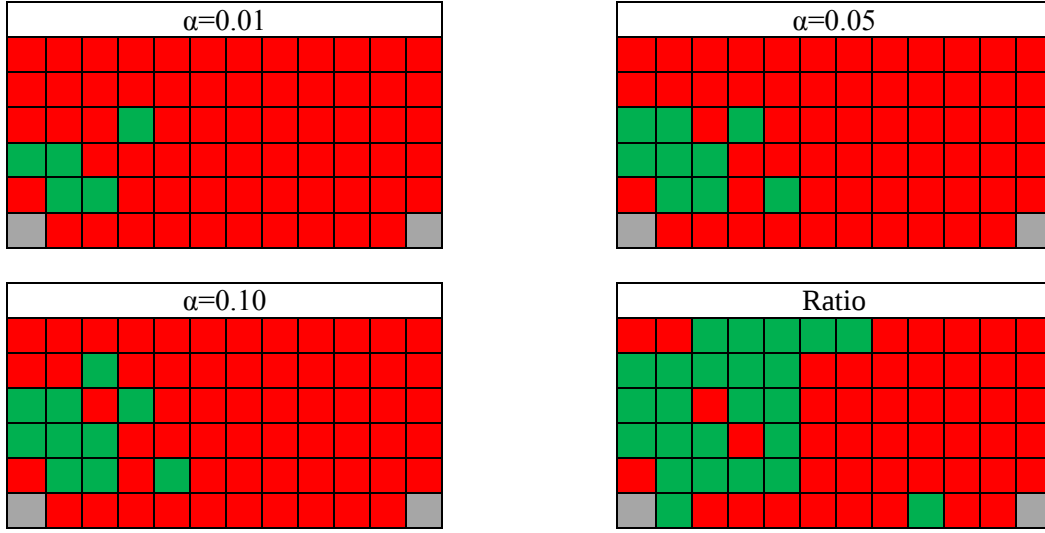


Figure 16 – Comparison $\omega = 10$ vs. $\omega = 25$. Cells in which we can reject the Null Hypothesis in green, cells in which we cannot in red and virtual cells in gray (i.e. cells that actually do not exist physically.) α denotes the level of significance. The *Ratio* table shows whether $F_{i,j} > 1$ (green) or $F_{i,j} \leq 1$ (red). Columns are different z -indices and rows are different r -indices (the azimuthal dependence has been averaged.) The window zone is on the left and the exterior wall is at the bottom (last row).

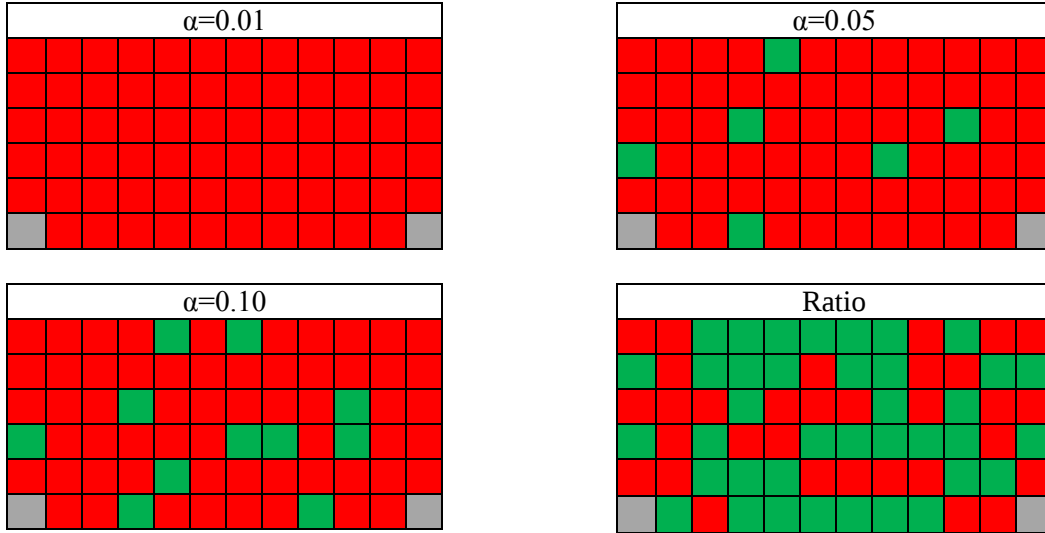


Figure 17 – Comparison $\omega \rightarrow \infty$ vs. $\omega = 25$. Cells in which we can reject the Null Hypothesis in green, cells in which we cannot in red and virtual cells in gray (i.e. cells that actually do not exist physically.) α denotes the level of significance. The *Ratio* table shows whether $F_{i,j} > 1$ (green) or $F_{i,j} \leq 1$ (red). Columns are different z -indices and rows are different r -indices (the azimuthal dependence has been averaged.) The window zone is on the left and the exterior wall is at the bottom (last row).

6.77	6.39	15.38	15.54	19.82	11.14	10.20	7.49	4.23	3.70	2.54	2.31
13.28	13.10	19.70	16.85	12.86	8.74	5.84	5.96	3.43	3.40	2.58	2.18
12.76	19.46	16.53	20.02	12.79	12.55	5.90	7.03	3.84	3.53	2.74	1.34
20.46	21.78	18.20	14.01	17.33	8.01	8.47	7.45	3.17	3.02	2.19	2.25
8.08	29.55	20.80	18.10	16.61	7.95	5.78	3.59	3.86	3.12	3.09	1.70
-	10.35	11.04	8.87	8.54	4.63	4.60	2.04	2.07	1.27	1.13	-

Table 4 – Reduction of CPU time for the radiative source term field from $\omega = 1$ (initial, non-optimized strategy) to $\omega = 25$ (new, optimized strategy). Columns are different z -indices and rows are different r -indices (the azimuthal dependence has been averaged.) The window zone is on the left and the exterior wall is at the bottom (last row).

3.7.2. Collision Based vs. Pathlength Based Method

All the details provided previously about the Monte Carlo Ray Tracing method correspond with the so-called collision-based, or standard, Monte Carlo. However, there exists another version of the MCRT method: the pathlength-based, or energy partitioning, technique. While absorption occurs in singular absorbing events (collisions between photons and absorbing particles) in the collision-based MCRT, the energy partitioning Monte Carlo distributes the absorbed energy throughout the pathlength (exponential decaying). Similarly, in the pathlength-based method the energy is distributed between absorption and reflection when a ray reaches the walls, and between absorption, reflection and transmission when it reaches the window. In the latter method, it is also necessary to define a cut-off level to establish when the rays have negligible energy and their tracing can be stopped (e.g. a cut-off level of 99% implies that the ray tracing stops when the energy of the rays is below 1% of its initial value. This residual energy is assigned to the cell in which the ray is located in that moment, although other strategies can be employed as well.) Of course, both methods converge to the exact solution in the limit of an infinite number of emissions and the best choice should be the one with the faster convergence. For that, each method has its own strengths: In the pathlength-based technique much more information is obtained from each ray (i.e., fewer rays are required to achieve convergence), while the CPU usage per ray is much smaller in the collision-based. Hence, the best Monte Carlo technique is problem-dependent and needs to be determined for each particular situation. Further details and discussion of the standard and the energy partitioning MCRT can be found, for example, in [55].

Both Monte Carlo methods have been implemented in the code developed for the receiver modeling in this *Proyecto Fin de Carrera* and the user is free to choose between them. This section aims to analyze the performance (product of the variance and the CPU time) of both methods when applied to the Small Particle Solar Receiver in order to facilitate such a decision. Each Monte Carlo technique has been employed to calculate the solution of the same radiative transfer problem one hundred and twenty one times, each of them with a different initial seed for the Random Number Generator. This way, an estimate of the variance and the CPU time is obtained. For the pathlength-based MCRT, three different cut-

off levels were employed (99%, 99.9% and 99.99%). Since the performance is expected to be a strong function of the radiative properties of the receiver walls, the analysis was performed for both black (blackbody) and Al_2O_3 walls (Figure 12 in Chapter 3 shows the spectral emissivity of aluminum oxide.) Finally, since the performance may also depend on the wavelength, this studio was split up into two sections: Rays coming from the heliostat field and rays emitted from inside of the receiver.

A FORTRAN code was written to post-process all the data and calculate the average, the variance and the CPU time per ray for each Monte Carlo strategy. Table 5 shows the performance (defined as the product of the variance and the CPU time *per ray*, and expressed in $\text{W}^2\text{-s}$) of different variables for the collision and the pathlength MCRT when the walls are modeled as blackbodies, both for the rays coming from the heliostat field and for the rays emitted from inside of the receiver. Table 6 collects the same information as Table 5 but with Al_2O_3 walls. From these tables it can be concluded that the pathlength-based MCRT has better performance than the collision-based in all the situations except for the rays emitted from inside of the receiver when using Al_2O_3 walls (note that the lower the performance is, the better.) This result is expected since, when modeling the walls as blackbodies, the rays are absorbed whenever they reach a wall and the CPU time is limited by this fact. Hence, the fact that much more information is obtained from each ray with the pathlength-based Monte Carlo makes it a better choice. However, the CPU time increases excessively when using the pathlength-based MCRT and Al_2O_3 walls since the ray tracing is not stopped by any perfect absorber. This is especially true for the rays emitted from the receiver as they have longer wavelengths and then the absorptivity of the carbon particles is lower. As for the best cut-off level of the pathlength-based Monte Carlo, the 99% option showed the best performance regardless the wavelength and the radiative properties of the walls. Also, the performance of the radiative source terms is lower (better) for short wavelengths (i.e. for the rays coming from the heliostat field) than for long wavelengths; while the opposite is true for the variable *window losses*. In any case, the difference between both MCRT techniques is below 50% and there is no order-of-magnitude gain as occurred with an optimized number of emissions from each cell (Section 3.7.1.3) and as will occur with an optimized, adaptive coupled solution procedure (Section 5.4).

3.7.3. Programming Efficiency

3.7.3.1. Inversion of Cumulative Distribution Functions

The expression of some Cumulative Distribution Functions can be inverted analytically and the vector $\mathbf{Y}$ can be easily calculated by evaluating the inverse of the CDF at R^* (the random number) during the ray tracing. However, other CDFs cannot be explicitly inverted and a transcendental equation needs to be solved to determine $\mathbf{Y}$. While many numerical methods (e.g. bisection, secant or Newton-Raphson methods) can be employed to solve this equation, it would be a very inefficient way to perform since this procedure needs to be

Variable	Collision	Pathlength		
		99.00%	99.90%	99.99%
RAYS FROM THE HELIOSTAT FIELD				
Window Losses	2.11E+02	1.56E+02	1.98E+02	1.43E+02
Fluid Source Term	9.61E+02	1.83E+02	2.15E+02	1.84E+02
Exterior Wall Source Term	4.83E+02	2.84E+01	4.09E+01	3.03E+01
Outlet Tube Source Term	2.40E+02	3.19E+01	4.00E+01	4.08E+01
Right Wall Source Term	1.38E+02	7.13E+00	9.48E+00	9.64E+00
Left Wall Source Term	4.03E+01	1.20E+01	1.71E+01	1.76E+01
Window Source Term	2.93E+01	2.26E+00	3.23E+00	2.42E+00
RAYS EMITTED FROM INSIDE OF THE RECEIVER				
Window Losses	2.19E+02	8.57E+01	9.97E+01	1.16E+02
Fluid Source Term	2.14E+03	5.23E+02	4.50E+02	6.54E+02
Exterior Wall Source Term	3.39E+03	2.24E+03	2.38E+03	2.27E+03
Outlet Tube Source Term	1.07E+03	1.16E+03	1.21E+03	1.09E+03
Right Wall Source Term	1.26E+03	1.05E+03	1.29E+03	1.18E+03
Left Wall Source Term	9.01E+02	8.32E+02	9.92E+02	8.41E+02
Window Source Term	5.03E+02	4.25E+02	4.57E+02	5.09E+02

Table 5 – Performance (W^2 -s) of different variables for the collision and the pathlength MCRT when the walls are modeled as blackbodies.

Variable	Collision	Pathlength		
		99.00%	99.90%	99.99%
RAYS FROM THE HELIOSTAT FIELD				
Window Losses	2.01E+02	1.47E+02	2.70E+02	5.33E+02
Fluid Source Term	3.77E+02	1.68E+02	3.03E+02	6.79E+02
Exterior Wall Source Term	8.80E+01	1.81E+00	3.28E+00	4.37E+00
Outlet Tube Source Term	5.73E+01	3.67E+00	5.77E+00	1.23E+01
Right Wall Source Term	3.93E+01	8.31E-01	1.38E+00	2.32E+00
Left Wall Source Term	8.91E+00	7.98E-01	8.05E-01	2.08E+00
Window Source Term	2.44E+01	3.07E+00	4.28E+00	1.09E+01
RAYS EMITTED FROM INSIDE OF THE RECEIVER				
Window Losses	8.715E+01	7.184E+01	1.163E+02	2.423E+02
Fluid Source Term	1.112E+03	8.517E+02	9.009E+02	2.673E+03
Exterior Wall Source Term	1.051E+03	1.260E+03	1.481E+03	3.012E+03
Outlet Tube Source Term	3.132E+02	8.012E+02	8.989E+02	1.619E+03
Right Wall Source Term	3.133E+02	5.701E+02	7.002E+02	1.142E+03
Left Wall Source Term	2.053E+02	4.006E+02	4.123E+02	1.088E+03
Window Source Term	2.785E+02	4.649E+02	6.512E+02	1.196E+03

Table 6 – Performance (W^2 -s) of different variables for the collision and the pathlength MCRT when using Al_2O_3 walls.

repeated several times per ray. Hence, for the sake of computational efficiency, the CDF with no analytical inverse are handled as described in Algorithm 2.

Algorithm 2

1. Calculate $CDF_i^{-1}(R_j)$ prior to starting the simulation, where R_j is a vector of N numbers uniformly distributed over $[0,1)$ (typically $100 < N < 1,000$ depending on the variable Y_i)
2. Store $CDF_i^{-1}(R_j)$ in proper vectors and matrices.
3. Pick a random number (R_γ) when Y_i needs to be determined during the ray tracing.
4. Linearly interpolate the values $CDF_i^{-1}(R_j)$ calculated in Step #1:

$$CDF_i^{-1}(R_1) + \frac{CDF_i^{-1}(R_2) - CDF_i^{-1}(R_1)}{R_2 - R_1} (R_\gamma - R_1)$$

Where $R_1 = \max(R_j) / R_j \leq R_\gamma$ and $R_2 = \min(R_j) / R_j \geq R_\gamma$. A binary search algorithm is used to find R_1 and R_2 .

3.7.3.2. Binary Search

The previously mentioned Cumulative Distribution Functions with no analytical inverse (e.g. the emission properties of the air-particle mixture, walls and window) are calculated prior to start the simulation (and stored in external .dat files) and need to be interpolated during the ray tracing. Hence, it is necessary to search these properties in multidimensional matrices several millions of times per iteration. To efficiently do so, a low complexity technique is required. In particular, the binary search algorithm [63], a dichotomic divide and conquer search algorithm with average case performance $\mathcal{O}(\log n)$ (n denotes the size of the array to be explored), is employed whenever possible.

3.7.3.3. Other considerations

On account of the structured character of the Monte Carlo mesh, all properties are stored in three-dimensional matrices that need to be looped repeatedly over the code. To reduce the CPU usage of this loops, the internal loop refers to the first index of the matrix in the Monte Carlo code (FORTRAN), while the opposite strategy is employed in the User-Defined Functions (C). Furthermore, some `if` statements were introduced and some equations/algorithms were simplified to avoid unnecessary computations.

3.8. Model Validation

With the availability of commodity computer hardware and software, the computation of solution to engineering problems has become a seemingly effortless task. However, this feeling of overconfidence is easily shattered when facing new problems and developing new models for its computer solution, such as the in-house Monte Carlo Ray Tracing code developed for the Small Particle Solar Receiver modeling. Indeed, there are three essential questions that must be answered before our simulation results can be trusted [64]: Does the mathematical model represent the relevant phenomena? Does the algorithm reproduce a

suitable approximation to the solution of the mathematical model? Does the software actually implement the solution algorithm?

The validity of the quasi-steady form of the Radiative Transfer Equation to model the radiation heat transfer in participating media and the Monte Carlo Ray Tracing method to solve the RTE have been repeatedly demonstrated [51,53]. Hence, the two first questions have a favorable response. Nonetheless, to guarantee the correctness of our simulation results is still necessary to prove that the software actually implements the MCRT algorithm. First, both black box tests and white (or glass) box tests were carried out under a number of different inputs to guarantee the correct programming of the different subroutines (unit testing). Then, the whole program was tested through integration tests.

Finally, and more importantly, the Monte Carlo software was verified and validated (V&V) by simulating several thermal radiation problems with known solution.

- Test #1: Surface to surface radiation exchange between two black, parallel, infinite plates at the same temperature.
- Test #2: Surface to surface radiation exchange between two black, parallel, infinite plates at different temperatures.
- Test #3: Surface to surface radiation exchange between two black, coaxial, infinite cylinders at the same temperature.
- Test #4: Surface to surface radiation exchange between two black, coaxial, infinite cylinders at different temperatures.
- Test #5: Radiation heat transfer between two black, parallel, infinite plates at different temperatures surrounding a participating, gray medium [51].
- Test #6: Radiation heat transfer between two black, coaxial, infinite cylinders at different temperatures surrounding a participating, gray medium [53].

The radiative heat transfer was predicted successfully by our code in all the six previous situations. For example, Figure 18 shows the dimensionless emissive power distribution, Φ_b , obtained in Test #5, which perfectly matches the analytical solution (see Appendix F) for the two optical thicknesses $\tau_L = 0.5$ (red) and $\tau_L = 2$ (green) tested. The results for the other tests are presented in Appendix F.

Several additional checks were also carried out to test those pieces of code unexplored by the previous benchmarks with successful results for all of them: Tracing the rays from the heliostat field, calculating the radiative properties of the air-particle mixture via Mie theory, randomness of the pseudorandom numbers generated by the RNG, etc. Furthermore, the MCRT software checks some relevant variables during the ray tracing and it is able to report when a ray is not been properly traced. This way some imprecisions in other codes developed by our group were found.

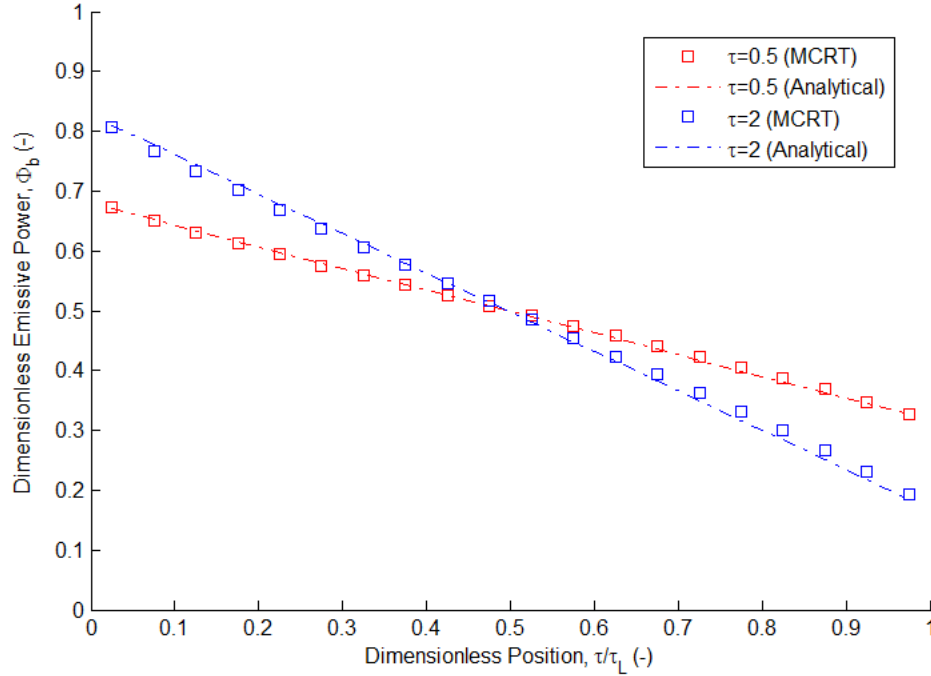


Figure 18 – Dimensionless emissive power distribution in the gas (Test #5 of the MCRT validation).

3.9. Other applications of the MCRT code: Radiative heat transfer inside the window

The Monte Carlo Ray Tracing code developed for the Small Particle Solar Receiver was modified so that it can also be applied to the radiation heat transfer in the window of the receiver. The main modifications introduced in the MCRT software were:

- Implement the optical properties of the fused quartz as a function of the wavelength.
- Implement the equations to calculate the reflectivity of the interfaces air-glass and glass-air (based on the electromagnetic theory), taking into account the possibility of total internal reflection in the latter case.
- Mapping the position and direction of the rays from the curved window to the “equivalent” flat window¹⁸.
- Load and trace the rays that enter into the window from the receiver, which is done in a similar fashion as described in this chapter for the rays from the heliostat field.
- Simplify and/or remove those parts of the code unnecessary for the window (e.g., scattering or Mie theory subroutines, etc.) in order to reduce the CPU time.

¹⁸ A circular, plane window whose radial coordinate equals the arc-length parameter of the intersection of the inner surface of the actual window and a $\varphi = \text{const}$ plane.

The thermal analysis of the window is being performed by Alex Whitmore using an in-house code that includes all the modes of heat transfer and the possibility of running transient analysis [65], in which the Monte Carlo code is simply the sub-model responsible for the radiation heat transfer calculation. The thermal study of the window is important for the following reasons:

1. Determine and reduce the thermal stresses in the window (for which the temperature field is required).
2. Determine and reduce the thermal losses in the receiver (due to radiation and convection to the outside).
3. Possible use of an anti-reflective coating if the temperature of the window was low enough (see Section 9.7).

Note, however, that the application of the MCRT method to the window involves several approximations that might need to be fixed if higher accuracy were required:

1. The mapping function from a spherical cap window to the “equivalent” flat window is not an isometric transformation, i.e. the distances between points are not preserved. This implies that neither the volume (and thus nor the emissive power) nor the optical thickness of the cells are preserved. Furthermore, the Cumulative Distributed Functions for the equivalent geometry will not exactly reproduce the spatial distribution of the emitted radiation. Although for a cap angle of 45° the error is small (for example, 2-3% in the volume of the cells, on average), both the volume and the optical thickness could be easily fixed with reasonable success by using proper correction factors. The CDF issue would require, however, a more involved solution.
2. The refracted angle and the transmissivity of the interface glass (absorbing) – air (non-absorbing) are calculated based on the behavior of electromagnetic waves going from a non-absorbing to an absorbing medium by switching the indices of the mediums. However, the process is not quite linear and the behavior of electromagnetic waves from an absorbing to a non-absorbing medium is more involved.
3. The electromagnetic spectrum is divided into N bands equally distributed between $0.1\ \mu\text{m}$ and $50\ \mu\text{m}$, while a non-uniform band distribution (more dense in the low wavelength region) would reduce the CPU time in the search of properties (remember the average performance of the binary search algorithm is $\sigma(\log N)$) and improve the accuracy of the solution due to the higher gradients of the complex refractive index of the quartz in the solar spectrum than in infrared wavelengths [21].

Chapter 4

Fluid Dynamics Model

As outlined in Chapter 2, the commercial CFD software ANSYS Fluent is employed to solve the mass, momentum, and overall energy equations of the fluid flow, as well as the extra equations required to represent the turbulent properties of the flow and close the problem. In this chapter, we will present and discuss the CFD mesh, the CFD solver, the turbulence model and the boundary conditions employed to simulate the Small Particle Solar Receiver.

4.1. CFD Mesh

After generating the geometry in proper CAD Software (SolidWorks), the geometrical domain needs to be discretized in order to numerically solve the governing PDEs of the fluid flow. This task was carried out in ANSYS Meshing Software through the ANSYS Workbench.

Mesh generation is one of the most critical aspects of engineering simulation, especially in Computational Fluid Dynamics. Too many cells may result in long solver runs, and too few may lead to inaccurate results as some flow features might not be captured. Hence, a compromise between these requirements needs to be achieved to obtain the right mesh for each situation. Moreover, fluid dynamics simulations require very high-quality meshes in both element shape (cell squish, aspect ratio, skewness) and smoothness of size changes, which plays a significant role in the accuracy, stability, rate of convergence and CPU time required to perform the numerical computation.

The best solution for the simulation of the Small Particle Solar Receiver is a hybrid mesh: A structured hexahedral mesh in both inlet and outlet zones (where the flow moves essentially parallel to the axis of symmetry) to prevent numerical diffusion and improve the accuracy of the solution, and a non-structured tetrahedral mesh for the recirculation zones. A drawback of this hybrid character of the mesh is that non-conformal interfaces do exist, which may lead to interpolation errors. After generating the previous mesh in ANSYS Meshing Software, the boundary layer meshing is performed directly in ANSYS Fluent through Boundary Adaption¹⁹. Further adaptive refinement may be required when the flow field is known.

¹⁹ A grid refinement method based on adapting the mesh in the proximity of specified surfaces (in our case, the window, the outlet tube and the walls for the boundary layer mesh generation.)

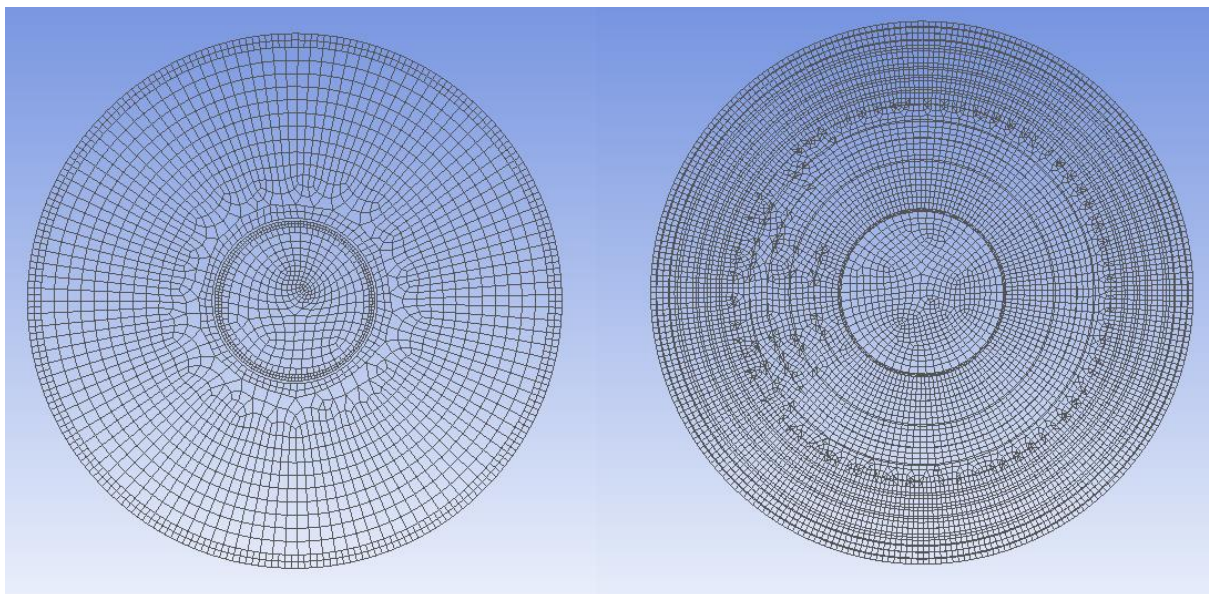


Figure 19 – Transverse section of the mesh in the inlet and outlet zones (left) and in the recirculation zone (right). Note the presence of the outlet tube in the left image and the much finer mesh in the right image to capture the features of the flow in the recirculation zone prior to entering the outlet tube.

While the meshes of the different designs analyzed in this *Proyecto Fin de Carrera* (see Chapter 7) are qualitatively similar, the grid size was varied (both because of the different volume of each design and the improved knowledge of the flow features in the last simulations.) The number of cells of the CFD mesh for the different designs of the Small Particle Solar Receiver is shown in Table 7. Note that the thermal efficiency of the receiver is virtually insensitive to the number of CFD cells as long as a minimum number of cells is used [20].

Model	# Cells
Parametric study of the operating conditions (Section 7.1)	413,487
Design optimization (Section 7.2)	
- Baseline	1,656,610
- Ellipsoidal window	1,216,320
- Geometry #2	2,181,763
- Geometry #3	2,346,852

Table 7 – Number of cells of the CFD mesh for the different designs of the Small Particle Solar Receiver presented in this *Proyecto Fin de Carrera*.

Finally, as advisable for most CFD simulations, both inlet and outlet have been extruded 0.5 m away from the domain so that the inlets/outlets of the CFD model are far enough from the region of interest and their influence on the solution is reduced.

4.2. CFD Solver

Two solver technologies are available in ANSYS Fluent to numerically solve the continuity, momentum and other scalars (energy, k , ω , etc.) equations: pressure-based solver and

density-based solver [66]. While both solvers are currently valid for the vast majority of fluid flows, one of them usually performs better than the other depending on the particular flow field. The pressure-based solver has been historically preferred for low-speed incompressible and mildly compressible flows and it is thus employed for the Small Particle Solar Receiver due to the incompressibility (as for pressure differences) of the flow.

The pressure-based solver can solve the fluid flow problem in either a segregated or coupled manner. The former is a semi-implicit solution method (momentum and pressure correction equations are solved separately) with slow convergence compared to the latter, a full implicit method²⁰ that solves the momentum and pressure-based continuity equations together [66]. However, the segregated method is more memory-efficient (its memory requirements are 1.5-2 times fewer than the ones of the density-based solver) because the individual governing equations are solved sequentially and only one discretized equation needs to be stored in the memory simultaneously. Since the computational limitation was memory rather than CPU capacity, the segregated pressure-based solver yields to more simulations per unit time and is then used. In particular, the SIMPLE algorithm is employed as convergence is limited by the convergence of the radiative source term field rather than by the pressure-velocity coupling.

The under-relaxation strategy utilized is also an important parameter of the CFD solver and is presented and discussed by convenience in Section 5.2 of Chapter 5.

4.3. Discretization Scheme

ANSYS Fluent only stores discrete values of the scalar variables (pressure, x-velocity, etc.) at the cell centroids, so that the face values (required for the convection terms) must be interpolated using a spatial discretization scheme. Moreover, gradients are needed to construct values of scalars at the cell faces, compute secondary diffusion terms and calculate velocity derivatives. For that, first-order accuracy and second-order accuracy schemes are available. A first-order discretization generally yields better convergence, but second-order schemes usually produce more accurate results. Nonetheless, the optimum choice of the discretization scheme is mesh- and problem-dependent.

A comparison was performed between first and second order discretization schemes for the particular case of the Small Particle Solar Receiver, with slower rate of convergence for the second-order schemes in all the cases. As for the accuracy of the results, no significant effect was observed for turbulent scalars, while small differences were found for the momentum and energy variables. This result is somehow expected since, with the exception of the recirculation zones, the flow is aligned with the mesh and the numerical diffusion is

²⁰ The full implicit coupling is achieved through an implicit discretization of pressure gradients term in the momentum equations, and an implicit discretization of the mass flux, including Rhie-Chow pressure dissipation terms [66].

low. Therefore, the discretization schemes employed for the different scalars are the ones shown in Table 8. In some cases, when higher accuracy was desired, second-order schemes were used for turbulent scalars as well.

Gradient	Least Squares Cell Based ⁽¹⁾
Pressure	Standard
Momentum	Second-Order Upwind
Turbulent Kinetic Energy	First-Order Upwind
Specific Dissipation Rate	First-Order Upwind
Energy	Second-Order Upwind

Table 8 – Discretization scheme for the different scalars employed in the CFD solver.

⁽¹⁾ On irregular (skewed and distorted) unstructured meshes, like in the recirculation zone of the Small Particle Solar Receiver, its accuracy is comparable to the one of the node-based gradient (and vastly superior compared to the cell-based gradient) and it is computationally less expensive [66].

4.4. Turbulence Model

The Shear Stress Transport (SST) formulation of the κ - ω turbulence model [23,33,67] is employed. The κ - and ω -equations were introduced in Eq. 2-1, while the closure coefficients, auxiliary relations and model constants of the SST κ - ω Turbulence Model employed in the numerical modeling of the Small Particle Solar Receiver are presented in Appendix G. This two-equation eddy-viscosity turbulence model has become very popular in the CFD community over the last years. The SST formulation combines the best of the κ - ε and the Standard κ - ω models. On the one hand, the use of a κ - ω formulation in the inner parts of the boundary layer makes the model directly usable all the way down to the wall through the viscous sub-layer. On the other hand, the SST formulation switches to a κ - ε behavior in the free-stream and thereby avoids the common κ - ω problem that the model is too sensitive to the inlet free-stream turbulence properties. Furthermore, this formulation exhibits a good behavior in adverse pressure gradients and separating flows, the latter present in the Small Particle Solar Receiver in both the front corner and the inlet of the outlet tube. Nonetheless, it does produce overly large turbulence levels in regions with large normal strain rates –like stagnation near the corner and high-acceleration regions prior to entering the outlet tube–. This tendency, however, is much less pronounced than in a κ - ε model and has little or no influence in the main outputs of the model, such as the outlet temperature, the thermal efficiency, the pressure drop, and the wall temperature distribution. At this point, the utilization of Large Eddy Simulation (LES), Direct Numerical Simulation (DNS) and the like is not considered as an option due to the exceedingly high CPU time required to achieve convergence with such turbulence models and the Monte Carlo Ray Tracing code. However, it constitutes an interesting alternative to be explored in the future (see Future Work, Chapter 9).

4.5. Boundary Conditions

The boundary conditions, summarized in Table 9, were carefully selected to reflect the actual conditions of the receiver as close as possible.

	Momentum B.C.	Thermal B.C.	Turbulence B.C.
Inlet	Mass Flow Rate ⁽¹⁾	Thermal Dirichlet B.C. $T = T^*$ ⁽²⁾	$I = 5\%$ Inlet hydraulic diameter ⁽¹⁾
Outlet	Pressure Dirichlet B.C. ⁽³⁾	Thermal Dirichlet B.C. ^(4,5)	$I = 5\%$ ⁽⁴⁾ $D_{h,outlet} = 0.6\text{ m}$ ⁽⁴⁾
Walls	No-Slip Condition	See below ⁽⁶⁾	Does not apply
Window	No-Slip Condition	Thermal Dirichlet B.C. $T_{win} = 1000\text{K}$ ⁽⁷⁾	Does not apply

Table 9 – Boundary conditions employed in the CFD model.

⁽¹⁾ The particular value of the boundary condition is simulation-dependent.

⁽²⁾ The inlet surface participates in the radiation heat transfer and a net radiative heat flux does exist on it. Hence, the inlet temperature is adjusted based on such a radiative source term via User-Defined Function (UDF). See Section 5.1 in Chapter 5 for further details and discussion.

⁽³⁾ Even neglecting the absorption and emission of the air-particle mixture, the flow in the outlet section is neither hydrodynamically nor thermally fully developed.

$$\frac{L_e}{D} \approx 4.4Re_D^{1/6} \Rightarrow L_e \approx 4.4Re_D^{1/6} D = 20.19\text{ m} \gg 1.5 - 3\text{ m} = L_{ot} \quad (4-1)$$

For $\mu(T = 1400\text{K}) = 5.3 \times 10^{-5}\text{ kg/m-s}$, $D_{OT} = 0.6\text{ m}$ and $\dot{m} = 5\text{ kg/s}$ (i.e., $Re_{D,ot} = 2 \cdot 10^5$).

Therefore, the *pressure-outlet* boundary condition from ANSYS Fluent is used to allow axial diffusive transport on the outlet surface. This is simply a Dirichlet boundary condition to specify the pressure on the outlet surface.

⁽⁴⁾ Only required when recirculation on the outlet surface occurs (recall an upwind interpolation scheme is employed), which does not exist in the final solution but may appear during the solution procedure. An estimate of the actual temperature and turbulence intensity on the outlet is employed to improve convergence if recirculation appears through the iterative procedure.

⁽⁵⁾ Actually, the outlet temperature is modified when post-processing the simulation results based on the radiative source term calculated by the MCRT code on the outlet surface (in a similar way as with the inlet temperature). In particular, the outlet surface is modeled in

Monte Carlo as a blackbody at the same temperature as the outlet air to simulate the deep cavity constituted by the piping.

⁽⁶⁾ The walls of the Small Particle Solar Receiver are modeled as volumetric media in the CFD model, rather than as boundary surfaces, for several reasons. First, three-dimensional heat transfer does exist in the receiver, along the outlet tube and along the walls. Second, this way it is possible to take advantage of the ANSYS Fluent's Under-Relaxation Factors to clip the wall temperature variations between iterations²¹. Otherwise, oscillations in the numerical solution may appear due to the high sensitivity of the radiation heat transfer to the wall temperature, as will be discussed in Section 5.2 of Chapter 5. It should be noted that an approximation has been introduced in this point: The radiative source term is supposed to be uniformly distributed in the thickness of the walls, while for opaque bodies surrounded by semitransparent media absorption/emission actually occurs in a thin layer of a few Å (metals) or μm (dielectrics). To verify the validity of this assumption, a one-dimensional analytical model has been developed to predict the average wall temperature as a function of the thickness of the layer in which the radiative source term is supposed to be uniformly distributed (Eq.4-2.a). The actual temperature of the inner surface can be calculated taking thicknesses arbitrarily small ($L \rightarrow 0$) in Eq. 4-2.a. The ratio between the average temperature using a thickness L (Eq. 4-2.a) and the actual temperature of the inner surface of the wall, $r(L) = T(L)/\lim_{L \rightarrow 0} T(L)$, for a stainless steel wall is shown in Figure 20. For a maximum error of 1% in the estimate of the emissive power, the thickness of the layer should be not greater than 3 cm for stainless steel walls and not greater than 3 mm for zirconia walls. Further analysis of the temperature profile revealed that the inner wall temperature is approximately equal to the exact solution regardless the thickness. Therefore, thicker layers are acceptable as long as only the CFD cells closer than a distance ε to the inner wall surface (around 1 cm and 1 mm respectively) are considered when averaging the temperature. Further details and discussion on the sensitivity of the inner wall temperature with respect to the thickness of the layer in which the radiative source term is supposed to be uniformly (L) are presented in Appendix H.

$$\begin{aligned}
 T(L) &= -\frac{1}{6} \frac{q_w}{k_w} L + \frac{1}{2} C_1 L + C_2 \\
 C_1 &= \frac{q_w + \frac{1}{2} h_{int} \frac{q_w}{k_w} L + h_{int} (T_{air} - T_{amb})}{k_w \left(1 + \frac{h_{int}}{\hat{h}_{ext}} \right) + h_{int} L} \\
 C_2 &= T_{amb} + \frac{q_w k_w + \frac{1}{2} h_{int} q_w L + h_{int} k_w (T_{air} - T_{amb})}{k_w (\hat{h}_{ext} + h_{int}) + \hat{h}_{ext} h_{int} L}
 \end{aligned} \tag{4-2}$$

²¹ When treated as surfaces in ANSYS Fluent, the temperature is calculated based on the thermal boundary condition and the Under-Relaxation of the temperature does not clip the wall temperature differences between consecutive iterations.

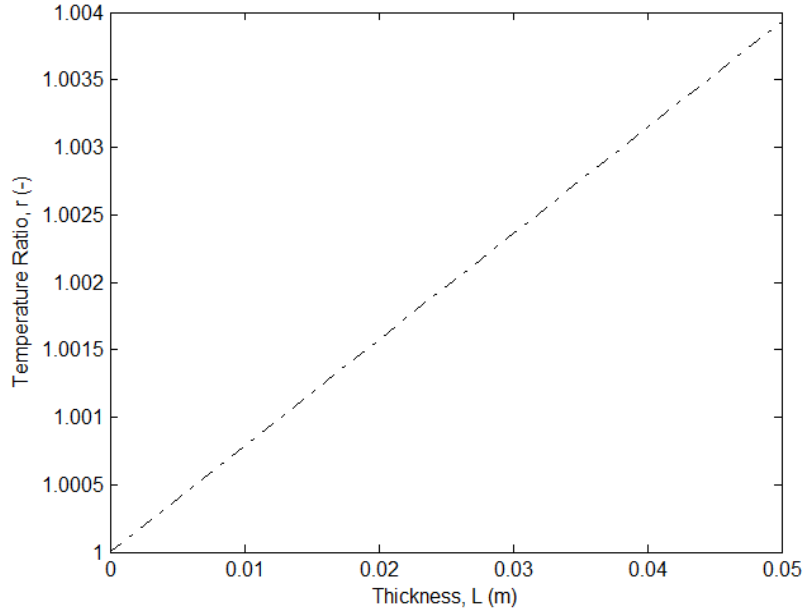


Figure 20 – Temperature ratio, $r(L) = T(L)/\lim_{L \rightarrow 0} T(L)$, in stainless steel walls.

On the fictitious outer surface of the CFD model's walls, the convective heat transfer coefficient was chosen so that the thermal resistance equals the combined conduction and convection thermal resistance of the non-computationally modeled domain (Eq. 4-3).

$$\frac{1}{\hat{h}_{ext}(\hat{t}_w)} = \frac{t_w - \hat{t}_w}{k_w} + \frac{1}{h_{ext}} \quad (4-3)$$

Where the effective exterior heat transfer coefficient, $\hat{h}_{ext}$, is a function of the thickness of the CFD model's walls, $\hat{t}_w$.

⁽⁷⁾ The temperature of the window must be kept below 800°C to ensure the integrity of the quartz. For this reason a Dirichlet thermal boundary condition $T_{win} = 1000 \text{ K}$ ²² is used on the inner surface of the window. This way, the thermal resistance to achieve the temperature goal can be calculated. For the simulations of Section 7.2, the preliminary results of the window heat transfer model developed by Alex Whitmore [65] were available and the temperature of the window was set at 850 K for $r \leq R_{ot}$ and at 800 K for $r > R_{ot}$. Finally, it should be pointed out that the way of keeping the window's temperature on target is via active cooling and is currently under research by Ara Hovhannisian, a graduate student in our group.

²² The maximum temperature of the window is reached on the inner surface, so that the thermal boundary condition in the CFD model should equal the upper temperature limit of quartz.

Chapter 5

Coupling between the MCRT method and the CFD solver

As discussed in Chapter 2, the governing equations of the fluid flow and the radiation heat transfer are, by their own nature, coupled. As it can be observed from Eq. 2-1, the energy equation –numerically solved by ANSYS Fluent– depends on the divergence of the radiative heat flux (third term in Eq. 2-1.c), while the Radiative Transport Equation –statistically solved by our in-house MCRT code– depends on the temperature field (both $i_{b\lambda}$ and some radiative properties in Eq. 2-1.f are a function of the temperature.) On account of this coupling between the Navier-Stokes (mass-, momentum- and energy-) equations and the RTE, it is necessary to couple the CFD solver and the MCRT code and iterate alternatively until convergence. A schematic representation of the solution procedure was illustrated in Figure 3, presented in Chapter 2.

5.1. User-Defined Functions to Couple the CFD Solver and the Monte Carlo Method

Several User-Defined Functions (UDFs) have been programmed in the C programming language to couple the CFD solver and the MCRT code. A User-Defined Function is a function provided by the user to interact with the CFD solver by providing external inputs, such as boundary conditions, material properties or source terms. In particular, the two main purposes of the UDFs utilized to couple the CFD solver and the MCRT code are the following:

- Impose the radiative source term calculated by the Monte Carlo method into the overall energy equation solved by ANSYS Fluent.
- Calculate the average temperature in every cell of the Monte Carlo grid –much coarser than the CFD mesh–, which the MCRT code needs to solve the RTE.

In order to do so, the User-Defined Functions described below are required. The main difficulty of all of them arises from the fact that they need to allow for an arbitrary axisymmetric geometry of the solar receiver, as well as different types of windows (flat, ellipsoidal or a spherical cap.) Moreover, it can accommodate the presence of an outlet tube for the air-particle mixture as long as its radius is smaller than the window radius. Hence, the programming must be general enough to consider all the possible situations and geometries. Finally, they can be used interchangeably for either the 2-D (axisymmetric) or the 3-D version of the CFD solver.

DEFINE_EXECUTE_ON_LOADING:

This User-Defined Function is executed at the same time the UDFs are loaded in ANSYS Fluent, i.e. when first hooking the UDFs to the Fluent model or when opening a Fluent file with the UDFs already attached. The main goals and steps performed in this UDF are collected in the subsequent paragraphs.

1. Generate the Monte Carlo mesh via FORTRAN subroutine.
2. Calculate the volume of each Monte Carlo cell in the CFD model, i.e. the volume of all the CFD cells inside a MCRT cell (recall that the MCRT mesh is coarser than the CFD mesh.) This process is split up into five zones: Air-particle mixture zone, exterior wall zone, left wall zone, outlet tube zone and window zone. The first zone is a fluid zone, while the other four are solid zones. Note, however, that the window is currently modeled as a boundary surface and the volume calculation is not performed in the simulations presented here (albeit the code is available to be eventually used when the window is modeled as a solid volume.) For each of these zones, all the CFD cells are looped following the subsequent procedure:
 - Calculate the global Cartesian coordinates of the centroid of the CFD cell.
 - Convert them to global cylindrical coordinates.
 - Determine whether the CFD cell is in the zone we are considering (air-particle mixture, outlet tube, etc.) If not, go to the next CFD cell of the loop. If so:
 - Determine the indices that characterize the Monte Carlo cell (recall the MCRT mesh is structured) in which the CFD cell is located. For that, Algorithm 4 is used.
 - In some cases, the radial and/or axial indices previously calculated are relative to the zone we are considering, instead of the global indices of the MCRT mesh. In such cases, the indices must be converted from local to global indices.
 - Add the volume of the CFD cell to the corresponding Monte Carlo cell in which it is located, using the indices just calculated.
3. Load the initial radiative source term and inlet temperature fields (specified via external files).
4. Show the initial radiative source term and inlet temperature fields in the ANSYS Fluent console to check whether they were successfully loaded. The kind of cell (air-particle mixture, window, left wall, exterior wall, outlet tube, inlet surface or outlet surface) is shown as well to facilitate the interpretation.

5. Equate the historical value of the radiative source term field and the inlet temperature field (necessary for future under-relaxation, see Section 5.2) to the initialization values.
6. Show through the ANSYS Fluent console a brief description of the features of the simulation (date, time of the day, mass flow rate, mass loading, radiative properties of the walls, etc.) to check whether the right UDF was loaded.

DEFINE_SOURCE:

These UDFs are executed before every iteration of the CFD solver to specify the radiative source term to be included in the energy equation (the UDF is called one time for each CFD cell.) Four different User-Defined Functions, one per volumetric zone, are required: air-particle mixture zone, exterior wall zone, left wall zone and outlet tube zone. Moreover, a fifth UDF is available for the window if it were eventually modeled as a volume (to calculate conduction heat transfer), rather than as a boundary surface with a proper Dirichlet boundary condition for the temperature. Each of these functions was programmed to accommodate the differences between the five zones. Nonetheless, all of them essentially follow the next three steps:

1. Calculate the global Cartesian coordinates of the centroid of the CFD cell.
2. Convert them to global cylindrical coordinates.
3. Determine the indices that characterize the Monte Carlo cell (recall the MCRT mesh is structured) in which the CFD cell is located. Algorithm 3 illustrates the general procedure to do it when the CFD cell is located in a zone whose corresponding MCRT cells are two-dimensional (i.e., the outlet tube, the exterior wall, the left wall and eventually also the window); while Algorithm 4 shows the process to be employed in CFD cells whose corresponding MCRT cells are three-dimensional (i.e., the air-particle mixture).

DEFINE_PROFILE:

While the outlet temperature of the recuperator in a recuperated gas turbine engine varies with a number of factors [61] (e.g., solar thermal input, guide vane angle or recuperator performance), an outlet temperature of 700 K was kept constant in this *Proyecto Fin de Carrera* in an effort to evaluate the solar receiver itself. However, the inlet surface of the receiver participates in the radiation heat transfer and a net radiative heat flux does exist on it; so that the inlet temperature of the receiver needs to be modified based on such a radiative source term.

Algorithm 3

1. Calculate the azimuthal index²³:

$$k = \text{INF}(\varphi/\Delta\varphi)$$

A *do while* loop is required to ensure that the azimuthal coordinate is such that $\varphi \in [0, 2\pi)$, since ATAN2 may return $\varphi < 0$ or $\varphi \geq 2\pi$.

2. Calculate the second index, i.e. the axial index for the outlet tube and the exterior wall or the radial index for the left wall and eventually the window. This is easily accomplished since the second coordinate of the nodes is known and does not depend on the azimuthal coordinate.
 4. Calculate the radiative source term in that Monte Carlo cell using the indices just calculated, and under-relax it if necessary. This is the source term that the CFD solver will use in the overall energy equation.
 5. Add the radiative source term passed to ANSYS Fluent in order to eventually check whether the source terms in the MCRT code and in ANSYS Fluent match.
-

Algorithm 4

1. Calculate the azimuthal index²³.

As in Algorithm 3, a *do while* loop is required to ensure that the azimuthal coordinate is such that $\varphi \in [0, 2\pi)$, since ATAN2 may return $\varphi < 0$ or $\varphi \geq 2\pi$.

2. Determine the type of cell (air-particle mixture, exterior wall, etc.) In the case of the air-particle mixture, it is also necessary to determine the type of cell (Type 1, 2 or 3).
3. Calculate a second index:

- For the outlet tube, the exterior wall and the air-particle mixture's cells of Type 1 or 2: Axial index.
- For the left wall, the air-particle mixture's cells of Type 3 and eventually the window: Radial index.

In both cases this is easily accomplished since the second coordinate of the nodes is known and does depend neither on the azimuthal index nor on the third index to be determined in Step #4.

4. In the case of the air-particle mixture cells (three-dimensional cells), calculate the third index: The radial index in cells of Type 1 and 2, or the axial index in cells of Type 3. This is relatively straightforward as it is possible to determine (although it may be not trivial) the minimum and maximum value of the third coordinate of the Monte Carlo cells once the first and second coordinates are known (Steps #1 and #3).
-

This UDF, which is called before every iteration of the CFD solver and for each cell on the inlet surface, is responsible for imposing such a thermal boundary condition. The way of doing it is by identifying the Monte Carlo cell in which the CFD cell of the inlet surface is

²³ The azimuthal index can be calculated directly, instead of having to use a search algorithm, since $\Delta\varphi$ is constant over the Monte Carlo mesh. Hence, this step can be performed with cost $\sigma(1)$ instead of, at least, $\sigma(\log n)$.

located and under-relaxing the value of the temperature (both in a similar way as in the UDF `DEFINE_SOURCE`):

1. Determine the indices that characterize the Monte Carlo cell (recall the MCRT mesh is structured) in which the CFD cell of the inlet surface is located. The azimuthal index is determined first and the radial index later (though, in this case, the indices are not coupled and the order may be inverted.) The axial index does not need to be calculated since all the cells in the inlet surface correspond with the last axial index of the MCRT mesh.
2. Provide the inlet temperature in that Monte Carlo cell –which is calculated in the MCRT code (see Section 3.5, Step #9)– and under-relax it if necessary.

`DEFINE_EXECUTE_AT_END`:

This User-Defined Function is executed after every iteration of the CFD solver. Its main goals are to calculate the temperature field in the Monte Carlo grid and execute the MCRT code to calculate the radiative heat transfer with the new temperature field. To accomplish it, the following steps are performed:

1. Show on the ANSYS Fluent console and write in an external file the total radiative source term passed to each zone of the CFD model (air-particle mixture, outlet tube, exterior wall, left wall and window). This information is required for both achieving a better understanding of the physics of the radiation heat transfer inside the solar receiver and checking whether the UDF properly passes the source term from the MCRT code to the CFD solver.
2. If the MCRT code was called in the previous CFD iteration, the historical value of both the radiative source term field and the inlet temperature field are updated to include the value in the last MCRT iteration.
3. Write the radiative source term field and the inlet temperature field in an external file so that if ANSYS Fluent is closed (either on purpose or due to a power failure) it is possible to continue the simulation from the last iteration performed.
4. Calculate the mass-weighted average temperature of all the CFD cells that are inside a Monte Carlo cell. This process is repeated for all the Monte Carlo cells so that the temperature field in the MCRT mesh is obtained. In this step it is necessary to determine the zone and the particular MCRT cell in which the CFD cell is located. This process can be quite involved and is accomplished in a similar way as the one to calculate the volume of every Monte Carlo cell (Step #2 of the UDF `DEFINE_EXECUTE_ON_LOADING`).
5. Under-relax the temperature field in the MCRT mesh using the temperature field just calculated in Step #4 and the historical value. The historical value is updated as well.

6. If the MCRT code needs to be executed (it is not called in all the CFD iterations, see Section 5.4) the following operations are required as well:

- Determine the number of rays to be traced by the MCRT method, both coming from the heliostat field and emitted from inside of the receiver. The number of rays to be traced varies throughout the iterative procedure as will be explained in Section 5.4.
- Calculate the initial seed for the Random Number Generator (RNG) of the MCRT code using the `localtime` function.
- Show in the ANSYS Fluent console and write in an external file the temperature field in the MCRT mesh.
- Execute the Monte Carlo Ray Tracing code.
- Clip the radiative source term just calculated by the MCRT method whenever necessary (excessively low or high values are possible during the iterative procedure so that clipping such unrealistic source terms improves convergence.) The information about the source terms that are clipped (the Monte Carlo cells where it occurs and the energy neglected) is printed in the ANSYS Fluent console and written in an external file. In general, this strategy is not necessary to achieve convergence.
- Show through the ANSYS Fluent console and write in an external file the radiative source term field and the inlet temperature field in the Monte Carlo grid (both the ones just calculated by the MCRT method and the ones that will be used by the CFD solver after under-relaxing the source terms and the inlet temperature.)

5.2. Under-Relaxation Strategy

The Under-Relaxation strategy is an important parameter of the CFD solver (Section 4.2), but it is treated separately in this chapter since the whole solution procedure (not only the fluid flow equations) needs to be strongly under-relaxed and it constitutes an important issue that requires a special treatment.

When using real solar irradiation (or in general non-collimated solar inputs) the walls of the solar receiver reach very high temperatures and the radiative heat transfer becomes extremely sensitive to their temperature. Consequently, small differences in the wall temperature lead to great differences in the radiative heat flux and the divergence of the radiative heat flux. Therefore, a strong under-relaxation strategy is required to avoid large temperature differences between iterations and achieve smooth convergence to the solution. The temperature field and the radiative source term field are under-relaxed before being passed to the MCRT code and to ANSYS Fluent respectively; and the equations of the fluid

dynamics solved in the CFD solver are under-relaxed as well²⁴. Moreover, the inlet temperature is also under-relaxed prior to imposing the inlet thermal boundary condition in the CFD solver. An overview of the under-relaxation strategy employed is presented below.

- Under-Relaxation of the temperature field passed from ANSYS Fluent to the MCRT code:

$$T_{MCRT}^{(i)} = (1 - URF_T) \cdot T_{CFD}^{(i)} + URF_T \cdot T_{hist}^{(i)} \quad (5-1)$$

$$T_{hist}^{(i)} = T_{MCRT}^{(i-1)}$$

Where the superscript i denotes the number of iteration of the Monte Carlo Ray Tracing method.

- Under-Relaxation of the radiative source term passed from the MCRT code to ANSYS Fluent:

$$S_{CFD}^{(i)} = (1 - URF_S) \cdot S_{MCRT}^{(i)} + URF_S \cdot S_{hist}^{(i)} \quad (5-2)$$

$$S_{hist}^{(i)} = S_{CFD}^{(i-1)}$$

Wherein S denotes either the divergence of the radiative heat flux in the 3-D cells ($S = \nabla \cdot \mathbf{q}^{rad}$) or the radiative heat flux through the 2-D cells ($S = -\mathbf{q}^{rad} \cdot \hat{\mathbf{n}}$). Since the MCRT code is not executed after every CFD iteration (see Section 5.4), the numerical values in Eq. 5-2 will be the same in all the iterations of the CFD solver that are performed between two consecutive MCRT iterations.

- Under-Relaxation of the inlet temperature passed from the MCRT code to ANSYS Fluent:

$$IT_{CFD}^{(i)} = (1 - URF_{IT}) \cdot IT_{MCRT}^{(i)} + URF_{IT} \cdot IT_{hist}^{(i)} \quad (5-3)$$

$$IT_{hist}^{(i)} = IT_{CFD}^{(i-1)}$$

Again, since the MCRT code is not executed after every CFD iteration, the numerical values in Eq. 5-3 will be the same in all the iterations of the CFD solver that are performed between two consecutive MCRT iterations.

- Under-Relaxation of the fluid dynamics equations in ANSYS Fluent:

$$\varphi^{(j)} = URF_\varphi \cdot \varphi_{calc}^{(j)} + (1 - URF_\varphi) \cdot \varphi^{(j-1)} \quad (5-4)$$

²⁴ Since the pressure-based solver is used, all equations have an associated under-relaxation factor available to be used.

Where here the superscript j denotes the number of iteration of the CFD solver, φ is a fluid flow variable and φ_{calc} is the value calculated, without under-relaxation, after the iteration of the CFD solver. Unlike URF_T , URF_S and URF_{IT} , the smaller the under-relaxation factor of a fluid flow variable in ANSYS Fluent is, the greater the under-relaxation is [66].

While high values of URF_T , URF_S and URF_{IT} would require more iterations to achieve convergence, they also consider the contribution of the rays traced in the previous iterations; which in the limit of convergence (when the temperature field is asymptotically close to the exact solution) is acceptable. This implies that much fewer rays can be traced per iteration (i.e. much less CPU time per iteration) without loss of accuracy. Actually, the advantages of under-relaxing the radiative source term and tracing fewer rays per iteration are apparent: This way, the radiative solution is not fully converged for all the temperature fields of the solution procedure, but rather the fluid flow and radiative solutions converge simultaneously (without achieving fully convergence in the radiative heat transfer solution in every iteration of the solution process.)

The difficulty resides in determining the under-relaxation strategy that yields the best compromise between both effects (less time per iteration vs. fewer iterations) and minimizes the CPU time to achieve convergence. An extensive variety of possibilities and strategies have been analyzed and compared in order to minimize the simulation time. The optimum under-relaxation parameters obtained from that analysis are presented in Table 10.

Equation	Under-Relaxation Factor
Temperature (URF_T)	0.50
Radiative source term (URF_S)	0.75
Inlet temperature (URF_{IT})	0.75
Fluid Flow Variables (URF_φ) ²⁵ :	
- Pressure	0.25
- Density	0.90
- Body Forces	1.00
- Momentum	0.60
- Turbulent Kinetic Energy	0.70
- Specific Dissipation Rate	0.70
- Turbulent Viscosity	0.80
- Energy	0.95 $\rightarrow$ 0.70 ²⁶

Table 10 – Optimum Under-Relaxation Strategy.

In reality, the best strategy depends on the ratio *solar thermal input vs. mass flow rate* as the temperature level in the receiver (and thereby the optimum under-relaxation strategy)

²⁵ Recall that, unlike URF_T , URF_S and URF_{IT} , the smaller the under-relaxation factor of a fluid flow variable in ANSYS Fluent is, the greater the under-relaxation is [66].

²⁶ Varied from 0.95 in the first iterations to 0.70 in the last iterations.

mainly depends on that. In general, the higher this ratio is, the higher the temperature is and the higher the under-relaxation of the fluid dynamics equations should be.

5.3. Interpolation Scheme

The radiative solution is provided in the Monte Carlo mesh by the MCRT code, while ANSYS Fluent requires the solution in the CFD mesh. Since the MCRT mesh is considerably coarser than the CFD grid (around 600 cells vs. over 1,000,000 cells), it is convenient to employ an interpolation scheme between both meshes in order to smooth the radiative source term field and improve the accuracy of the final solution. The main difficulty associated with the interpolation scheme is that it must be conservative, i.e. the integral of the interpolation function over $\bar{\Omega}$ must equal the total radiative source term in the receiver. If not, the error in the main outputs of the model (useful thermal power and thermal efficiency of the receiver) would be of the same order as the error in the total source term due to the non-conservative character of the interpolation scheme, which would make the simulation results unreliable.

The difficulty arises from the fact that known conservative interpolation schemes [68-70] require the solution of a linear system of N equations, where N is the number of cells of the objective mesh (in our case the CFD mesh, i.e. $N > 1,000,000$); which is computationally expensive. The only affordable method is the first-order Galerkin projection (see [68] for further details on Galerkin projections), which leads to the degenerate case of a diagonal matrix and is computationally efficient. However, this first-order Galerkin projection is equivalent to simply imposing the radiative source term of the MCRT cell in which the CFD cell is located, which means that the source term is actually not interpolated and this is the strategy previously employed [20].

Therefore, a conservative interpolation scheme should be developed specifically for the Small Particle Solar Receiver. While in 1-D this is easily accomplished with a linear interpolation scheme, in higher dimensions multi-linear interpolations schemes are not conservative. Moreover, in axisymmetric geometries, the volume is linear in the variables z , φ and r^2 , but not in r . While it is possible to fix the latter problem by employing the coordinates (r^2, φ, z) , the mathematical domain of the Monte Carlo cells in such a coordinate system would become much more complicated and the difficulty of the overall problem would be even greater.

The mathematical formulation of a possible conservative interpolation scheme for the Small Particle Solar Receiver is presented in Appendix I (not shown here for the sake of clarity.) Note, however, that all the results presented in Chapter 7 correspond with the case with no interpolation scheme, or rather, with just a first-order discontinuous Galerkin projection.

5.4. Solution Procedure

In addition to the physico-mathematical difficulties of the model itself, presented in Section 2.1, there exist important issues associated to the convergence of the coupled model. In general, when coupling CFD solvers with external, field-dependent source terms, it is necessary to design and optimize the solution procedure in order to prevent numerical oscillations and ensure stability and convergence to the solution. Indeed, this known potential problem requires special attention in the numerical modeling the Small Particle Solar Receiver as explained in Section 5.2.

In addition to the under-relaxation strategy, it is also necessary to pay attention to the way the MCRT method and the CFD solver iterate alternatively. For example, if too many Fluent iterations are performed between two consecutive MCRT iterations, the temperature field varies too much (between Monte Carlo iterations) and the numerical solution oscillates around the actual solution²⁷. If too few Fluent iterations are employed, the numerical solution smoothly converges to the right solution but the CPU time becomes significantly longer for the calculation. Furthermore, the number of rays traced by the MCRT method is another variable that can be varied to optimize convergence. Hence, an optimized adaptive strategy is employed. This strategy gradually varies both the ratio ANSYS Fluent vs. MCRT iterations and the number of rays traced by the MCRT. This way, the solution smoothly converges in an optimized CPU time. Table 11 collects the main parameters that are varied during the solution process. Moreover, the under-relaxation of the fluid flow variables in the CFD solver is adaptively varied during the solution procedure as well (see Table 10).

	First iterations	Last iterations
Ratio CFD vs. MCRT Iterations	10:1 Reason: The numerical solution rapidly goes to a region close to the actual solution.	1:1 Reason: This way, the temperature field almost does not vary between MCRT iterations and, thus, no oscillations in the solution occur.
Total number of rays traced	200,000 (100,000 from the heliostat field + 100,000 emitted from inside of the receiver) Reason: The temperature and velocity fields are far from the actual solution and there is no necessity to reduce the statistical uncertainty of the MCRT solution.	400,000 (200,000 from the heliostat field + 200,000 emitted from inside of the receiver) Reason: It is possible to keep the statistical uncertainty of the final solution on target with such a reduced number of rays due to the under-relaxation strategy of the radiative source term (see Section 5.2)

Table 11 – Main parameters that are varied during the solution procedure (the under-relaxation strategy of the fluid flow variables in ANSYS Fluent is varied as well and is shown in Table 10.)

²⁷ These oscillations can be as large as ± 300 K in the outlet temperature, and the exact solution may not even be close to the value around which the solution oscillates.

It should be noted that integrated and averaged quantities, such as the outlet temperature, the thermal efficiency or the pressure drop, frequently converge before the local flow variables do and then the simulations do not require the full precision available. Therefore, the convergence criterion is based on the convergence of these integrated variables rather than the flow field itself. Of course, the fully converged solution would be preferred, but the additional computational time required does not justify the negligible accuracy gain in the outputs of the model. In particular, the simulation is assumed to be converged when the outlet temperature levels out and the oscillations are within the range ± 0.5 K. By then, the pressure drop and inlet temperature are already converged. Note, however, that if an accurate prediction of the wall temperature were required, some extra iterations would be necessary (especially if the walls were treated as blackbodies.)

Chapter 6

Design Optimization

“Assuming that one has the ability to predict the performance, the question then arises of how to modify the design to improve the performance”, Antony Jameson [71].

In the always highly competitive energy market it is of the utmost importance to optimize the design of the different components of a power plant in order to maximize the efficiency, reduce the initial and operating costs, increase the lifespan of the different components and, in turn, reduce the generation cost of the electricity. For example, increasing one percent the efficiency of a 100 MW CSP plant would increase the profit several M\$/year. In particular, the main purposes of the Multidisciplinary Design Optimization of the 5 MW_{th} Small Particle Solar Receiver to be design under the U.S. DOE’S SunShot program are:

1. Increase the thermal efficiency of the solar receiver (with the ultimate goal of maximizing the overall efficiency of the CSP power plant.)
2. Reduce the wall temperature, which in turn would avoid material problems, increase the lifespan of the receiver, reduce maintenance costs and, again, increase the receiver efficiency.
3. Reduce manufacturing, operation and maintenance costs.

The methodology to perform such a design optimization is the subject of the present chapter, while the numerical results will be presented in Chapter 7.

6.1. Optimization Problem

The design optimization of the Small Particle Solar Receiver constitutes an extremely complex PDE-constrained optimization problem that can be written as in Eq. 6-1:

$$\begin{aligned}
 & \max_{\mathbf{u}, \boldsymbol{\alpha}} g(\mathbf{u}, \boldsymbol{\alpha}) \\
 & s. t. \mathcal{F}(\mathbf{u}, \boldsymbol{\alpha}) = \mathbf{0} \\
 & \quad \mathbf{h}(\boldsymbol{\alpha}) = \mathbf{0} \\
 & \quad \mathbf{p}(\mathbf{u}, \boldsymbol{\alpha}) \leq \mathbf{0}
 \end{aligned} \tag{6-1}$$

Where $\mathbf{u} \in \mathbb{R}^d$ is the fluid flow and radiative solution and $\boldsymbol{\alpha} \in \mathbb{R}^n$ is the vector of design variables. $\mathcal{F}$ are the governing equations of the problem (namely, the N-S equations

and the RTE, Eq. 2-1), g is the objective functional (which in general may depend on both $\mathbf{u}$ and α), $\mathbf{h}$ is the set of additional restrictions applied to the design variables (maximum and minimum dimensions of the receiver, radiative properties available for the walls, etc.), and $\mathbf{p}$ are the material limits (maximum wall temperature, etc.), which depend on the material itself (i.e., on the design variables) and will be imposed via a penalty method.

6.2. Difficulties of the Design Optimization

Whenever the sensitivities of the objective function with respect to the design variables can be computed, conventional gradient descent methods can be used to find the solution to an optimization problem. The main difficulty to optimize the design of the Small Particle Solar receiver lies in the fact that the objective functional depends on the problem solution $\mathbf{u}$, which in turn depends on the design variables α through the governing equations $\mathcal{F}(\mathbf{u}, \alpha)$ (the Navier-Stokes equations and the RTE, i.e. Eq. 2-1 in compact form.)

After the dualization of the constraint, the objective function can be written as $G(\mathbf{u}, \alpha, \phi) = g(\mathbf{u}, \alpha) + \phi^T \mathcal{F}(\mathbf{u}, \alpha)$ and, thus, the sensitivities with respect to the design variables are:

$$\frac{\partial}{\partial \alpha} G(\mathbf{u}, \alpha, \phi) = \mathbf{0} \Leftrightarrow \frac{\partial g}{\partial \alpha} + \frac{\partial g}{\partial \mathbf{u}} \frac{\partial \mathbf{u}}{\partial \alpha} + \phi^T \left(\frac{\partial \mathcal{F}}{\partial \alpha} + \frac{\partial \mathcal{F}}{\partial \mathbf{u}} \frac{\partial \mathbf{u}}{\partial \alpha} \right) = \mathbf{0} \quad (6-2)$$

The main difficulty is now obvious: In order to compute the sensitivities of the objective function it is necessary to compute the sensitivities of $\mathbf{u}$ with respect to the design variables, which is computationally expensive and unaffordable in our case. One way of avoiding the computation of the sensitivities of $\mathbf{u}$ with respect to the design variable is by picking ϕ satisfying Eq. 6-3, which is called the Adjoint Equation.

$$\frac{\partial g}{\partial \mathbf{u}} + \phi^T \frac{\partial \mathcal{F}}{\partial \mathbf{u}} = \mathbf{0} \quad (6-3)$$

Thus, we can readily compute the sensitivities as expressed in Eq. 6-4.

$$\frac{\partial g}{\partial \alpha} = -\phi^T \frac{\partial \mathcal{F}}{\partial \alpha} \quad (6-4)$$

The Adjoint Navier-Stokes equations are well-known [72-74], while the RTE adjoint operator is such that $L^*(\mathbf{x}, \Omega) = L(\mathbf{x}, -\Omega)$ [75,76], where Ω denotes direction, $\mathbf{x}$ denotes position, L is the RTE operator and L^* is the adjoint RTE operator. This means that the Monte Carlo Ray Tracing software developed in this *Proyecto Fin de Carrera* can, with small modifications, be employed to solve the adjoint thermal radiation problem. However, the development of such a solver is much beyond the scope of the project for several reasons. Moreover, computing the sensitivities via finite differences would also require an unaffordable CPU time, and we should then limit ourselves to explore the design space in a finite number of points (rather than finding the actual solution using descent methods), which leads to a discrete optimization problem. As solving binary or discrete optimization

problems is NP-hard²⁸, we should cleverly define the design space to avoid introducing irrelevant or insensitive variables, which would excessively increase the required effort.

6.3. Design Space

The design space consists of the geometry of the receiver, the geometry of the window, the optical (radiative) properties of the walls and the direction of the fluid flow with respect to the concentrated solar irradiation. It is convenient to point out that we are optimizing the design of the receiver rather than the operating conditions (mass flow rate, inlet particle size, inlet mass loading, etc.)

6.4. Constraints

The constraints are based on material limits (for example, the maximum operating temperature of aluminum oxide is around 1560°C), the space available on the top of the tower of the National Solar Thermal Test Facility where the solar receiver will be located, and other technical issues. The former constraints are imposed via a penalty method as they depend on the problem solution.

6.5. Objective Function

A wide variety of objective functions can be defined, such as:

- Thermal efficiency on a particular day and time (e.g. 12:00 PM on March 21st, the Spring equinox):

$$g_1(\mathbf{u}, \boldsymbol{\alpha}) = \frac{1}{Q_{sol}^{input}} \left(\iint_{\Gamma_{outlet}} \rho h(u_i n_i) dA - \iint_{\Gamma_{inlet}} \rho h(u_i n_i) dA \right) \Big|_{03/21 \text{ at } 12.00pm} \quad (6-5)$$

- Total useful energy throughout a particular day (e.g. March 21st):

$$g_2(\mathbf{u}, \boldsymbol{\alpha}) = \int_{12.00 \text{ am}}^{11.59pm} \left(\iint_{\Gamma_{outlet}} \rho h(u_i n_i) dA - \iint_{\Gamma_{inlet}} \rho h(u_i n_i) dA \right) dt \Big|_{03/21} \quad (6-6)$$

- Total useful energy throughout the year:

$$g_3(\mathbf{u}, \boldsymbol{\alpha}) = \int_{Jan \ 1st}^{Dec \ 31st} \left(\iint_{\Gamma_{outlet}} \rho h(u_i n_i) dA - \iint_{\Gamma_{inlet}} \rho h(u_i n_i) dA \right) dt \quad (6-7)$$

²⁸ NP-hard means that any algorithm developed for its numerical computation has a cost greater than any polynomial order, i.e., the time required to compute a solution grows faster than $N^p \forall p \in \mathbb{N}$, where N is the size of the problem (in our case, the dimension of the design space.)

- Cost of the generated electricity: For a more multidisciplinary approach the cost of the generated electricity can be minimized. For that, the cost of the components and their expected life span need to be known.

Here we will employ the efficiency at 12:00 PM on an average day, namely on March 21st (the Spring equinox), as a preliminary objective function ($g = g_1$) since the cost of the components and their expected lifespan cannot be accurately predicted yet. Objective functionals that consider the weighted-average efficiency at different times and days would be more accurate to elucidate the best design, but would yield a prohibitive CPU time.

6.6. Optimization Technique

The design space is explored via parametric study in order to identify important and sensitive variables, determine appropriate design variable ranges to meet the material limits, $\mathbf{p}(\mathbf{u}, \boldsymbol{\alpha}) \leq \mathbf{0}$, and obtain a first estimate of the optimum design and the maximum thermal efficiency that the 5 MW_{th} Small Particle Solar Receiver can achieve. Hence, only one variable of the design space will be varied at the same time with respect to the so-called *baseline case*, and the objective function, g , will be evaluated in such designs. This way $g|_{x_i=x_i^*} \forall i \neq j$ will be explored, where x_j is the variable with respect to which the parametric study is conducted and x_i^* is the value of the design variable x_i in the baseline case.

Design Parameter	Value	Design Parameter	Value
Receiver:		Direction of the flow	Countercurrent
- Shape	Cylindrical	Inlet Temperature	700 K
- Length	3 m	Walls:	
- Diameter	2 m	- Radiative Properties	Aluminum Oxide (Al ₂ O ₃)
- Tilt angle	26.5°	- Thermal Resistance	2 m ² -K/W
Window:		(including the insulation)	
- Material	Fused quartz (HOQ-310 [21])	Solar Irradiation:	
- Shape	Spherical cap (45° cap angle)	- Time	12.00 PM
- Diameter	1.7 m	- Day	March 21 st
- Thickness	2.54 cm	- Input power	4.25 MW
Outlet Tube:		Operating Pressure	5 bar
- Length	2.1 m	Mass Loading of Particles	0.5 g/m ³
- Diameter	0.6 m	Particle Diameter	200 nm
- Thickness	1 cm		

Table 12 – Design parameters and operating conditions of the baseline case of the design optimization.

The design of the baseline case was chosen based on preliminary results (see Section 7.1) and its design parameters are collected in Table 12. The operating conditions, which are not varied throughout the parametric study, are included for completeness as well. Note that the operating pressure has been changed from 10 bar (parametric study of the operation conditions, results in Section 7.1) to 5 bar (Multidisciplinary Design Optimization, results in

Section 7.2). In the former case, 10 bar was chosen for consistency with previous results [19,20]; while in the latter 5 bar is employed since this the pressure at which the 5 MW_{th} Small Particle Solar Receiver (whose design is to be optimized) will operate. Moreover, the optical properties of the fused quartz in the visible spectrum have been updated due to the availability of new data.

Note that parameter studies do not capture interaction between variables and the optimum design will not most likely be obtained. However, it is a cheap²⁹ method to perform a preliminary design space exploration and determine important and sensitive variables, which is the main goal at this point of the project.

A one-at-a-time optimization technique, however, is suggested for the final design optimization (to be performed once the oxidation code, currently being developed by Trent Martin, is available to be coupled to the model.) This optimization strategy captures some interaction between variables –even though the result may depend on the order of the factors– and has an expense $1 + n \cdot (l - 1)$ as well. Table 13 [77] aims to summarize the differences between a parameter study and a one-at-a-time technique, and presents a schematic representation of how they perform. Note that A^* is the value of A that optimizes the objective function (Experiments No. 1 and 2), and similarly with B^* (Experiments No. 1, 3 and 4), C^* (1 and 5) and D^* (1, 6 and 7). The “best design” is then A^* , B^* , C^* , D^* . In the case of the design optimization of the Small Particle Solar Receiver, A, B, C and D represent the direction of the fluid flow with respect to the concentrated solar irradiation coming from the heliostat field, the radiative properties of the walls, the geometry of the window and the geometry of the receiver, respectively.

Expt. No.	Parameter Study				One At a Time			
	A	B	C	D	A	B	C	D
1	A1	B1	C1	D1	A1	B1	C1	D1
2	A2	B1	C1	D1	A2	B1	C1	D1
3	A1	B2	C1	D1	A^*	B2	C1	D1
4	A1	B3	C1	D1	A^*	B3	C1	D1
5	A1	B1	C2	D1	A^*	B^*	C2	D1
6	A1	B1	C1	D2	A^*	B^*	C^*	D2
7	A1	B1	C1	D3	A^*	B^*	C^*	D3

Table 13 – Schematic representation of a parameter study and a one-at-a-time technique.

²⁹ The expense is $1 + n \cdot (l - 1)$, where l is the number of levels and n the number of factors (or variables) of the parametric study.

Chapter 7

Numerical Results

This chapter summarizes the results obtained in this *Proyecto Fin de Carrera* using the methodology presented in previous chapters. It is split up into two sections: The first part corresponds to the parameter study of the operating conditions (time of the day and mass flow rate), whereas the second section presents the multidisciplinary design optimization of the 5 MW_{th} Small Particle Solar Receiver.

7.1. Parametric Study of the Operating Conditions

This sections collects the results of the parameter study of the operating conditions (time of the day and mass flow rate) using the most efficient design found in the preliminary design optimization process (illustrated in Figure 2 and whose design parameters are collected in Table 14.) In Figure 2, the mixture of air and carbon nanoparticles enters the rear of the receiver (blue arrows), travels towards the front absorbing concentrated solar irradiation (which penetrates through the ellipsoidal window displayed in gleaming light gray, as illustrated with yellow arrows), and finally exits the receiver going backwards through the central outlet tube (red arrows).

Design Parameter	Value	Design Parameter	Value
Receiver:		Walls:	
- Shape	Cylindrical	- Thermophysical Properties	Aluminum Oxide (Al ₂ O ₃)
- Length	3 m	- Radiative Properties	Blackbody
- Diameter	3 m	- Thermal Resistance	2 m ² -K/W
- Tilt angle	23.8°	(including the insulation)	
Window:		Operating Conditions:	
- Material	Generic fused quartz [89]	- Inlet Temperature	700 K
- Shape	Oblate spheroid (ellipsoid)	- Operating Pressure	10 bar
- Principal axes	1.7 m x 1.7 m x 1.21 m	- Inlet particle mass loading	0.5 g/m ³
- Thickness	2.54 cm	- Inlet particle diameter	200 nm
Outlet Tube:			
- Length	1.9 m		
- Inner diameter	0.6 m		
- Thickness	1 cm		

Table 14 – Preliminary design parameters and operating conditions of the Small Particle Solar Receiver.

The size of the window has been chosen to optimize the transmitted solar irradiation without excessively increasing the radiative losses coming from the inside of the receiver; while the length of the outlet tube provides enough path length to absorb solar irradiation and allows an easy flow recirculation. Note also that gravity forces are not included in the model and buoyancy forces are thereby neglected. Since a strong thermal stratification is

expected inside the solar receiver, it constitutes a complicated problem itself that should be first addressed separately. Particle oxidation is not yet included, as the oxidation code is currently being developed by Trent Martin, a graduate student in our group.

For this preliminary design of the Small Particle Solar Receiver, three solar irradiation conditions have been simulated to predict the receiver's behavior at different times: 12:00 PM, 2:00 PM and 4:00 PM on March 21st –the Spring equinox–. The location employed for the CSP plant is the National Solar Thermal Test Facility (Albuquerque, NM), where the Small Particle Solar Receiver will be tested. The spectral intensity field on the window for these three times was generated by proper ray tracing software. The incoming rays from the heliostat field (transmitted, absorbed and reflected rays) are generated by our coupled MIRVAL and window model, developed by Sandia National Laboratories [78] and Mecit [21] respectively. In particular, 100 million rays are traced in MIRVAL, which leads to about 13 million ray entering into the receiver and 1.4 million rays being absorbed by the window. Then, the Monte Carlo software reads the location, direction, wavelength and energy of all these rays and traces them throughout the receiver. Therefore, the spatial, directional and wavelength dependence of the concentrated solar irradiation is considered and modeled by our software.

For each solar thermal input, the mass flow rate has been varied to accommodate the irradiation differences and thus optimize the efficiency. Table 15 collects a summary of the fifteen simulations performed for different cross combinations of time of the day and mass flow rate.

	12:00 PM	2:00 PM	4:00 PM
1 kg/s	-	-	Sim. 3-1
1.5 kg/s	-	-	Sim. 3-2
2 kg/s	Sim. 1-1	Sim. 2-1	Sim. 3-3
2.5 kg/s	-	-	Sim. 3-4
3 kg/s	Sim. 1-2	Sim. 2-2	Sim. 3-5
4 kg/s	Sim. 1-3	Sim. 2-3	-
5 kg/s	Sim. 1-4	Sim. 2-4	-
6 kg/s	Sim. 1-5	Sim. 2-5	-
Input Power	3.93 MW	3.48 MW	1.75 MW

Table 15 – Summary of simulations performed (March 21st in Albuquerque, NM).

Figures 21 and 22 show the outlet temperature and the thermal efficiency of the Small Particle Solar Receiver, respectively, for the fifteen simulations presented in Table 15. The thermal efficiency is defined as the useful power over the solar thermal power that goes through the window and enters the receiver. Hence, the losses due to absorption and reflection in the window are not included in the definition of *thermal efficiency*, but rather they are accounted for by the so-called *optical efficiency* of the receiver. In the set of simulations presented in this parametric study (Section 7.1) the transmissivity of the window (i.e. the optical efficiency) is 85.2%, 88.3% and 88.3% at 12:00 PM, 2:00 PM and 4:00 PM,

respectively. However, the actual optical efficiency of the receiver will actually be higher since the optical properties of the fused quartz employed in this section [89] lead to an unrealistically high absorptivity (for example, with the updated properties [21] used in the simulations of Section 7.2 the optical efficiency at 12:00 PM is 93.1%, see Table 20.) Note also that the useful power is simply proportional to the thermal efficiency for a particular time of the day. As expected, the outlet temperature is a monotonic decreasing function of the mass flow rate; which implies that the smaller the mass flow rate is, the greater the thermodynamic efficiency of the power block could be. However, since thermal losses increase with temperature, the thermal efficiency of the solar receiver shows the opposite trend.

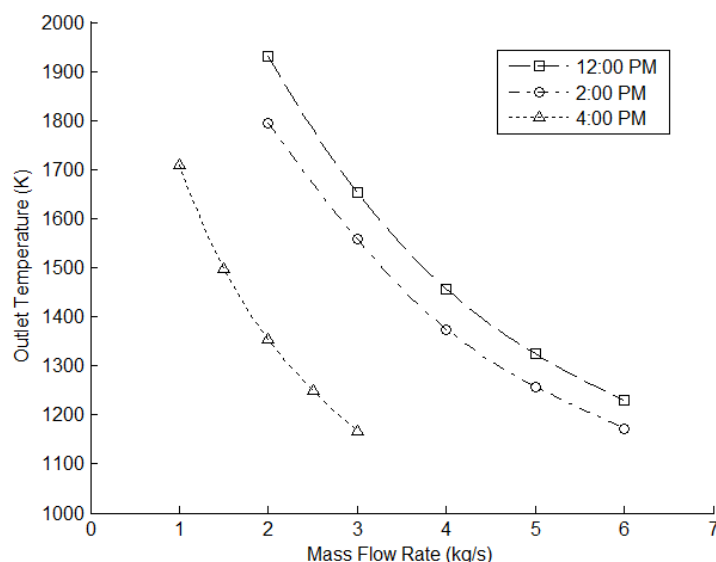


Figure 21 – Outlet temperature of the Small Particle Solar Receiver for different times and mass flow rates.

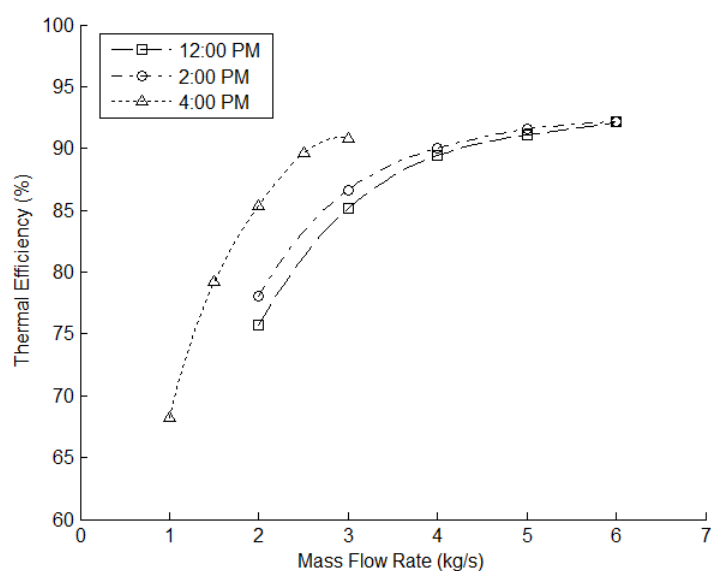


Figure 22 – Thermal efficiency of the Small Particle Solar Receiver for different times and mass flow rates.

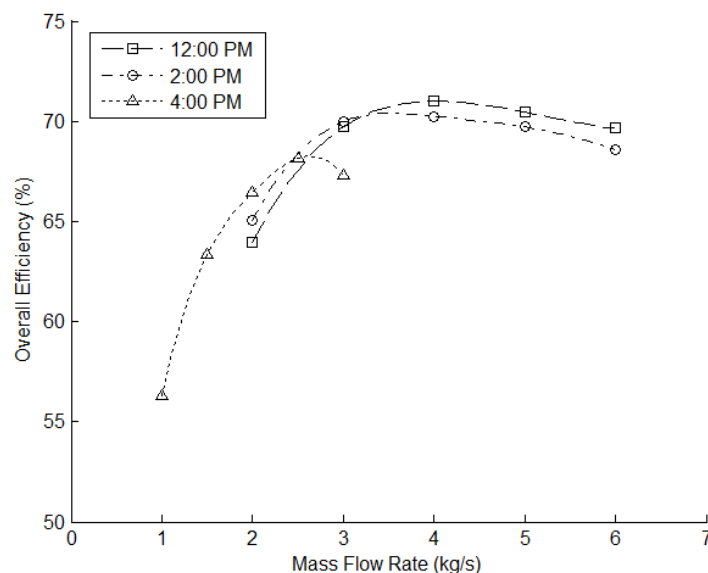


Figure 23 – Overall efficiency of the Small Particle Solar Receiver driving a gas turbine for different times and mass flow rates (Carnot efficiency is employed for the power block.) Only the optimum mass flow rate is desired to be pointed out.

Therefore, an intermediate mass flow rate that maximizes the overall efficiency must exist and should be determined. For that, the thermodynamic efficiency of the power block as a function of the useful thermal power, pressure ratio, isentropic efficiency of compressor and turbine, recuperator effectiveness and pressure drops needs to be known. As a first approximation and with the only purpose of estimating the optimum mass flow rate (rather than predicting the overall efficiency), the Carnot efficiency can be employed for the power block. Under such assumption, the overall efficiency of the system is shown in Figure 23 and the (discrete) optimum mass flow rates are 4 kg/s at 12:00 PM, 4 kg/s at 2:00 PM and 2.5 kg/s at 4:00 PM.

It is noteworthy that, utilizing the overall optimum mass flow rate defined above, the outlet temperature can be kept over 1250 K from 7:30 AM to 4:00 PM³⁰ on an average day, namely March 21st. This outlet temperature is right on target for driving a Brayton cycle [60], which is the ultimate goal of the Small Particle Solar Receiver. Furthermore, it is possible to achieve these temperatures with thermal efficiencies over 89% at all times.

The temperature field in horizontal and vertical sections for the optimum mass flow rate at 12:00 PM (4 kg/s) is shown in Figure 24. The hot spot next to the window is caused by the lack of an oxidation model and is more spread out in the horizontal than in the vertical direction. This is mainly due to the fact that the heliostat field of the National Solar Thermal Test Facility (Albuquerque, NM) spans 90° laterally and only 29° vertically when viewed from the top of the tower. Note also that the temperature field is slightly higher in the top

³⁰ The maximum concentrated solar irradiation that reaches the window occurs approximately at 12:00 PM, and 7:30 AM is the equivalent time in the morning to 4:00 PM [21] (Albuquerque, NM, on March 21st.)

half of the solar receiver –especially near the window– which indicates that the tilt angle should be increased. Actually, the optimum tilt angle has been recently found to be 26.5° [22], while 23.8° is used here due to the lack of knowledge about the optimum angle when the simulations were run. Finally, the length to obtain good mixing in the outlet tube will be considerably reduced when particle oxidation is included in the model since the high temperature zone near the window wouldn't exist and a much more homogeneous temperature profile at the beginning of the outlet tube would be obtained.

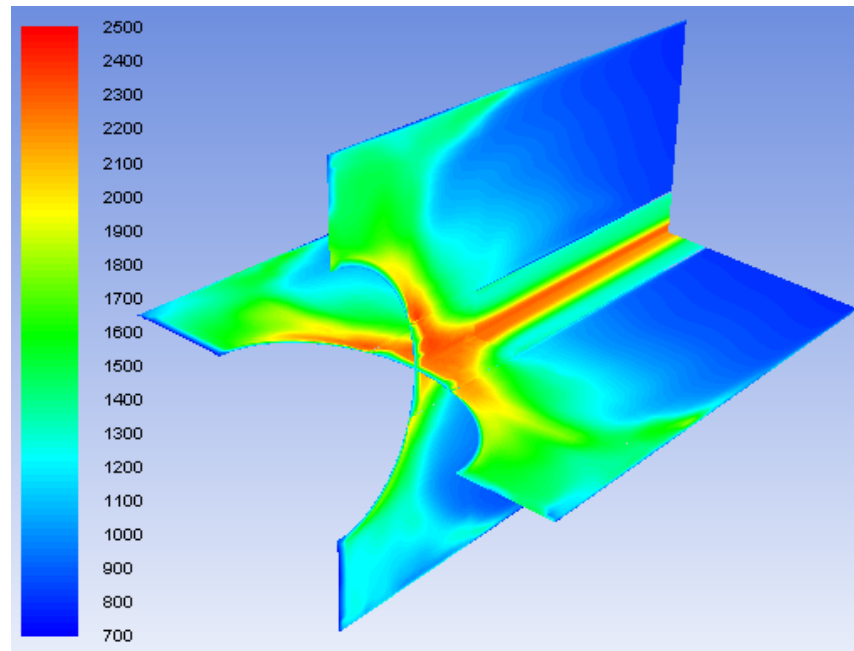


Figure 24 – Temperature field (K) in horizontal and vertical sections at 12:00 PM with a mass flow rate of 4 kg/s.

The temperature field at 4:00 PM is clearly asymmetric with respect to the vertical plane (see Figure 25) since the receiver is fixed on the top of the tower and does not have solar tracking. Nevertheless, the maximum wall temperature is lower than at 12:00 PM (to be discussed below) due to the also lower solar irradiation at that time.

As for the flow field inside the solar receiver, it should be noted that, even in this preliminary design, the air-particle mixture has a smooth recirculation prior to entering the outlet tube. Moreover, the pressure drop is in the asymptotic behavior zone and is limited to 90 Pa even in the most unfavorable (optimum) situation (4 kg/s at 12:00 PM). This value is well below current tubular solar receivers and additionally does not diminish the thermodynamic efficiency due to pressure drop between the compressor and the turbine (the expansion ratio through the turbine is essentially the same.)

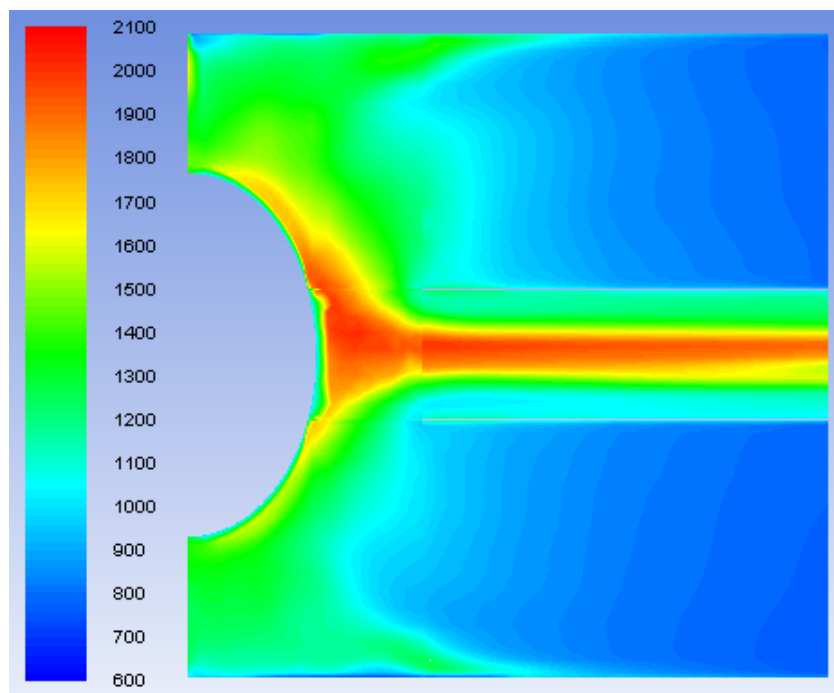


Figure 25 – Horizontal section of the temperature field (K) at 4:00 PM with a mass flow rate of 2.5 kg/s (bottom view of the receiver. Recall it is a southward heliostat field in the Northern Hemisphere.)

The maximum wall temperature is reached at the beginning of the outlet tube and on the exterior cylindrical wall at a distance between 0.3 m (4:00 PM) and 0.7 m (12:00 PM) from the window side. In particular, the maximum wall temperature is reached at 12:00 PM and is around 1400 K when the optimum mass flow rate (4 kg/s) is employed. However, the walls are treated as blackbodies here, which is unrealistic and represents the worst case scenario. In the actual receiver, aluminum oxide walls will be most likely employed (see Section 7.2.2) and, on account of their selective behavior, its temperature will be much below the blackbody case. Actually, one additional simulation was performed at 12:00 PM with Al_2O_3 radiative properties on the walls and 4 kg/s to determine the wall temperature distribution in such more realistic situation (all other parameters are kept constant, see Table 14). The maximum temperature found was 1175 K on the exterior wall and 1350 K on the outlet tube; albeit the latter can be reduced just by distancing the outlet tube from the window. A further discussion of the radiative properties of the walls as a design variable will be presented in Section 7.2.2. Furthermore, convergent geometries (from the fluid flow point of view) will reduce the wall temperature and will be explored in the multidisciplinary design optimization of Section 7.2. These convergent geometries will also contribute to increase the thermal efficiency and improve the fluid flow inside the solar receiver.

Another extra simulation was performed at 12:00 PM with 4 kg/s and 5 bar inside the solar receiver. All other parameters than pressure were kept constant with respect to Table 14 in an effort to assess the effect of the operating pressure. It was found that both the thermal efficiency and the temperature field are approximately constant regardless the

pressure. However, the pressure drop doubled from 10 bar (91.8 Pa) to 5 bar (184.1 Pa) as the air flows twice faster. Note that the pressure was varied from 10 bar in this parametric study (Section 7.1) to 5 bar in the design optimization process (Section 7.2), which justifies the analysis presented in this paragraph.

It is of great interest to analyze the origin of the losses in order to optimize the design and increase the thermal efficiency of the Small Particle Solar Receiver. Table 16 collects the contribution of the main losses mechanisms at 12:00 PM with a mass flow rate of 4 kg/s (note that the input power is 3.93 MW in such conditions). Several conclusions can be drawn from these results. First, radiative losses clearly dominate over convective losses. Second, emission from the window is the main mechanism of losses when it is at 1000 K (such temperature was imposed via boundary condition). However, the temperature of the window will actually be lower [65] (especially on the outer surface) and the losses have been overestimated. At any rate, this shows the importance of keeping the window as cool as possible for additional reasons aside from lessening the thermal stresses. Moreover, anti-reflective coatings could be used if the temperature of the window was low enough, with the corresponding reduction of optical losses.

Note finally that the results presented above correspond with the preliminary design of the Small Particle Solar Receiver shown in Figure 2 and whose design parameters are summarized in Table 14. However, an optimized design (spherical cap window, new receiver geometries, selective wall surfaces, etc.) will increase the thermal efficiency. For example, losses (4) and (5) could be reduced through a no-particles zone near the window; while losses (6) would be considerably diminished with an optimized geometry. The design optimization of the Small Particle Solar Receiver is the subject of the next section.

Mechanism of Losses	Energy (kW)
<i>Convection:</i>	
1. From the window	32.1
2. From the walls	8.9
<i>Radiation:</i>	
3. Emitted from the window (mostly from the exterior surface)	139.6
4. Emitted from the air-particle mixture	122.8
5. Back-scattered solar irradiation	73.3
6. Emitted from the inner part of the exterior wall (see Figure 2)	71.9
7. Emitted from the left wall (as displayed in Figure 2)	21.1
8. Emitted from the outlet tube	7.6

Table 16 – Contribution of the different losses mechanisms at 12:00 PM and with a mass flow rate of 4 kg/s.

7.2. Design Optimization

7.2.1. Direction of the Flow

The ideal direction of the fluid flow with respect to the solar irradiation (cocurrent vs. countercurrent) was analyzed. Previous work conducted by Ruther [19] showed that the countercurrent direction of flow has slightly better efficiency than the cocurrent, at least for a particle diameter of 200 nm. However, two main factors limited the validity of this result:

1. Lack of an oxidation model.
2. The design of the receiver and the operating conditions were quite different to the ones currently considered.

To elucidate this question three different oxidation models were implemented (for the sake of robustness) in the 2-D model previously developed by Ruther [19]. While simple, this model can serve as a first approximation to the best flow direction. Therefore, in this section (and only in this section) we will not employ the three-dimensional model presented in this *Proyecto Fin de Carrera* since the best flow direction is very sensitive to particle oxidation and this effect, although currently under research, has not been included yet in the three-dimensional model. The solution procedure of this two-dimensional model was under-relaxed (temperature and source term fields) respect to the original model by Ruther to prevent numerical oscillation due to oxidation effects. Several other parts of the code were modified as well (pure programming issues) to accommodate different particle sizes and mass loadings throughout the receiver.

In particular, the three kinetic models employed are:

- Kinetic Theory model:

$$\dot{m}'' = \frac{Arr \cdot p_{O_2}}{\sqrt{T}} e^{-\frac{E}{RT}} \quad (7-1)$$

Where $\dot{m}''$ is the rate of carbon oxidation per unit time and unit particle surface area, Arr is the Arrhenius coefficient, E is the activation energy and R is the universal gas constant. Lee and coworkers [79] used such a model to determine soot oxidation rates in flames, and provided $Arr = 1.085 \cdot 10^5 \text{ kg } K^{0.5}/m^2 \text{ s atm}$ and $E = 39,300 \text{ cal/mol}$ for carbon soot.

- Nagle and Strickland-Constable model:

$$\frac{\dot{m}''}{120} = \left(\frac{k_A p_{O_2}}{1 + k_z p_{O_2}} \right) \chi + k_B p_{O_2} (1 - \chi) \left[\frac{\text{kg}}{m^2 - s} \right] \quad (7-2)$$

With:

$$\chi = [1 + k_T/(k_B p_{O_2})]^{-1}$$

$$k_A = 20e^{-30,000/RT} \quad k_B = 4.46 \cdot 10^{-3} e^{-15,200/RT} \quad (7-3)$$

$$k_T = 1.51 \cdot 10^5 e^{-97,000/RT} \quad k_Z = 21.3e^{4,100/RT}$$

While the constants were determined from measurements on bulk pyrolytic graphite [80], they can also be used to predict oxidation rates for soot quite well [81].

- Bechtel model [82]:

$$\dot{m}'' = Arr_B \cdot p_{O_2} e^{-\frac{E_B}{T}} \quad (7-4)$$

Where $Arr_B = 3,000 \text{ kg/m}^2 \text{ s atm}$ and $E_B = 19,000 \text{ K}$, albeit the exact values actually depend on the particular type of carbon.

A further discussion on these three oxidation models can be found in [83]. Once the oxidation kinetics are known, the mass loading φ can be calculated by integration of Eq. 7-5 along the streamlines:

$$\varphi = \varphi_0 - \int_{t_0}^t \dot{m}''(T) A(t) dt \quad (7-5)$$

Note that it is necessary to know $T = T(t)$ along the streamlines to calculate the mass loading: $T = T(x)$ is known from the Monte Carlo solution and $x = x(t)$ can be readily obtained since a simple slug flow travels across the receiver in this 2-D model. Although T is constant over each cell, the effective surface available for oxidation diminishes due to oxidation and the integrand in Eq. 7-5 varies even across isothermal cells. Therefore, a numerical quadrature technique is used to improve the accuracy of the solution.

Operating Conditions	Value	Design Parameter	Value
Solar Input:		Receiver:	
- Power	4.2 MW	- Shape	Cylindrical
- Spatial distribution over the window	Uniform	- Length	3 m
- Directional distribution	45° Cone Angle	- Diameter	2 m
Mass Flow Rate	4 kg/s	Window:	
Operating Pressure	5 bar	- Optical Properties	Transparent
Air-Particle Mixture Inlet Conditions:		- Shape	Flat
- Mass Loading	0.5 g/s	- Diameter	1.6 m
- Particle Diameter	200 nm	Walls:	
- Temperature	700 K	- Radiative Properties	Aluminum Oxide (Al ₂ O ₃)

Table 17 – Design parameters and operating conditions of the receiver (study to elucidate the best fluid flow direction with respect to the concentrated solar irradiation.)

The case of no oxidation, which physically corresponds to a receiver operated with a nitrogen-particle mixture, was simulated as well. The design parameters and operating conditions of the receiver employed, which were chosen to reproduce the actual design as close as the model allows, are summarized in Table 17.

Table 18 collects the average outlet temperature and the average outlet mass loading obtained for the eight simulations performed. For further details, Figure 26 shows the average temperature as a function of the axial position for the cocurrent (circles) and countercurrent (squares) flow directions employing the three oxidation models previously mentioned. The results without oxidation model are shown as well. The average mass loading as a function of the axial position is plotted in Figure 27.

	Temperature (K)	Mass Loading (g/m ³)
No Oxidation		
- Cocurrent	1481.12	0.5
- Countercurrent	1408.30	0.5
Nagle Model		
- Cocurrent	1309.19	$8.13 \cdot 10^{-3}$
- Countercurrent	1293.86	$4.44 \cdot 10^{-3}$
Kinetic Theory Model		
- Cocurrent	1241.93	0.00
- Countercurrent	1173.33	$1.47 \cdot 10^{-3}$
Bechtel Model		
- Cocurrent	1224.17	0.00
- Countercurrent	1122.76	$8.29 \cdot 10^{-4}$

Table 18 – Average temperature and mass loading on the outlet surface (study to elucidate the best fluid flow direction with respect to the concentrated solar irradiation.)

The Nagle and Strickland-Constable model predicts the slower oxidation rate, followed by the Kinetic Theory and the Bechtel model respectively, which is consistent with [83]. Two main conclusions can be inferred from these results:

1. The cocurrent direction of the flow provides higher thermal efficiency than the countercurrent one for the three oxidation models implemented. The same result was observed with no oxidation, which indicates that the geometry of the solar receiver (the only variable modified in this case with respect to [19]) has an influence in the best direction of the flow. Hence, the Small Particle Solar Receiver would show better performance with the cocurrent flow direction regardless of whether it is operated by air (oxidation) or nitrogen (no oxidation), at least for the baseline design employed here.
2. The kinetic theory and the Bechtel model predict lower outlet mass loading with the cocurrent flow direction than with the countercurrent one, while the Nagel model shows the opposite trend. Anyway, the particles are essentially oxidized prior to exiting the

solar receiver for either flow direction³¹. This implies that the outlet air is fully ready to drive a gas turbine (high temperature, no particles).

Note that the greater efficiency of the cocurrent flow direction is expected when particle oxidation is included in the model since: (1) The outlet temperature (and thereby the thermal efficiency) is essentially limited by the temperature at which the particles fully oxidize³²; (2) the more abrupt the temperature increases, the higher the temperature the carbon particles reach before completely oxidizing (see Proof 1); and (3) the rate of heating is higher with the cocurrent flow direction (see Figure 28) as the particles experience the highest irradiation level when entering the receiver.

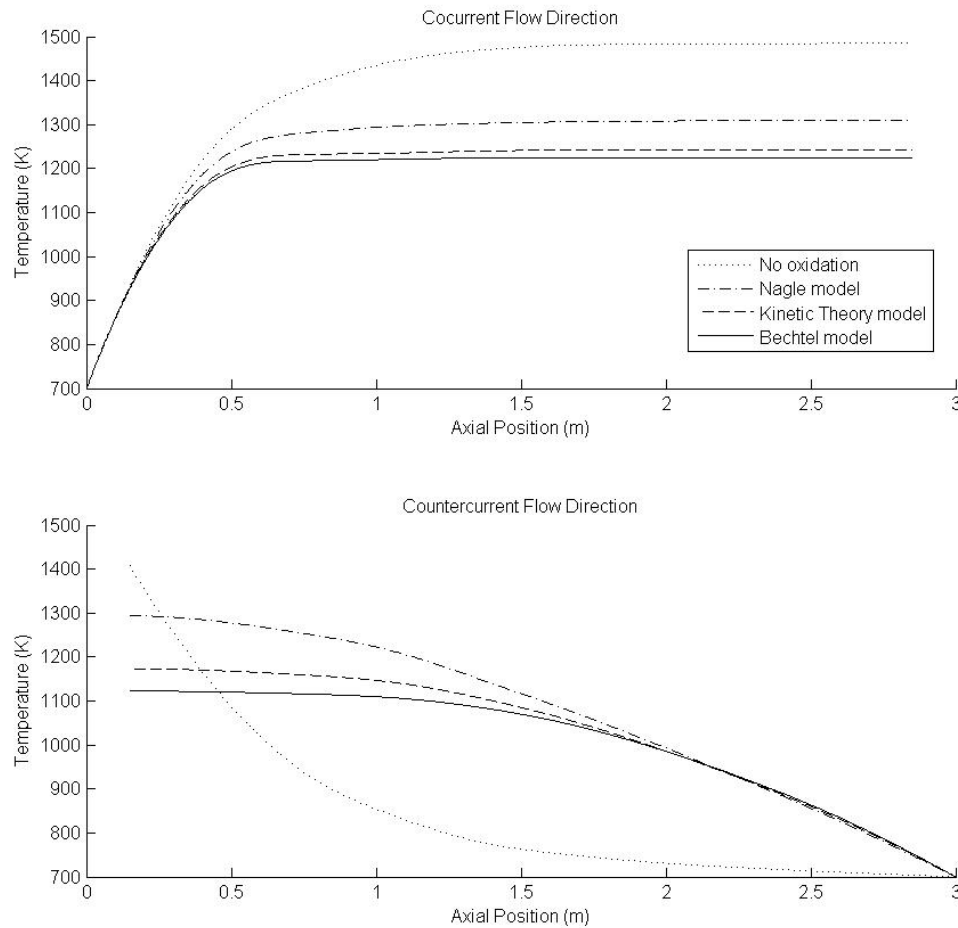


Figure 26 – Average temperature as a function of the axial position for the cocurrent (top) and countercurrent (bottom) flow directions.

³¹ First, the coarse Monte Carlo mesh (especially important in the radial direction) and the simple slug flow assumed diminish the oxidation rate. Second, the oxidation models fail with very small particles, when the exponential behavior is no longer valid. Third, even if the models were right, the particles on the outlet would be of 32 nm at 1170 K in the worst case (kinetic theory, countercurrent) and would oxidize completely prior to entering the turbine of the engine.

³² Volumetric absorption is the main mechanism to absorb solar irradiation.

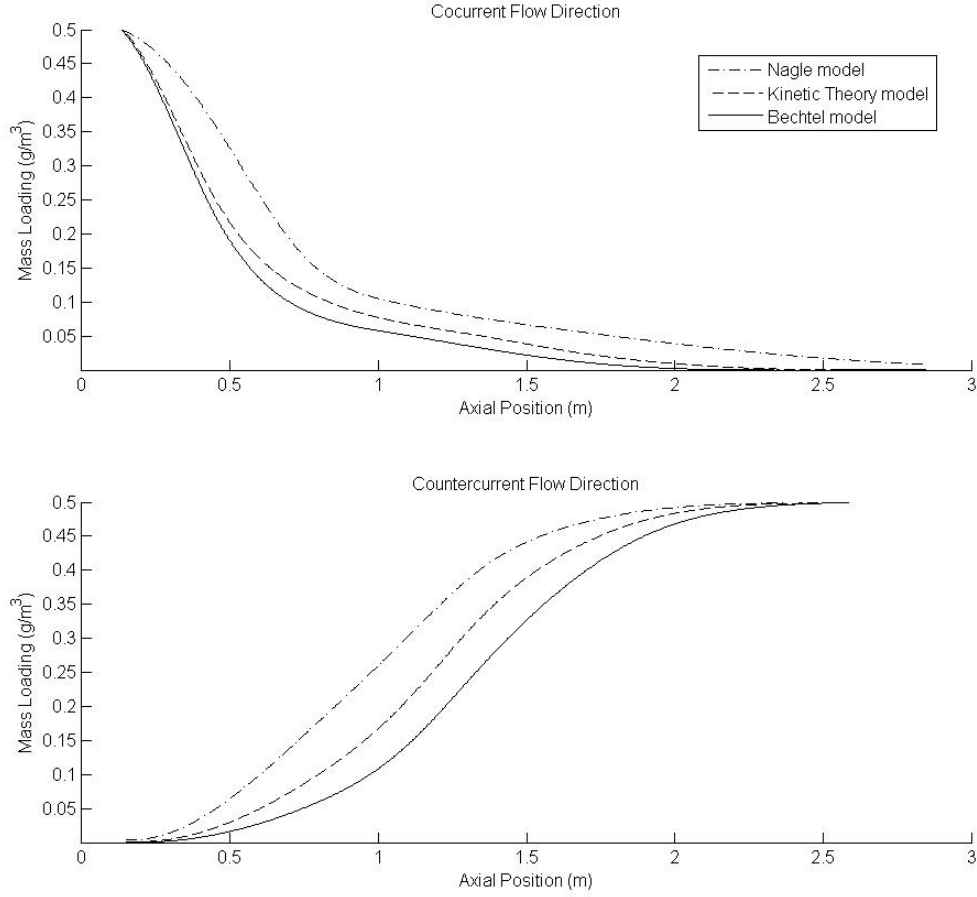


Figure 27 – Average mass loading as a function of the axial position for the cocurrent (top) and countercurrent (bottom) flow directions.

Proof 1

We will compute the sign of dT_{ox}/da for the heating rate $T = T_0 + at$, where T_{ox} is the temperature at which the particles oxidize, which is supposed to happen when the mass of the carbon particles m is smaller than a critical mass m_{cr} :

$$m_0 - m_{cr} = \int_0^{t_{ox}} \dot{m}''(t)A(t)dt = \int_{T_0}^{T_{ox}} \dot{m}''(T)A(T) \frac{dT}{a} = \int_{T_0}^{T_{ox}} \dot{m}''(T) \frac{3m^{2/3}(T)m_0^{1/3}}{N\rho_p R_0} \frac{dT}{a}$$

Where $R(t) = R_0 \left(\frac{m(t)}{m_0}\right)^{1/3}$, $A = \frac{3m}{N\rho_p R} = \frac{3m^{2/3}m_0^{1/3}}{N\rho_p R_0}$ and $\dot{m}$ are the radius, the surface area and the oxidation rate per surface area of the carbon particles, respectively. Employing the Leibniz integral rule:

$$\frac{dT_{ox}}{da} = -\frac{a}{\dot{m}''(T_{ox})m^{2/3}(T_{ox})} \int_{T_0}^{T_{ox}(a)} \dot{m}''(T) \frac{\partial}{\partial a} \left(\frac{m^{2/3}(T)}{a} \right) dT > 0, \text{ where } \frac{\partial}{\partial a} \left(\frac{m^{2/3}(T)}{a} \right) = -\frac{m^{2/3}(T)}{a^2} + \frac{2}{3am^{1/3}(T)} \frac{\partial m(T)}{\partial a}$$

Since $a, \dot{m}''(T), m(T) > 0$ and $\frac{\partial m(T)}{\partial a} = \frac{\partial}{\partial a} \left(m_0 - \int_0^T \dot{m}''(T)A(T) \frac{dT}{a} \right) = \frac{1}{a^2} \int_0^T \dot{m}''(T)A(T) dT > 0$, we can conclude that $\frac{dT_{ox}}{da} > 0$. Therefore, the higher the heating rate is, the higher the temperature the carbon particles reach before oxidizing completely.

While this proof was given for a constant heating rate, $dT/dt = a$, it can be readily extended to non-constant heating rates since they are actually an infinite succession of constant heating rates of infinitesimal duration and with different values of a .

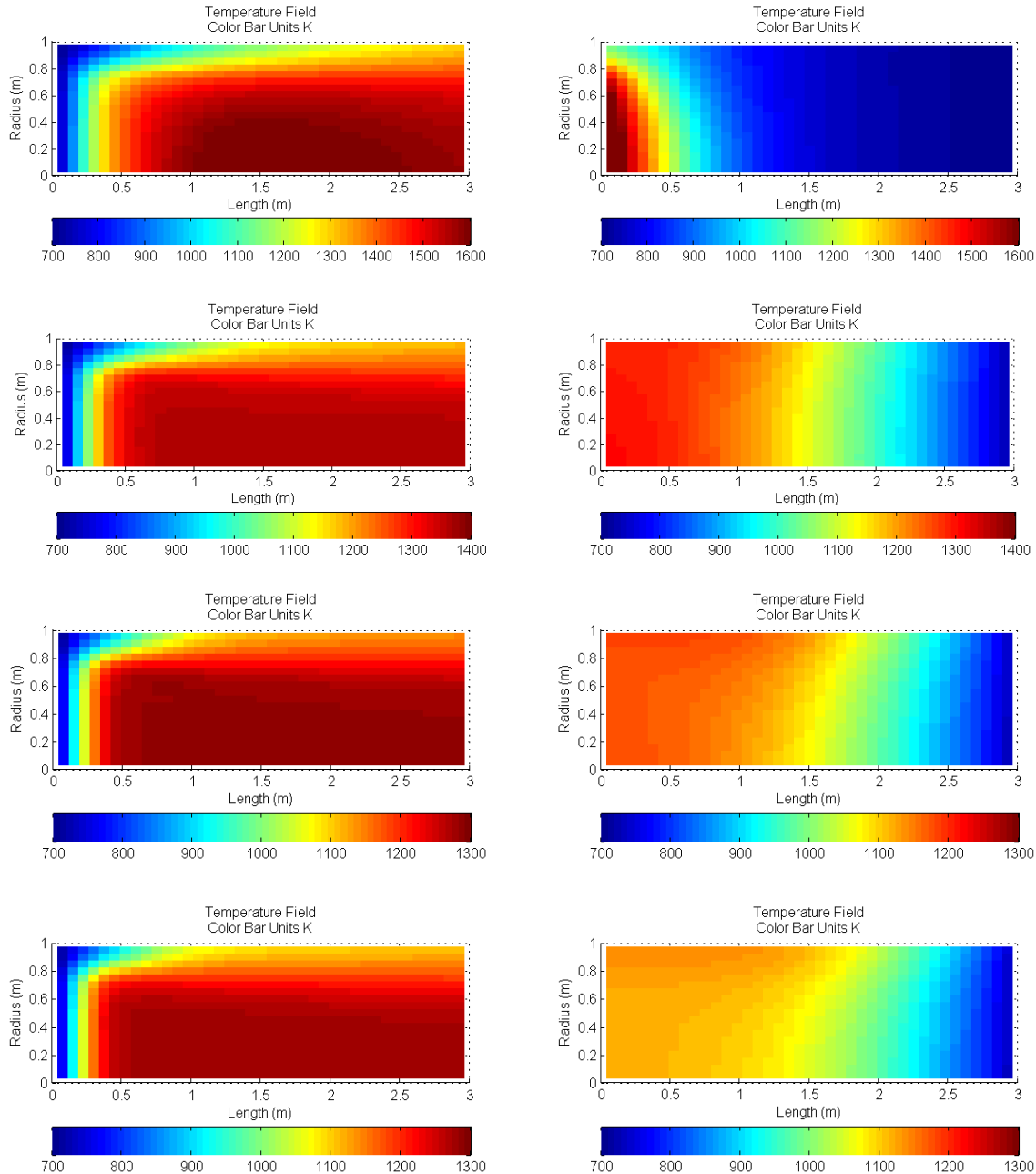


Figure 28 – Temperature field for cocurrent (left column) and countercurrent (right column) flow directions. Each row corresponds to a different oxidation model: (1) No oxidation, (2) Nagel model, (3) Kinetic Theory model, and (4) Bechtel model. The solar irradiation travels always from left to right. Note that the color scale is the same for each oxidation model but can vary between them.

It should also be noted that the lack of a window in the radiative heat transfer calculation in this two-dimensional model (modeled as a simple transparent aperture) penalizes the designs whose fraction of losses due to emission from inside of the receiver (long wavelength $\rightarrow$ small transmissivity) is large compared to the losses due to backward scattering of solar irradiation (short wavelength $\rightarrow$ large transmissivity). This ratio will be probably higher for the countercurrent flow direction and the simulation results could be

biased in favor of the cocurrent direction. In addition, one cannot neglect the fact that it is much more difficult to inject the air-particle mixture and obtain a homogeneous fluid flow when the inlet is located in the window side. Nonetheless, these results are only valid for an inlet particle size of 200 nm. For a robust decision, a wider variety of particles sizes should be simulated (larger inlet particles are expected to benefit the cocurrent flow direction; while smaller particles should help the countercurrent one [19]).

Finally, Figure 28 shows the temperature field for both cocurrent and countercurrent flow directions with (1) no oxidation, (2) the Nagel model, (3) the Kinetic Theory model, and (4) the Bechtel model.

Despite the previous results, the countercurrent flow direction was chosen for the baseline case of the design space exploration for two main reasons:

1. Consistency with previous results [19,20].
2. The difficulty of injecting the air-particle mixture and obtain a homogeneous fluid flow when the inlet is located on the window side, which may compromise the superiority of the cocurrent flow direction.

Nevertheless, further analysis of the cocurrent direction of the flow and how to inject the air-particle mixture in such a case is a pending task to be addressed in the future.

7.2.2. Radiative Properties of the Walls

The infinite degrees of freedom necessary to describe the spectral dependence of the radiative properties of the walls can be essentially reduced to four types of properties, denoted by S1, S2, S3 and S4:

- S1: High absorptivity in the solar spectrum and low emissivity at longer, infrared wavelengths (e.g. selective coatings of solar collectors.)
- S2: High absorptivity and emissivity in the whole spectrum (blackbody).
- S3: Low absorptivity in the solar spectrum and high emissivity at infrared wavelengths (e.g. Al_2O_3).
- S4: Low absorptivity and emissivity in the whole spectrum (reflective walls).

A schematic representation of the spectral absorptivity of these four types of radiative properties is shown in Figure 29. The directional behavior is assumed diffuse in all cases.

Table 19 shows a summary of the simulation results with the radiative properties S2, S3 and S4. The surface S1 is not simulated as it would lead to (unacceptable) wall temperatures over the blackbody case (S2). From Table 19 we can infer that the radiative properties S3 (Al_2O_3) show the best compromise between thermal efficiency and wall temperature. Note

that the high temperature of the exterior wall is due to the reduced diameter and simple, right-cylindrical geometry of the receiver utilized in the baseline design. Optimized geometries will dramatically reduce the wall temperature and increase the thermal efficiency of the receiver, as will be discussed later. Finally, as expected, pressure drop is essentially insensitive to the radiative properties of the walls.

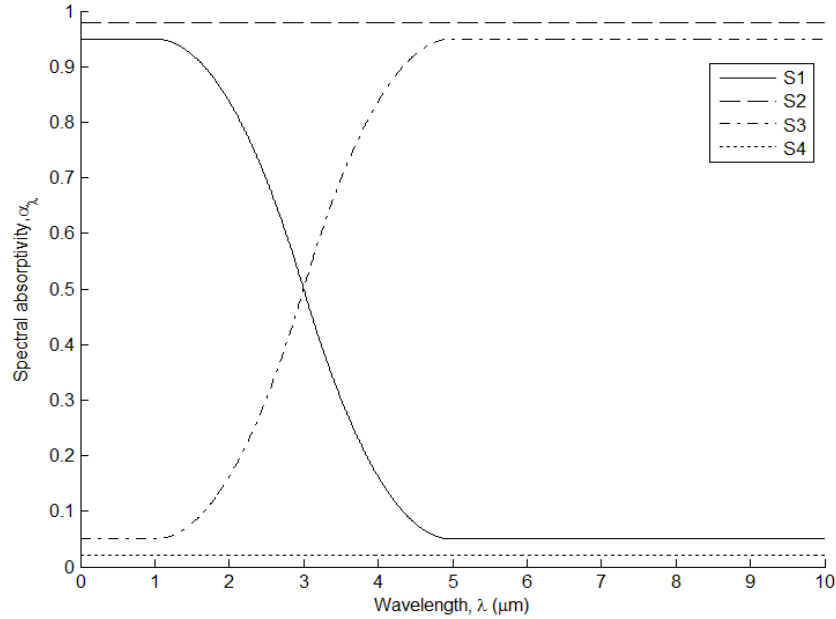


Figure 29 – Schematic representation of the spectral absorptivity of the four types of surface radiative properties considered. Note that, under local thermodynamic equilibrium, the spectral emissivity equals the spectral absorptivity in diffuse surfaces.

	S2	S3	S4
Radiative properties employed to simulate this case	$\alpha_\lambda = 1$	Al ₂ O ₃ (see Figure 12)	$\alpha_\lambda = 0.1$
Thermal efficiency	77.46%	79.63%	80.46%
Outlet temperature	1414.5 K	1433.3 K	1440.4 K
Maximum temperature:			
- Exterior wall	~ 1725 K	~ 1600 K	~ 1750 K
- Outlet tube	~ 1600 K	~ 1450 K	~ 1500 K
Pressure drop	163.6 Pa	165.0 Pa	165.5 Pa

Table 19 – Summary of simulation results with the different types of surface radiative properties considered.

7.2.3. Window Geometry

A curved window is required to withstand the mechanical loading due to the pressurized environment inside the receiver (around 5 bar in the 5 MW_{th} Small Particle Solar Receiver considered here and greater when eventually introducing the receiver in the high-pressure side of a gas turbine engine.) The material selected for the window is fused quartz (or fused silica) due to its selective optical behavior (high transmissivity in the solar spectrum and low

transmissivity at infrared wavelengths) and very high compressive strength (around 1100 MPa). Hence, a fused quartz window will perform well as long as only small tensile stresses are allowed to develop (thereby the curved geometry.) Moreover, its extremely low coefficient of thermal expansion accounts for its remarkable ability to undergo large, rapid temperature changes (e.g. during cloudy transient periods³³) without cracking.

Regarding its shape, spherical-cap and ellipsoidal windows are considered and compared (the latter is simply a prolate spheroid with ratio between principal axes $r = \sqrt{2}$.) As for mechanical considerations, the ellipsoidal geometry would eliminate tensile stresses and the window would be entirely in compression. Moreover, it may be preferable from a seal design perspective. However, spherical windows are much easier to fabricate and polish than ellipsoidal shapes as they are a portion of a sphere. With a spherical cap window, the amount of required material to avoid buckling of the window is minimized for a 60° cap angle [88]. Nevertheless, tensile stresses are not minimized for this shape and near the sealing edge the glass is under tension. It may be possible to reduce these stresses by a proper seal design that flexes in response to the window being under internal pressure.

Previous studies conducted by Mecit [21] showed that the optical efficiency of spherical-cap windows has a global minimum at 45° cap angle and then increases in both directions (towards 0° and towards 90°). The optical efficiency of the ellipsoidal window equals the one of a 70° cap angle window. However, these results only account for the transmittance of concentrated solar irradiation from the heliostat field to the inside of the receiver; while the transmission of radiation from the inside to the outside of the receiver constitutes the main loss mechanism (see Section 7.1) and needs to be considered as well. Thus, the optimum window geometry would be a compromise between both effects; not to mention that the efficiency is only one of the many aspects to be considered in this multidisciplinary decision-making process.

As stated previously, the ellipsoidal window ($r = \sqrt{2}$) and the 45° spherical-cap window have been compared in the design space exploration presented in this *Proyecto Fin de Carrera*. A summary of the simulation results with both window geometries is shown in Table 20. The optical efficiency is, as expected [21], greater with the ellipsoidal window, but the overall efficiency is higher with the 45° spherical-cap geometry. This result is mainly because the ellipsoidal window penetrates deeper into the solar receiver than the 45° spherical-cap window and the radiative losses are thereby higher. The maximum wall temperature and outlet tube temperature are insensitive to the window geometry (note, again, that such high temperatures are due to the reduced diameter and simple, right-cylindrical geometry of the receiver employed in the baseline design case.) Finally, the pressure drop is

³³ Note, however, that the heliostat field would be gradually covered by a transient cloud and the temperature gradient with respect to time would be considerably reduced.

kept constant as the position of the outlet tube was chosen in both cases to maintain a distance to the window of 0.5 m.

	45° Spherical-Cap Window	Ellipsoidal Window
Efficiency of the receiver:		
- Optical	92.14%	93.08%
- Thermal	79.63%	76.03%
- Total	73.37%	70.77%
Maximum temperature:		
- Exterior wall	~ 1600 K	~ 1600 K
- Outlet tube	~ 1450 K	~ 1450 K
Radiation absorbed in the window:		
- From the heliostat field	273.1 kW	294.7 kW
- From the solar receiver	33.0 kW	33.2 kW
- From the solar receiver	240.1 kW	261.5 kW
Pressure drop	165.0 Pa	165.6 Pa

Table 20 – Summary of simulation results with the ellipsoidal window and with the 45° spherical-cap window.

From Table 20, the total radiation absorbed by the ellipsoidal window is 8% greater than with the 45° spherical-cap window. However, the absorption per unit area is smaller with the ellipsoidal window (see Figure 30) due to its higher surface. Note, finally, that the optimum window geometry should be a compromise between efficiency, mechanical behavior, manufacturing issues and economic aspects. Hence, the 45° spherical-cap window is preferred over the ellipsoidal window as it provides higher efficiency, is more inexpensive and easier to manufacture.

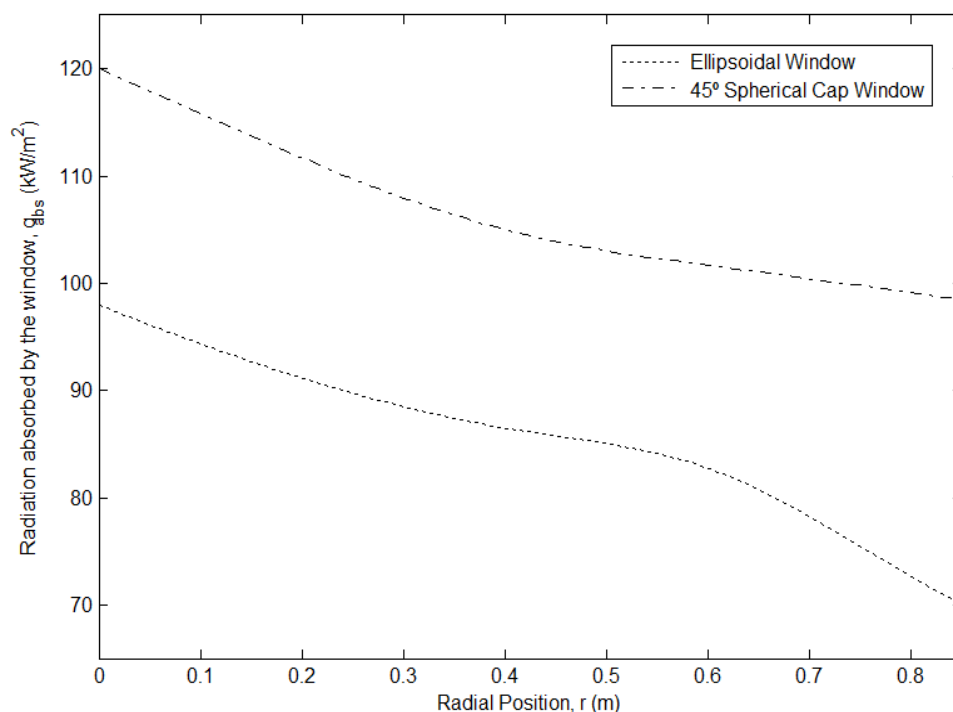


Figure 30 – Radiation absorbed by the 45° spherical-cap window and by the ellipsoidal window as a function of the radial position (the azimuthal dependence is averaged).

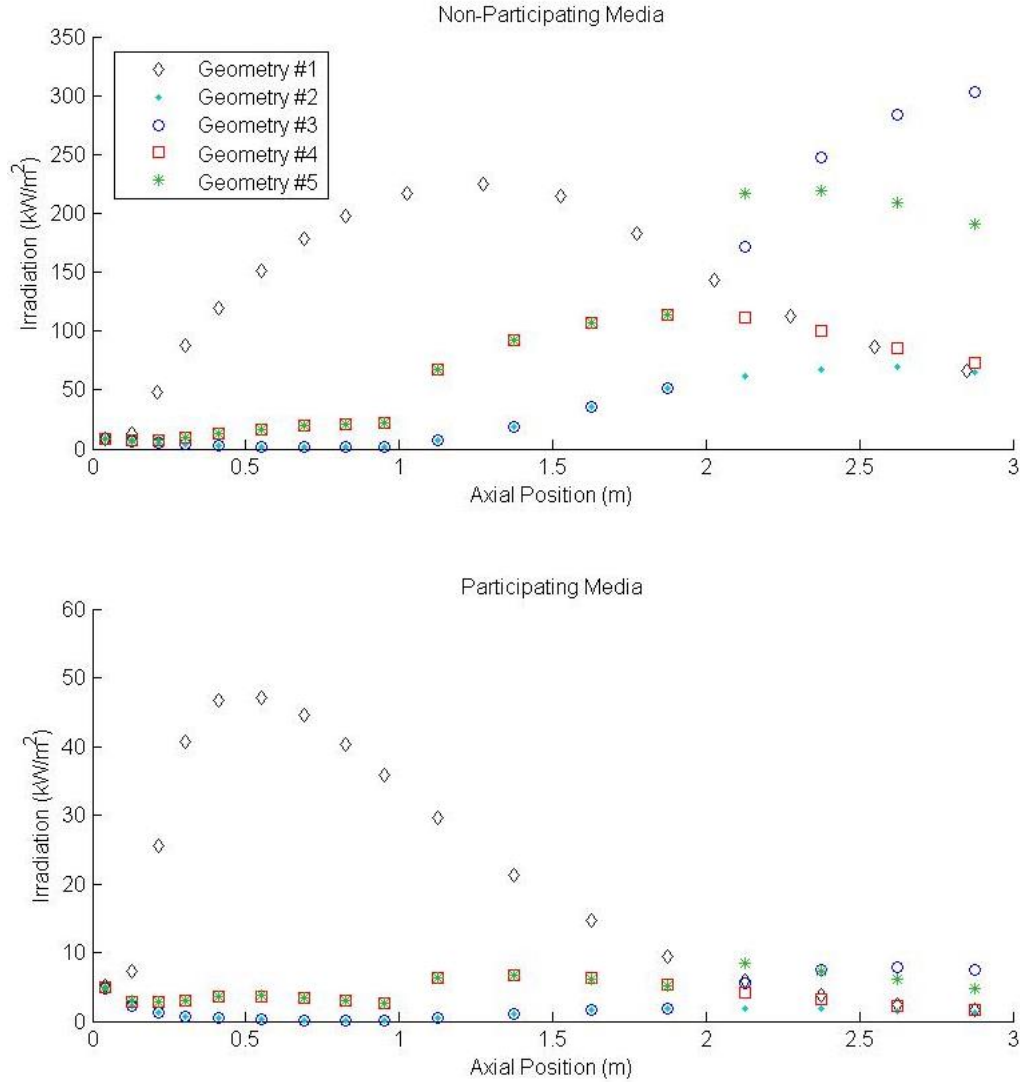


Figure 31 – Solar irradiation on the exterior wall as a function of the axial position for a non-participating media (air, top figure) and a participating media (bottom, air-particle mixture with $\phi = 0.5 \text{ g/m}^3$ and $a = 100 \text{ nm}$.) Note the different scale of solar irradiation between both figures.

7.2.4. Receiver Geometry

To simplify the analysis, only the angle between the front wall and the initial part of the exterior wall –or, equivalently, between the rear wall and the end of the exterior wall– is varied (see Figure 32 for greater clarity.) The length and the front diameter of the receiver are kept constant (3 m and 2 m, respectively) in all the designs. This way, the continuous function to describe the generatrix of the solar receiver (infinite degrees of freedom) is reduced to only one variable (one degree of freedom). Thus, the two geometries illustrated in Figure 32 were simulated, which correspond with the cases of 0° and 45° . The choice of these designs is based on preliminary studies of the distribution of solar irradiation on the walls for different receiver geometries. In particular, the five geometries described below, whose results are collected in Figure 31, were analyzed:

- Geometry #1: Same geometry as *Design 1* (see Figure 32).
- Geometry #2: Same geometry as Geometry #3 but without the rear “chamfer” (the front “chamfer” still exists.)
- Geometry #3: Same geometry as *Design 2* but with an angle of 26.6° (instead of 45°) between the front wall and the initial part of the exterior wall, as well as between the rear wall and the end of the exterior wall.
- Geometry #4: Same geometry as Geometry #5 but without the rear “chamfer” (the front “chamfer” still exists.)
- Geometry #5: Same geometry as *Design 2* (see Figure 32).

The front diameter of the receiver is 2 m in the five geometries analyzed, i.e. regardless the existence of the “chamfers” and their angles.

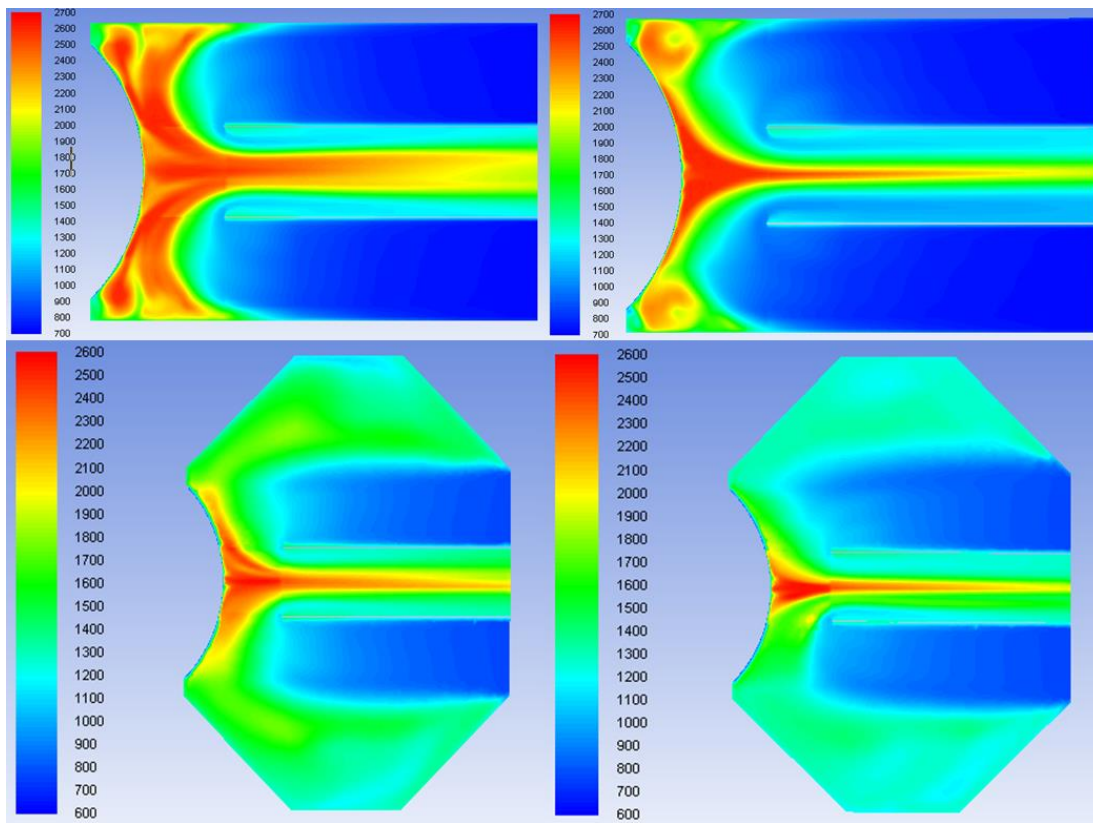


Figure 32 – Temperature field (K) in longitudinal section on the left and vertical section on the right of the solar receiver. The first row corresponds with the *Design 1* (0°) and the second row with the *Design 2* (45°). The color scale varies between both designs. Note also that both designs are not to the same scale for an easier visualization of the temperature field. In reality, both designs are the same length (3 m).

The main simulation outputs for the two geometries analyzed are collected in Table 21, while Figure 32 shows the temperature field inside the receiver. The so-called *Design 2* (45°) maximizes the thermal efficiency and minimizes the temperature of the exterior wall, which is now acceptable unlike in previous sections (recall it was because *Design 1* was chosen for the baseline case.) Note also that the outlet tube temperature can be easily

reduced just by distancing it from the window; although this would also affect the thermal efficiency and the window temperature.

The extremely high temperature in some regions of the receiver (see Figure 32) is due to the lack of particle oxidation in the current model. In reality, these high temperature zones cannot exist as particles would immediately oxidize and no absorption would occur. This, in turn, would increase the thermal efficiency of the receiver since the radiative losses due to emission from the air-particle mixture (the main losses mechanism in all the designs analyzed in the design optimization) would dramatically diminish. Actually, the outlet temperature of the Small Particle Solar Receiver will most likely be limited by the temperature at which the particles fully oxidize; although the efficiency can be raised by increasing the mass flow rate even if premature oxidation occurs. Note, however, that this strategy would reduce the solar share since the natural gas consumption would increase due to both higher carbon particle requirements (to maintain the mass loading and thus the optical thickness) and a higher fuel demand in the combustor to achieve the turbine inlet temperature desired.

	Design 1 (0°)	Design 2 (45°)
Thermal efficiency	79.63%	85.47%
Outlet temperature	1433.3 K	1485.8 K
Maximum temperature:		
- Exterior wall	~ 1600 K	~ 1325 K
- Outlet tube	~ 1450 K	~ 1500 K
Pressure drop	165.0 Pa	173.3 Pa

Table 21 – Summary of simulation results with the two geometries of the solar receiver considered.

Therefore, the 45° geometry (*Design 2*) is suggested for the 5 MW_{th} Small Particle Solar Receiver to be designed and tested under the U.S. DOE's SunShot Initiative. Note, however, that this geometry has greater cross sectional area than *Design 1*, which would increase the residence time of the particles inside the receiver and could lead to premature oxidation and then limit the outlet temperature that can be reached. It is also advisable to locate the air-particle inlets in different axial positions of the exterior surface for several reasons. First, the operational flexibility (important for experimental plants) would increase since different flow patterns and strategies could be analyzed. This, in turn, would improve the robustness of the design with respect to the oxidation kinetics. And second, these inlets would avoid no-particle zones near the walls³⁴, which is necessary to keep the wall temperature below material limits. A disadvantage of this multiple-inlet design is that the small holes required would increase the pressure drop through the receiver. Hence, they should be designed to

³⁴ If no action was taken in *Design 2*, a no-particle zone would appear near the exterior wall due to particle oxidation and the lack of convective transport to replace the oxidized particles.

ensure that the pressure drop remains low and the thermodynamic efficiency of the power block is not significantly reduced.

Chapter 8

Conclusions

A three-dimensional, coupled software to numerically simulate the fluid flow and radiative heat transfer in a Small Particle Solar Receiver has been successfully developed, programmed and validated. This solar receiver, developed under the support of the U.S. DOE's SunShot Initiative, aims to volumetrically absorb concentrated solar irradiation using an air-particle mixture to drive a gas turbine in Solar Tower Power plants at much higher temperatures than the state-of-the-art molten salt solar receivers. The steady-state Reynolds-Averaged Navier Stokes equations, together with the two equations of the SST κ - ω turbulence model and the corresponding constitutive relations, are solved numerically by the CFD package ANSYS Fluent. An in-house Monte Carlo Ray Trace (MCRT) method is employed for the radiative heat transfer due to the highly directional intensity distribution from the heliostat field and the strong spectral dependence of the radiative properties of the particles, which cannot be properly solved by conventional numerical methods such as the Spherical Harmonics or the Discrete Ordinates method.

The CFD solver and the MCRT code have been coupled together via User-Defined Functions (UDFs) and iterate alternatively until convergence. The (adaptive) solution procedure was optimized to prevent numerical oscillations and reduce the CPU time by approximately two orders of magnitude compared to the non-optimized version of the code. For that, an efficient programming of the Monte Carlo code, the application of variance reduction techniques (mainly stratified sampling) and the availability of two different MCRT methods (collision-based and pathlength-based) were of great help. The Monte Carlo method is also coupled with a heliostat field model and allows for real solar irradiation, i.e. the spatial, directional and wavelength dependence of the concentrated solar irradiation is properly modeled. Moreover, this software can simulate any axisymmetric geometry for the solar receiver, as well as flat, ellipsoidal and spherical cap windows, the latter necessary to withstand the pressurized environment inside the receiver. Both the UDFs and the MCRT method were written specifically for this *Proyecto Final de Carrera* and consist of over 12,500 lines of code. Furthermore, they can be used interchangeably for either the two-dimensional (axisymmetric) or the three-dimensional version of the CFD solver.

This software was first utilized to perform a parametric study of the operating conditions (time of the day and mass flow rate) using a preliminary design of the solar receiver. The mass flow rate that optimizes the overall (thermal of the receiver + thermodynamic of the power block) efficiency of the system was found to be between 1 and $1.5 \text{ kg}\cdot\text{s}^{-1}\cdot\text{MW}^{-1}$, depending on the solar irradiation. For such overall optimum mass flow rates, the thermal efficiency of the receiver can be kept over 89% and the outlet temperature

over 1250 K at all times from 7:30 AM to 4:00 PM. This outlet temperature is right on target to drive a gas turbine [60], which is the ultimate goal of the Small Particle Solar Receiver. Furthermore, the pressure drop is limited to 90 Pa even in the most unfavorable situation, which does not diminish the thermodynamic efficiency due to pressure drop between the compressor and the turbine (the expansion ratio through the turbine is essentially the same.) Radiative losses were proven to dominate over convective losses. In particular, emission from the window, emission from the air-particle mixture, back-scattered solar irradiation and emission from the inner part of the exterior wall (see Figure 2) are, in this order, the main loss mechanisms in the design employed for this parametric study. Nevertheless, the temperature of the window was imposed via boundary condition (1000 K in these parametric study), but in reality it will be lower [65] and the radiative losses due to emission from the window will be considerably reduced.

A multidisciplinary design optimization of a 5 MW_{th} Small Particle Solar Receiver, to be designed and tested under the U.S. DOE's SunShot Initiative, was conducted later. The design space was explored through parametric studies and consisted of the geometry of both window and receiver, the optical (radiative) properties of the walls and the direction of the fluid flow with respect to the incoming solar irradiation. The cocurrent flow direction showed higher thermal efficiency than the countercurrent one both with and without particle oxidation, i.e., regardless of whether the receiver is actually operated by air (oxidation) or nitrogen (no oxidation). A mathematical proof of this result for air-driven receivers was provided as well. Furthermore, the temperature levels and residence time ensure that the particles are completely oxidized when they exit the solar receiver for either flow direction and for any of the three oxidation kinetics employed. The aluminum oxide (Al₂O₃) walls, which would also serve as insulation, showed the best compromise between wall temperature and thermal efficiency compared to the other three main types of radiative properties that can be employed. As for the window geometry, the receiver efficiency is higher with a 45° spherical-cap window than with an ellipsoidal window; while the wall temperature and pressure drop are virtually insensitive to its shape. In addition, the 45° spherical-cap window is much more inexpensive and easier to manufacture. Finally, the geometry of the receiver labeled as *Design 2* was the best geometry analyzed as it maximizes the thermal efficiency and minimizes the wall temperature.

Although interactions between design variables are not properly captured by parameter studies, it is thought that they are small in our design space and the conclusions inferred for each variable have general validity. At any rate, using Al₂O₃ walls, the so-called *Design 2* and the 45° spherical-cap window, the maximum wall temperature can be kept below 1350 K and the thermal efficiency over 85% (for the operating conditions used in this parametric study) even with the countercurrent flow direction. It is possible, however, to raise the efficiency at the expense of the solar share by increasing the mass flow rate [84]. Using a further optimized geometry and the cocurrent flow direction, it is thought that the thermal

efficiency of the receiver can be increased to over 90%. This, in turn, would lead to a greater overall efficiency of the CSP plant than the state-of-the-art Rankine cycles employed in current commercial plants, due to the considerably higher thermodynamic efficiency of the higher-temperature gas turbine engine [85]. Finally, several ideas and considerations to further improve the design were presented and discussed as well. For example, it is advisable to locate the air-particle inlets in different axial positions of the exterior surface for several reasons, such as increasing the operational flexibility, improving the robustness of the design with respect to the oxidation kinetics, or avoiding no-particle zones near the walls (necessary to keep the wall temperature below material limits.)

Chapter 9

Future Work

Although a number of difficulties have been overcome and many results have been obtained in this work, the following lines of research and improvements to the current model are proposed.

9.1. Parallelization of the MCRT method via GPU Computing

A huge effort was made to speed up the Monte Carlo Ray Tracing code (variance reduction, efficient programming) so that it is currently optimized for single CPU execution. In fact, the CPU time to perform one MCRT iteration is over fifty times lower than the one required for the two-dimensional version of the model [19], even though one could expect the three-dimensional MCRT to be around fifteen times more CPU demanding. Nevertheless, the Monte Carlo method still takes over 50% of the total CPU time and its parallelization would considerably speed up the computation. An alternative view is that a finer MCRT mesh could be used to improve the accuracy of the radiative heat transfer modeling. Moreover, after the parallelization of the Monte Carlo code, the parallel solver of ANSYS Fluent could be used to further reduce the computational time.

By its own nature, Monte Carlo methods are highly parallelizable and have a high speed-up ratio, as defined by Amdahl's law:

$$S = \frac{1}{(1 - P) + \frac{P}{N}} \approx N \quad (9-1)$$

Where S is the expected speedup, P is the portion of code susceptible to parallelization (measured as the fraction of CPU time before the parallelization) and N is the number of parallel threads. The value of P in Monte Carlo simulations is close to unity and the expected speedup is thereby close to N . In reality, the speedup of most parallel applications is worse than what is predicted by the Amdahl's law due to the parallel overhead.

In order to facilitate its eventual parallelization, the Monte Carlo Ray Tracing code was structured in different subroutines so that the parallel code (essentially) only requires introducing proper distribution and synchronization instructions. Perhaps the simplest way to parallelize the code would be to trace all the rays emitted from a particular Monte Carlo cell in the same thread, which would also easily avoid load imbalance between processors if a proper processor scheduling is used.

9.2. Couple the oxidation code to the whole model

Once the oxidation model, which is currently being developed by Trent Martin –a graduate student in our group–, is ready to be used, it should be coupled to the software presented in this *Proyecto Fin de Carrera*. Once again, the MCRT code and the User-Defined Functions were programmed to facilitate this eventual coupling. Note also that a new, more complex iterative solution procedure will be required when coupling the oxidation code, as the variation of the optical properties of the air-particle mixture (due to oxidation) between MCRT iterations will increase the amplitude of the numerical oscillations. As with the MCRT method, computing only a partially converged solution between CFD iterations and under-relaxing it will most likely be the best strategy.

9.3. Couple the thermal window model to the whole software

A numerical model to calculate conduction, convection and radiation heat transfer in the window of the receiver is currently being developed by Alex Whitmore, another graduate student in our group. After developing and validating the window model, it could be coupled to the software presented in this *Proyecto Fin de Carrera* to impose the thermal boundary condition on the window via User-Defined Function. The total convection heat transfer through the inner surface of the window would need to be computed via UDF as well, as it constitutes a boundary condition of the thermal window model. As for the iterative procedure, employing a partially converged solution for the temperature field of the window when the window model is executed and under-relaxing it would probably optimize the rate of convergence. Furthermore, the window model could be executed only every fifty or one hundred iterations of the CFD solver due to the relatively slight sensitivity of the receiver solution to the window temperature field.

9.4. Employ Large Eddy Simulation (LES) for turbulence modeling

While the thermal efficiency of the Small Particle Solar Receiver is virtually independent of the fluid flow features themselves, higher fidelity in the flow solution would improve the accuracy of the wall temperature prediction, which in turn would also modify the thermal efficiency. In this regard, Large Eddy Simulation (LES) would provide a more realistic turbulence modeling and thereby a better wall temperature estimate. On account of the extremely high CPU time required to perform a LES+MCRT simulation, Large Eddy Simulation has not been employed up to now. However, it would be an interesting improvement to the model, especially to evaluate the differences in the numerical solution using SST κ - ω and LES and to determine up to what extent the more CPU-efficient SST κ - ω turbulence model worsens the numerical results.

9.5. Further Design Optimization

Once the oxidation code is ready and coupled to the whole model, a one-at-a-time optimization technique is proposed to conduct further design optimization. Post-optimality analysis (sensitivity analysis, uncertainty quantification) are also suggested to quantify the uncertainties of the model and test the robustness of the design respect to the oxidation kinetics, optical properties of the window, inlet air-particle mixture conditions (particle size and mass loading) and peaks of concentrated solar irradiation.

Finally, since the solar irradiation that reaches the window from the heliostat field is not (directionally) axisymmetric³⁵, an elliptical geometry for the solar receiver (with the largest principal axis in the horizontal direction) might reduce the wall temperature and increase the thermal efficiency. For that, the MCRT code and UDFs would need to be modified to accommodate such a non-axisymmetry. Note, however, that an elliptical geometry would increase the manufacturing costs of the receiver, which is an important factor when performing system optimization from a multidisciplinary approach.

9.6. Thermal Stratification

Buoyancy forces within the solar receiver dominate the fluid motion over pressure gradients in the radial and azimuthal directions. This implies that, if no action was taken, a strong thermal stratification in the receiver would occur, as has been demonstrated numerically. In order to solve this issue, it is proposed to inject the air-particle mixture into the solar receiver with a swirl component. Thus, the inertial forces –which wouldn't be negligible anymore– would dominate the fluid motion and would mix the fluid flow. The pressure drop would increase due to the higher shear stress on the walls; although it would be still small and wouldn't reduce the thermodynamic efficiency of the gas turbine due to pressure drop between the compressor and the turbine. Therefore, different inlet flow swirl levels and injection locations should be analyzed to study of how to prevent thermal stratification within the solar receiver.

9.7. High Temperature Anti-Reflective Coatings

The transmissivity of unpolarized light traveling from air to glass is given by Equations 9-2, while the reflectivity is simply $\rho = 1 - \tau$.

³⁵ The heliostat field of the National Solar Thermal Test Facility (where the 5 MW_{th} Small Particle Solar Receiver will be located) spans 90° laterally and only 29° vertically when viewed from the top of the tower.

$$\begin{aligned}
\tau &= \frac{1}{2}(\tau_p + \tau_s) \\
\tau_p &= 1 - \frac{(p - n_1 \sin \theta_1 \tan \theta_1)^2 + q^2}{(p + n_1 \sin \theta_1 \tan \theta_1)^2 + q^2} (1 - \tau_s) \quad \tau_s = 1 - \frac{(n_1 \cos \theta_1 - p)^2 + q^2}{(n_1 \cos \theta_1 + p)^2 + q^2} \\
p^2 &= \frac{1}{2} \left[\sqrt{(n_2^2 - k_2^2 - n_1^2 \sin^2 \theta_1)^2 + 4n_2^2 k_2^2} + (n_2^2 - k_2^2 - n_1^2 \sin^2 \theta_1) \right] \\
q^2 &= \frac{1}{2} \left[\sqrt{(n_2^2 - k_2^2 - n_1^2 \sin^2 \theta_1)^2 + 4n_2^2 k_2^2} - (n_2^2 - k_2^2 - n_1^2 \sin^2 \theta_1) \right]
\end{aligned} \tag{9-2}$$

Since there are two interfaces between glass and air and radiation can be reflected back and forth within the glass an infinite number of times; the total transmissivity, reflectivity and absorptivity of the window (assuming k_2 is small enough so that Equations 9-2 reduce to Fresnel equations. The conditions under which this hypothesis is acceptable are presented in [21]) is the sum of a geometric series, as expressed in Equations 9-3.

$$\begin{aligned}
T &= \frac{(1 - \rho)^2 e^{-k_2 d / \cos \theta_2}}{1 - \rho^2 e^{-2k_2 d / \cos \theta_2}} \\
R &= \rho \left[1 + \frac{(1 - \rho)^2 e^{-2k_2 d / \cos \theta_2}}{1 - \rho^2 e^{-2k_2 d / \cos \theta_2}} \right] \quad A = \frac{(1 - \rho)(1 - e^{-k_2 d / \cos \theta_2})}{1 - \rho e^{-k_2 d / \cos \theta_2}}
\end{aligned} \tag{9-3}$$

Based on these equations, it may seem that the transmissivity of the window only depends on the complex index of refraction of the glass (and the angle of incidence). However, two hypotheses were assumed when deriving Equations 9-3. First, interference effects were neglected (which is true when the glass thickness is much greater than the wavelength of the electromagnetic waves, as is true in regular windows.) Second, the index of refraction varies abruptly from the air to the glass. It is actually possible to take advantage of these two effects (interference and gradual variation of the refractive index) to increase the transmissivity, so that Equations 9-2 would be no longer valid. The first phenomenon is the one employed in current anti-reflective coatings and is accomplished by using thin coatings where interference occurs. The materials employed for these coatings suffer from thermal degradation and the state-of-the-art anti-reflective coatings cannot be utilized at the high temperatures present in the window of the Small Particle Solar Receiver. As for the second strategy, further details can be found, for example, in [90].

Since the majority of the losses of the solar receiver are due to reflection of incoming solar irradiation, new materials and technologies to improve the transmissivity of the window at high temperature would dramatically increase the efficiency of the receiver. Hence, it is proposed to simulate an ideal window with, say, transmissivity of 96% in the solar spectrum (a typical value for low-temperature glass coatings) in order to assess the benefits of high temperature glass coatings and determine future lines of research.

References

- [1] H. Le Treut *et al.* “IPCC Climate Change 2007: The Physical Science Basis”, Eds. S. Solomon *et al.*, pp. 93–127, Cambridge University Press, 2007.
- [2] R. A. Pielke J. “Climate predictions and observations”, *Nature Geoscience*, vol. 1, p. 206, 2008.
- [3] A. Kattenberg *et al.* “IPCC Climate Change 1995: The Science of Climate Change”, Eds. J. T. Houghton *et al.*, Ch. 6, Cambridge University Press, 1995.
- [4] U. Cubasch *et al.* “IPCC Climate Change 2001: The Scientific Basis”, Eds. J. T. Houghton *et al.*, pp. 525–581, Cambridge University Press, 2001.
- [5] G. A. Meehl *et al.* “IPCC Climate Change 2007: The Physical Science Basis”, Eds. S. Solomon *et al.*, pp. 748–845, Cambridge University Press, 2007.
- [6] D. J. Frame and D. A. Stone. “Assessment of the first consensus prediction on climate change”, *Nature Climate Change*, vol. 3, pp. 357-359, 2013.
- [7] “Climate Change: The IPCC Scientific Assessment”, Eds. J. T. Houghton, G. J. Jenkins and J. J. Ephraums, Cambridge University Press, 1990.
- [8] F. P. Bretherton, K. Bryan and J. D. Woods. “Climate Change: The IPCC Scientific Assessment”, Eds. J. T. Houghton, G. J. Jenkins and J. J. Ephraums, pp. 173–194, Cambridge University Press, 1990.
- [9] “Ivanpah Solar Electric Generating Station”, Concentrating Solar Power Projects, National Renewable Energy Laboratory (NREL), 2011.
- [10] “DOE Finalizes \$737 Million Loan Guarantee to Tonopah Solar Energy for Nevada Project”, Loan Programs Office (LPO), U.S. Department of Energy, September 2011.
- [11] Enermodal Engineering Ltd. and Marbek Resource Consultants Ltd. “Cost Reduction Study for Solar Thermal Power Plants. Final Report”, Report prepared for The World Bank, May 1999.
- [12] Greenpeace International, European Solar Thermal Electricity Association and IEA SolarPACES. “Concentrating Solar Power Outlook 09. Why Renewable Energy is Hot”, Technical Report, 2009.
- [13] International Renewable Energy Agency. “Concentrated Solar Power”, *Renewable Energy Technologies: Cost Analysis Series*, vol. 1, Issue 2, June 2012.

- [14] J. Lillan. “Extensive US project pipeline awaiting dollars and transmission”, *Solar Industry*, No. 4, 2010.
- [15] A. Hunt. “A New Solar Thermal Receiver Utilizing a Small Particle Heat Exchanger”, *14th Intersociety Energy Conversion Engineering Conference*, Boston, MA, 1979.
- [16] A. Hunt. “A New Solar Thermal Receiver Utilizing Small Particles”, *Proceedings of the International Solar Energy Society Conference*, pp. 1362-1366, Atlanta, GA, 1979.
- [17] A. J. Hunt and C. Brown. “Solar Test Results of an Advanced Direct Absorption High Temperature Gas Receiver”, *Proceedings of the 1983 Solar World Conference*, Perth, Australia, 1983.
- [18] A. Z’Graggen and A. Steinfeld. “Heat and Mass Transfer Analysis of a Suspension of Reacting Particles Subjected to Concentrated Solar Irradiation – Application to the Steam-Gasification of Carbonaceous Materials”, *International Journal of Heat and Mass Transfer*, vol. 52, pp. 385-395, 2009.
- [19] S. J. Ruther. “Radiation Heat Transfer Simulation of a Small Particle Solar Receiver using the Monte Carlo Method”, Master’s Thesis, San Diego State University, 2010.
- [20] A. Crocker. “Coupled Fluid Flow and Radiation Modeling of a Small Particle Solar Receiver”, Master’s Thesis, San Diego State University, 2012.
- [21] A. M. Mecit. “Optical Analysis and Modeling of a Window of the Small Particle Solar Receiver using the Monte Carlo Ray Trace Method”, Master’s Thesis, Department of Mechanical Engineering, San Diego State University, 2013.
- [22] A. M. Mecit and F. J. Miller. “Optical Analysis of a Window for Small Particle Solar Receiver using the Monte Carlo Ray Trace method”, *ASME 2013 7th International Conference on Energy Sustainability*, Minneapolis, MN, July 14th-19th, 2013.
- [23] F. R. Menter, M. Kuntz and R. Langtry. “Ten Years of Industrial Experience with the SST Turbulence Model”, *Turbulence, Heat and Mass Transfer 4*, pp. 625 – 632, 2003.
- [24] M. F. Modest. “Radiative Heat Transfer”, Academic Press, Second Edition, 2011.
- [25] S. Mazumder and M. F. Modest. “Turbulence-radiation interactions in nonreactive flow of combustion gases”, *Journal of Heat Transfer*, vol. 121, pp. 726-728, 1999.
- [26] S. Mazumder and M. F. Modest. “A probability density function approach to modeling turbulence-radiation interactions in nonluminous flames”, *International Journal of Heat and Mass Transfer*, vol. 42, pp. 971-991, 1999.

- [27] G. Li and M. F. Modest. “Application of composition PDF methods in the investigation of turbulence-radiation interactions”, *Journal of Quantitative Spectroscopy and Radiative Transfer*, vol. 73, pp. 461-472, 2002.
- [28] G. Li and M. F. Modest. “Importance of turbulence-radiation interactions in turbulent diffusion jet flames”, *Journal of Heat Transfer*, vol. 125, pp. 831-838, 2003.
- [29] M. F. Modest. “Multiscale modeling of turbulence, radiation and combustion interactions in turbulent flames”, *International Journal for Multiscale Computational Engineering*, vol. 5, pp. 85-106, 2005.
- [30] A. Habibi, B. Merci and D. Roekaerts. “Turbulence radiation interaction in Reynolds-averaged Navier-Stokes simulations of nonpremixed piloted turbulent laboratory-scale flames”, *Combustion and Flame*, vol. 151, pp. 303-320, October 2007.
- [31] P. J. Coelho. “Assessment of a presumed joint PDF for the simulation of turbulence-radiation interaction in turbulent reactive flows”, *Applied Thermal Engineering*, vol. 49, pp. 22-30, 2012.
- [32] V.P. Kabashnikov. “Thermal Radiation in Turbulent Flows - in the Case of Large Fluctuations of the Absorption Coefficient and the Planck Function”, *Journal of Engineering Physics and Thermophysics*, vol. 49, pp. 778–784, 1985.
- [33] C. Rumsey, B. Smith and G. Huang. “Turbulence Modeling Resource”, Report by the NASA Langley Research Center, 2013.
- [34] W. Yuen, F. J. Miller and A. J. Hunt. “Heat Transfer Characteristics of a Gas-Particle Mixture under Direct Radiant Heating”, *International Communications in Heat and Mass Transfer*, vol. 13, pp. 145-154, 1986.
- [35] L. Frederickson, K. Kitzmiller and F. Miller. “Carbon particle generation and preliminary Small Particle Heat Exchange Receiver lab scale testing”, *ASME 2013 7th International Conference on Energy Sustainability*, Minneapolis, MN, USA, 2013.
- [36] E. Cunningham. “On the velocity of steady fall of spherical particles through fluid medium”, *Proceedings of The Royal Society A*, vol. 83, pp. 347-356, 1910.
- [37] C. N. Davies. “Definite equations for the fluid resistance of spheres”, *Proceedings of the Physical Society*, vol. 57, p. 18, 1945.
- [38] J. H. Jeans. “The equations of radiative transfer of energy”, *Monthly Notices Royal Astronomical Society*, vol. 78, pp. 28-36, 1917.

- [39] V. Kourganoff. “Basic Methods in Transfer Problems”, Dover Publications, New York, 1963.
- [40] B. Davison. “Neutron Transport Theory”, Oxford University Press, London, 1958.
- [41] R. L. Murray. “Nuclear Reactor Physics”, Prentice Hall, Englewood Cliffs, NJ, 1957.
- [42] D. A. Andrienko, S. T. Surzhikov and J. S. Shang. “Spherical harmonics method applied to multi-dimensional radiation heat transfer, *Computer Physics Communications*, In Press.
- [43] S. Chandrasekhar. *Radiative Transfer*, Dover Publications, 1960.
- [44] K. D. Lathrop. “Use of discrete-ordinate methods for solution of photon transport problems”, *Nuclear Science and Engineering*, vol. 24, pp. 381-388, 1966.
- [45] B. G. Carlson and K. D. Lathrop. “Transport theory –the method of discrete ordinates”, *Computing Methods in Reactor Physics*, Eds. H. Greenspan, C. N. Kelber and D. Okrent, Gordon & Breach, New York, 1968.
- [46] W. A. Fiveland. “Three-dimensional radiative heat-transfer solutions by the discrete-ordinates method”, *Journal of Thermophysics and Heat transfer*, vol. 2, no. 4, pp.309-316, October 1988.
- [47] J. S. Truelove. “Three-dimensional radiation in absorbing-emitting-scattering media using the discrete-ordinates approximation”, *Journal of Quantitative Spectroscopy and Radiative Transfer*, vol. 39, no. 1, pp. 27-31, 1988.
- [48] E. S. Chalhoub. “Discrete-ordinates solution for radiative-transfer problems”, *Journal of Quantitative Spectroscopy and Radiative Transfer*, vol. 76, pp. 193-206, 2003.
- [49] J. A. Fleck. “The calculation of nonlinear radiation transport by a Monte Carlo method”, Technical Report UCRL-7838, Lawrence Radiation Laboratory, 1961.
- [50] J. A. Fleck. “The calculation of nonlinear radiation transport by a Monte Carlo method: Statistical physics”, *Methods in Computational Physics*, vol. 1, pp. 43-65, 1961.
- [51] J. R. Howell and M. Perlmutter. “Monte Carlo solution of thermal transfer through radiant media between gray walls”, *ASME Journal of Heat Transfer*, vol. 86, no. 1, pp. 116-122, 1964.
- [52] J. R. Howell and M. Perlmutter. “Monte Carlo solution of radiant heat transfer in a nongrey nonisothermal gas with temperature dependent properties”, *AIChE Journal*, vol. 10, no. 4, pp. 562-567, 1964.

- [53] M. Perlmutter and J. R. Howell. “Radiant transfer through a gray gas between concentric cylinders using Monte Carlo”, *ASME Journal of Heat Transfer*, vol. 86, no. 2, pp. 169-179, 1964.
- [54] J. R. Howell. “The Monte Carlo method in radiative heat transfer”, *ASME Journal of Heat Transfer*, vol. 120, no. 3, pp. 547-560, 1998.
- [55] J. T. Farmer and J. R. Howell. “Comparison of Monte Carlo Strategies for Radiative Transfer in Participating Media”, *Advances in Heat Transfer*, vol. 31, pp. 333-429, 1998.
- [56] P. Bratley, B. L. Fox and E. L. Schrage. “A Guide to Simulation”, Springer-Verlag, New York, pp. 180-213, 1983.
- [57] S. K. Park and K. W. Miller. “Random Number Generators: Good ones are hard to find”, *Communications of the ACM*, vol. 31, no. 10, pp. 1192-1201, October 1988.
- [58] G. Mie. “Beiträge zur Optik trüber Medien, speziell kolloidaler Metallösungen”, *Annalen der Physik*, vol. 330, Issue 3, pp. 377-445, 1908.
- [59] B. Leckner. “Spectral and total emissivity of water vapor and carbon dioxide”, *Combustion and Flame*, vol. 19, pp. 33-48, 1972.
- [60] K. Kitzmiller and F. J. Miller. “Thermodynamic Cycles for Small Particle Solar Receivers used in Concentrating Solar Power Plants”, *ASME Journal of Solar Engineering*, vol. 133, 031014, August 2011.
- [61] K. Kitzmiller and F. J. Miller. “Effect of Variable Guide Vanes and Natural gas Hybridization for Accommodating Fluctuations in Solar Input to a Gas Turbine”, *ASME Journal of Solar Energy Engineering*, vol. 134, 041008, November 2012.
- [62] R. Y. Rubinstein and D. P. Kroese. “Simulation and the Monte Carlo method”, Wiley, 2008.
- [63] R. L. Kruse. “Data Structures and Program Design in C++”, Prentice-Hall, p. 280, 1999.
- [64] J. Peraire. “Computational Mechanics: Linear Functional Outputs and Certificates”, ACDEL Seminar, Massachusetts Institute of Technology, April 2005.
- [65] A. M. Mecit, A. Whitmore and F. J. Miller. “Optical Analysis and Thermal Modeling of a Window for a Small Particle Solar Receiver”, *19th SolarPACES Conference*, Las Vegas, NV, USA, September 2013.
- [66] “ANSYS Fluent User’s Guide”, ANSYS, Inc., Release 14.0, November 2011.

- [67] F. R. Menter. “Zonal Two Equation κ - ω Turbulence Models for Aerodynamic Flows”, AIAA Paper 93-2906, 1993.
- [68] P. E. Farrell and J. R. Maddison. “Conservative interpolation between volume meshes by local Galerkin projection”, *Computer Methods in Applied Mechanics and Engineering*, vol. 200, pp. 89-100, 2011.
- [69] P. E. Farrell, M. D. Piggott, C. C. Pain *et al.* “Conservative interpolation between unstructured meshes via supermesh construction”, *Computer Methods in Applied Mechanics and Engineering*, vol. 198, pp. 2632-2642, 2009.
- [70] S. Menon and D. P. Schmidt. “Conservative interpolation on unstructured polyhedral meshes: An extension of the supermesh approach to cell-centered finite-volume variables”, *Computer Methods in Applied Mechanics and Engineering*, vol. 200, pp. 2797-2804, 2011.
- [71] A. Jameson. “Aerodynamic design via control theory”, *Journal of Scientific Computing*, vol. 3, no. 3, pp. 233–260, September 1988.
- [72] M. S. Campobasso, M. C. Duta and M. B. Giles. “Adjoint methods for turbomachinery design”, *ISOABE Conference*, Bangalore, Indian, September 2001.
- [73] G. Carpentieri, B. Koren and M. J. L. van Tooren. “Adjoint-based aerodynamic shape optimization on unstructured meshes”, *Journal of Computational Physics*, vol. 224, pp. 267-287, 2007.
- [74] S. Kim, J. J. Alonso and A. Jameson. “Design optimization of high-lift configurations using a viscous continuous adjoint method”, AIAA Paper 2002-0844, 40th AIAA Aerospace Sciences Meeting and Exhibit, Reno, NV, USA, January 2002.
- [75] V. V. Rozanov and A. V. Rozanov. “Generalized form of the direct and adjoint radiative transfer equation”, *Journal of Quantitative Spectroscopy and Radiative Transfer*, vol. 104, pp. 155-170, 2007.
- [76] A. Doicu and T. Trautmann. “Adjoint problem of radiative transfer for a pseudo-spherical atmosphere and general viewing geometries”, *Journal of Quantitative Spectroscopy and Radiative Transfer*, vol. 110, pp. 464-476, 2009.
- [77] K. Willcox. “Design Space Exploration”, Lectures of 16.888 Multidisciplinary Design Optimization, Massachusetts Institute of Technology, Spring 2010.
- [78] P. L. Leary and J. D. Hankins. “User’s Guide for MIRVAL – A Computer Code for Modeling the Optical Behavior of Reflecting Solar Concentrators”, Sandia National Laboratories, Livermore, CA, SAND77-8280, 1979.
- [79] K. B. Lee, M. W. Thring and J. M. Beer. “On the Rate of Combustion of Soot in a Laminar

- Soot Flame”, *Combustion and Flame*, vol. 6, pp. 137-145, 1962.
- [80] J. Nagle and R. F. Strickland-Constable. “Oxidation of Carbon between 1000-2000°C”, *Proceedings of the Fifth Carbon Conference*, vol. 1, pp. 154-164, 1962.
- [81] C. Park and J. Appleton. “Shock-Tube Measurements of Soot Oxidation Rates”, *Combustion and Flame*, vol. 20, pp. 369-379, 1973.
- [82] S. Schoenung, P. D. Laquil and R. Loyd. “Particle Suspension Heat Transfer in a Solar Central Receiver”, *Proceedings of the ASME-JSME Joint Thermal Engineering Conference*, Honolulu, Hawaii, USA, 1987.
- [83] F. J. Miller. “Experiments with a Laboratory Scale Small Particle Solar Receiver”, DLR Report, 1990.
- [84] P. Fernández, F. Miller and A. Crocker. “Three-Dimensional Fluid Dynamics and Radiative Heat Transfer Modeling of a Small Particle Solar Receiver”, *ASME 2013 7th International Conference on Energy Sustainability*, Minneapolis, MN, USA, July 2013.
- [85] P. Fernández and F. Miller. “Assessment of the Overall Efficiency of Gas Turbine-Driven CSP Plants using Small Particle Solar Receivers”, *19th SolarPACES Conference*, Las Vegas, NV, USA, September 2013.
- [86] F. M. White. “Viscous Fluid Flow”, McGraw-Hill Higher Education, Third Edition, 2006.
- [87] P. Fernández, F. Miller, M. McDowell and A. Hunt. “Design Space Exploration of a 5 MW_{th} Small Particle Solar Receiver”, *19th SolarPACES Conference*, Las Vegas, NV, USA, September 2013.
- [88] F. Miller and A. Hunt. “Developing the Small Particle Heat Exchange Receiver for a Prototype Test”, *ASME 2012 6th International Conference on Energy Sustainability*, San Diego, CA, USA, July 23-26, 2012.
- [89] R. Kitamura, L. Pilon and M. Jonasz. “Optical constants of silica glass from extreme ultraviolet to far infrared at near room temperature”, *Applied Optics*, vol. 46, no. 33, pp. 8118-8133, 2007.
- [90] L. Amsbeck, G. Hensch, M. Röger and R. Uhlig. “Development of a Broadband Antireflection Coated Transparent Silica Window for a Solar-Hybrid Microturbine System”, *15th SolarPACES Conference*, Berlin, Germany, September 2009.
- [91] J. Saà-Seoane. “Simulation and Design Optimization for Linear Wave Phenomena on Metamaterials”, Master’s Thesis, Computation for Design and Optimization, Massachusetts Institute of Technology, 2011.

Appendix A

Area of the two-dimensional cells of the Monte Carlo mesh

CONICAL CELLS

We can assume, without loss of generality, that the cell starts at $\varphi = z = 0$ and the generatrix of the cone is given by Eq. A-1.

$$r(z) = \left[R_W + \frac{R_E - R_W}{\Delta z} z \right] \quad (\text{A-1})$$

The area of the cell can be calculated as:

$$A = \int_0^{\Delta\varphi} \int_0^{\Delta z} \frac{1}{\cos \alpha} r(z) dz d\varphi = \dots = \Delta\varphi \Delta z \frac{R_E + R_W}{2} \sqrt{1 + \left(\frac{R_E - R_W}{\Delta z} \right)^2} \quad (\text{A-2})$$

Which reduces to the area of a cylinder, $A = R\Delta\varphi\Delta z$, when $R = R_W = R_E$.

SPHERICAL CELLS

$$A = \int_{\theta_1}^{\theta_2} \int_0^{\Delta\varphi} a^2 \sin(\theta) d\theta d\varphi = \dots = \Delta\varphi a^2 \left[\cos\left(\tan^{-1} \frac{R_S}{Z_S + Z_0}\right) - \cos\left(\tan^{-1} \frac{R_N}{Z_N + Z_0}\right) \right] \quad (\text{A-3})$$

ELLIPSOIDAL CELLS

$$\begin{aligned} A &= \Delta\varphi \int_{Z_N}^{Z_S} \sqrt{c_r^2 + (\alpha^4 - \alpha^2)z^2} dz = \dots \\ &= \frac{1}{2} \Delta\varphi \left[Z_S \sqrt{c_r^2 + (\alpha^4 - \alpha^2)Z_S^2} - Z_N \sqrt{c_r^2 + (\alpha^4 - \alpha^2)Z_N^2} \right. \\ &\quad \left. + \frac{c_r^2}{\sqrt{\alpha^4 - \alpha^2}} \ln \left(\frac{Z_S \sqrt{\alpha^4 - \alpha^2} + \sqrt{c_r^2 + (\alpha^4 - \alpha^2)Z_S^2}}{Z_N \sqrt{\alpha^4 - \alpha^2} + \sqrt{c_r^2 + (\alpha^4 - \alpha^2)Z_N^2}} \right) \right] \end{aligned} \quad (\text{A-4})$$

It should be noted that the previous equation is only valid for oblate spheroids (i.e. $\alpha > 1$). A prolate spheroid window ($\alpha < 1$) would lead to excessively high radiative losses and is not considered as an option for Small Particle Solar Receiver.

Appendix B

Volume of the three-dimensional cells of the Monte Carlo mesh

FLUID CELLS TYPE 2

Cone – Cone:

$$r_N(z) = R_{NW} + \frac{R_{NE} - R_{NW}}{\Delta z} z \quad r_S(z) = R_{SW} + \frac{R_{SE} - R_{SW}}{\Delta z} z \quad (\text{B-1})$$

And the volume:

$$V = \frac{1}{6} \Delta \varphi \Delta z (R_{NW}^2 + R_{NE}^2 + R_{NW} R_{NE} - R_{SW}^2 - R_{SE}^2 - R_{SW} R_{SE}) \quad (\text{B-2})$$

Which reduces to the volume of a cylinder, $V = \frac{1}{2} \Delta \varphi \Delta z (R_N^2 - R_S^2)$, when $R_{NW} = R_{NE}$ and $R_{SW} = R_{SE}$.

FLUID CELLS TYPE 3

Plane – Plane:

$$V = \frac{1}{2} \Delta \varphi \Delta z (R_N^2 - R_S^2) \quad (\text{B-3})$$

Ellipsoid – Ellipsoid:

$$V = \frac{1}{3} \Delta \varphi \left[\frac{(c_{r,W}^2 - R_N^2)^{3/2} - (c_{r,W}^2 - R_S^2)^{3/2}}{\alpha_W} - \frac{(c_{r,E}^2 - R_N^2)^{3/2} - (c_{r,E}^2 - R_S^2)^{3/2}}{\alpha_E} \right] \quad (\text{B-4})$$

Ellipsoid – Plane:

$$V = \Delta \varphi \left[\frac{1}{2} Z_E (R_N^2 - R_S^2) + \frac{(c_{r,W}^2 - R_N^2)^{3/2} - (c_{r,W}^2 - R_S^2)^{3/2}}{3\alpha_W} \right] \quad (\text{B-5})$$

Sphere – Ellipsoid:

$$V = \Delta\varphi \left[-\frac{(c_{r,E}^2 - R_N^2)^{3/2} - (c_{r,E}^2 - R_S^2)^{3/2}}{3\alpha_E} + \frac{1}{2}Z_0(R_N^2 - R_S^2) + \frac{(a^2 - R_N^2)^{3/2} - (a^2 - R_S^2)^{3/2}}{3} \right] \quad (\text{B-6})$$

Sphere – Plane:

$$V = \Delta\varphi \left[\frac{1}{2}(Z_E + Z_0)(R_N^2 - R_S^2) + \frac{(a^2 - R_N^2)^{3/2} - (a^2 - R_S^2)^{3/2}}{3} \right] \quad (\text{B-7})$$

Where:

$$Z_0 = \frac{R_{win}}{\tan(\theta_{cap})} \quad a = \frac{R_{win}}{\sin(\theta_{cap})} \quad (\text{B-8})$$

Cone – Cone:

$$V = \left\{ \frac{1}{2} \left[Z_{SE} - Z_{SW} + \frac{Z_{SE} + Z_{NW} - Z_{NE} - Z_{SW}}{R_N - R_S} R_S \right] (R_N^2 - R_S^2) + \frac{1}{3} \left[\frac{Z_{NE} + Z_{SW} - Z_{SE} - Z_{NW}}{R_N - R_S} \right] (R_N^3 - R_S^3) \right\} \Delta\varphi \quad (\text{B-9})$$

Which reduces to the volume of a cylinder when $Z_{SW} = Z_{NW}$ and $Z_{SE} = Z_{NE}$.

Appendix C

Location of emission from two-dimensional Monte Carlo cells

CONICAL CELLS

r-coordinate:

$$R_r = \frac{\int_0^s r(s) d\varphi ds}{\int_0^{s_{max}} r(s) d\varphi ds} \quad (C-1)$$

Where the coordinate s represents the length of the generatrix. It can be assumed, without loss of generality, that the origin of the s coordinate is located at $z = Z_W$. Hence,

$$r = R_W + (R_E - R_W) \frac{z}{Z_E - Z_W} \text{ and } ds = \sqrt{1 + \left(\frac{R_E - R_W}{\Delta z}\right)^2} dz:$$

$$R_r = \frac{\int_0^s r(s') d\varphi ds'}{\int_0^{s_{max}} r(s') d\varphi ds'} = \frac{\int_0^z r(z') d\varphi dz' \sqrt{1 + \left(\frac{R_E - R_W}{\Delta z}\right)^2}}{\int_0^{\Delta z} r(z') d\varphi dz' \sqrt{1 + \left(\frac{R_E - R_W}{\Delta z}\right)^2}} = \dots = \frac{r^2 - R_W^2}{R_E^2 - R_W^2} \quad (C-2)$$

Therefore:

$$r = \sqrt{R_W^2 + R_r(R_E^2 - R_W^2)} \quad (C-3)$$

Note that this is the same expression as for cylindrical fluid cells (Appendix D), which is due to the fact that both area and volume are proportional to $d(r^2)$ in cylindrical coordinates.

z-coordinate:

$$z = Z_W + \frac{Z_E - Z_W}{R_E - R_W} (r - R_W) \quad (C-4)$$

SPHERICAL CELLS

z-coordinate:

$$R_z = \frac{\int_{\theta_S}^{\theta} \sin(\theta') d\theta'}{\int_{\theta_S}^{\theta_N} \sin(\theta') d\theta'} = \frac{\cos \theta_S - \cos \theta}{\cos \theta_S - \cos \theta_N} \Rightarrow \theta = \cos^{-1}[\cos \theta_S - R_z[\cos \theta_S - \cos \theta_N]] \quad (C-5)$$

Or, equivalently,

$$\tan^{-1} \frac{r}{z + Z_0} = \cos^{-1} \left[\cos \left(\tan^{-1} \frac{R_S}{Z_S + Z_0} \right) - R_z \left[\cos \left(\tan^{-1} \frac{R_S}{Z_S + Z_0} \right) - \cos \left(\tan^{-1} \frac{R_N}{Z_N + Z_0} \right) \right] \right] \quad (\text{C-6})$$

Which can be rewritten as:

$$\frac{\sqrt{a^2 - (z + Z_0)^2}}{z + Z_0} = C \quad (\text{C-7})$$

$$\text{Where } C = \tan \left\{ \cos^{-1} \left[\cos \left(\tan^{-1} \frac{R_S}{Z_S + Z_0} \right) - R_z \left[\cos \left(\tan^{-1} \frac{R_S}{Z_S + Z_0} \right) - \cos \left(\tan^{-1} \frac{R_N}{Z_N + Z_0} \right) \right] \right] \right\}.$$

Therefore, the axial location of emission can be computed as:

$$z = \frac{-Z_0(C^2 + 1) \pm \sqrt{Z_0^2(C^2 + 1)^2 - (C^2 + 1)[Z_0^2(C^2 + 1) - a^2]}}{(C^2 + 1)} \quad (\text{C-8})$$

r-coordinate:

$$r = \sqrt{a^2 - (z + Z_0)^2} \quad (\text{C-9})$$

ELLIPSOIDAL CELLS

z-coordinate:

$$\begin{aligned} R_z &= \frac{\int_{Z_N}^z \sqrt{c_r^2 + (\alpha^4 - \alpha^2)z^2} dz}{\int_{Z_N}^{Z_S} \sqrt{c_r^2 + (\alpha^4 - \alpha^2)z^2} dz} = \dots \\ &= \frac{z\sqrt{c_r^2 + (\alpha^4 - \alpha^2)z^2} - Z_N\sqrt{c_r^2 + (\alpha^4 - \alpha^2)Z_N^2} + \frac{c_r^2}{\sqrt{\alpha^4 - \alpha^2}} \ln \left(\frac{z\sqrt{\alpha^4 - \alpha^2} + \sqrt{c_r^2 + (\alpha^4 - \alpha^2)z^2}}{Z_N\sqrt{\alpha^4 - \alpha^2} + \sqrt{c_r^2 + (\alpha^4 - \alpha^2)Z_N^2}} \right)}{Z_S\sqrt{c_r^2 + (\alpha^4 - \alpha^2)Z_S^2} - Z_N\sqrt{c_r^2 + (\alpha^4 - \alpha^2)Z_N^2} + \frac{c_r^2}{\sqrt{\alpha^4 - \alpha^2}} \ln \left(\frac{Z_S\sqrt{\alpha^4 - \alpha^2} + \sqrt{c_r^2 + (\alpha^4 - \alpha^2)Z_S^2}}{Z_N\sqrt{\alpha^4 - \alpha^2} + \sqrt{c_r^2 + (\alpha^4 - \alpha^2)Z_N^2}} \right)} \end{aligned} \quad (\text{C-10})$$

Note, again, that the previous equation is only valid for oblate spheroids ($\alpha > 1$).

r-coordinate:

$$r = \sqrt{c_r^2 - \alpha^2 z^2} \quad (\text{C-11})$$

Appendix D

Location of emission from three-dimensional Monte Carlo cells

FLUID CELLS TYPE 2

For cells Type 2, AA – BB means that the r^- face of the cell is an AA and the r^+ face, a BB (AA and BB are geometrical shapes).

Cone – Cone:

$$r_N(z) = R_{NW} + (R_{NE} - R_{NW}) \frac{z - Z_W}{Z_E - Z_W} \quad r_S(z) = R_{SW} + (R_{SE} - R_{SW}) \frac{z - Z_W}{Z_E - Z_W} \quad (D-1)$$

z-coordinate:

$$R_z = \frac{A(z - Z_W) + \frac{1}{2}B(z^2 - Z_W^2) + \frac{1}{3}C(z^3 - Z_W^3)}{A(Z_E - Z_W) + \frac{1}{2}B(Z_E^2 - Z_W^2) + \frac{1}{3}C(Z_E^3 - Z_W^3)} \quad (D-2)$$

r-coordinate:

$$r = \sqrt{\left(R_{SW} + (R_{SE} - R_{SW}) \frac{z - Z_W}{Z_E - Z_W}\right)^2 + R_r \left[\left(R_{NW} + (R_{NE} - R_{NW}) \frac{z - Z_W}{Z_E - Z_W}\right)^2 - \left(R_{SW} + (R_{SE} - R_{SW}) \frac{z - Z_W}{Z_E - Z_W}\right)^2 \right]} \quad (D-3)$$

Where,

$$\begin{aligned} A &= \left(R_{NW} - \frac{R_{NE} - R_{NW}}{Z_E - Z_W} Z_W\right)^2 - \left(R_{SW} - \frac{R_{SE} - R_{SW}}{Z_E - Z_W} Z_W\right)^2 \\ B &= 2 \left(R_{NW} - \frac{R_{NE} - R_{NW}}{Z_E - Z_W} Z_W\right) \left(\frac{R_{NE} - R_{NW}}{Z_E - Z_W}\right) - 2 \left(R_{SW} - \frac{R_{SE} - R_{SW}}{Z_E - Z_W} Z_W\right) \left(\frac{R_{SE} - R_{SW}}{Z_E - Z_W}\right) \\ C &= \left(\frac{R_{NE} - R_{NW}}{Z_E - Z_W}\right)^2 - \left(\frac{R_{SE} - R_{SW}}{Z_E - Z_W}\right)^2 \end{aligned} \quad (D-4)$$

FLUID CELLS TYPE 3

For cells Type 3, AA – BB means that the z^- face of the cell is an AA and the z^+ face, a BB (AA and BB are geometrical shapes).

Ellipsoid – Ellipsoid:

$$z_W(r) = \sqrt{\frac{c_{r,W}^2 - r^2}{\alpha_W^2}} \quad z_E(r) = \sqrt{\frac{c_{r,E}^2 - r^2}{\alpha_E^2}} \quad (\text{D-5})$$

r-coordinate:

$$R_r = \frac{\frac{1}{\alpha_W} \left[(c_{r,W}^2 - r^2)^{3/2} - (c_{r,W}^2 - R_S^2)^{3/2} \right] - \frac{1}{\alpha_E} \left[(c_{r,E}^2 - r^2)^{3/2} - (c_{r,E}^2 - R_S^2)^{3/2} \right]}{\frac{1}{\alpha_W} \left[(c_{r,W}^2 - R_N^2)^{3/2} - (c_{r,W}^2 - R_S^2)^{3/2} \right] - \frac{1}{\alpha_E} \left[(c_{r,E}^2 - R_N^2)^{3/2} - (c_{r,E}^2 - R_S^2)^{3/2} \right]} \quad (\text{D-6})$$

z-coordinate:

$$z = \sqrt{\frac{c_{r,W}^2 - r^2}{\alpha_W^2}} + R_z \left[\sqrt{\frac{c_{r,E}^2 - r^2}{\alpha_E^2}} - \sqrt{\frac{c_{r,W}^2 - r^2}{\alpha_W^2}} \right] \quad (\text{D-7})$$

Ellipsoid – Plane:

$$z_W(r) = \sqrt{\frac{c_{r,W}^2 - r^2}{\alpha_W^2}} \quad z_E(r) = Z_E \quad (\text{D-8})$$

r-coordinate:

$$R_r = \frac{Z_E(r^2 - R_S^2) + \frac{2}{3\alpha_W} \left[(c_{r,W}^2 - r^2)^{3/2} - (c_{r,W}^2 - R_S^2)^{3/2} \right]}{Z_E(R_N^2 - R_S^2) + \frac{2}{3\alpha_W} \left[(c_{r,W}^2 - R_N^2)^{3/2} - (c_{r,W}^2 - R_S^2)^{3/2} \right]} \quad (\text{D-9})$$

z-coordinate:

$$z = \sqrt{\frac{c_{r,W}^2 - r^2}{\alpha_W^2}} + R_z \left[Z_E - \sqrt{\frac{c_{r,W}^2 - r^2}{\alpha_W^2}} \right] \quad (\text{D-10})$$

Sphere – Ellipsoid:

$$z_W(r) = \sqrt{a^2 - r^2} - Z_0 \quad z_E(r) = \sqrt{\frac{c_{r,E}^2 - r^2}{\alpha_E^2}} \quad (\text{D-11})$$

r-coordinate:

$$R_r = \frac{-\frac{1}{\alpha_E} \left[(c_{r,E}^2 - r^2)^{3/2} - (c_{r,E}^2 - R_S^2)^{3/2} \right] + \frac{3}{2} Z_0 (r^2 - R_S^2) + (a^2 - r^2)^{3/2} - (a^2 - R_S^2)^{3/2}}{-\frac{1}{\alpha_E} \left[(c_{r,E}^2 - R_N^2)^{3/2} - (c_{r,E}^2 - R_S^2)^{3/2} \right] + \frac{3}{2} Z_0 (R_N^2 - R_S^2) + (a^2 - R_N^2)^{3/2} - (a^2 - R_S^2)^{3/2}} \quad (\text{D-12})$$

z-coordinate:

$$z = \sqrt{a^2 - r^2} - Z_0 + R_z \left[\sqrt{\frac{c_{r,E}^2 - r^2}{\alpha_E^2}} + Z_0 - \sqrt{a^2 - r^2} \right] \quad (\text{D-13})$$

Sphere – Plane:

$$z_W(r) = \sqrt{a^2 - r^2} - Z_0 \quad z_E(r) = Z_E \quad (\text{D-14})$$

r-coordinate:

$$R_r = \frac{(r^2 - R_S^2)(Z_E + Z_0) + \frac{2}{3}[(a^2 - r^2)^{3/2} - (a^2 - R_S^2)^{3/2}]}{(Z_E + Z_0)(R_N^2 - R_S^2) + \frac{2}{3}[(a^2 - R_N^2)^{3/2} - (a^2 - R_S^2)^{3/2}]} \quad (\text{D-15})$$

z-coordinate:

$$z = z_W(r) + R^*[z_E(r) - z_W(r)] = \sqrt{a^2 - r^2} - Z_0 + R_z [Z_E + Z_0 - \sqrt{a^2 - r^2}] \quad (\text{D-16})$$

Note that all the equations in Appendices C and D are injective functions. Therefore, their inverses are single-valued functions and can be inverted unequivocally.

Appendix E

Intersection between a ray and Monte Carlo mesh faces

The equation of the line through which the ray travels is given by:

$$\mathbf{x}(t) = \mathbf{x}_o + \mathbf{v} \cdot t \quad (\text{E-1})$$

Where $\mathbf{x}(t) \in \mathbb{R}^3$ is the locus of the ray –characterized by the parameter $t \in \mathbb{R}$, which is such that $\mathbf{x}(0) = \mathbf{x}_o$ is the current location of the ray– and $\mathbf{v}$ is a unit vector in the direction of the ray.

DISTANCE LINE-SPHERE

On account of the axisymmetry of the Small Particle Solar Receiver, only spheres with center at $(x, y) = (0, 0)$ need to be considered, i.e., $x^2 + y^2 + (z + Z_0)^2 = a^2$ where a is the radius of the sphere. The distance to the intersection, t , can be readily obtained as expressed in Eq. E-2.

$$t = \frac{-C_2 \pm \sqrt{C_2^2 - 4C_1C_3}}{2C_1} \quad (\text{E-2})$$

$$C_1 = \frac{1}{2} \quad C_2 = (x_o v_x + y_o v_y + z_o v_z + v_z Z_0) \quad C_3 = \frac{1}{2}(x_o^2 + y_o^2 + z_o^2 + Z_0^2 + 2z_o Z_0 - a^2)$$

DISTANCE LINE-ELLIPSOID

Again, only axisymmetric ellipses with the center at $(x, y) = (0, 0)$, Eq. E-3, need to be considered.

$$\frac{x^2}{c_r^2} + \frac{y^2}{c_r^2} + \alpha^2 \frac{z^2}{c_r^2} = 1 \quad (\text{E-3})$$

Where c_r is the size parameter and α is the shape parameter ($\alpha = \sqrt{2}$ is used in all the simulations with an ellipsoidal window). The distance to intersection, t , is expressed in Eq. E-4.

$$t = \frac{-C_2 \pm \sqrt{C_2^2 - 4C_1C_3}}{2C_1} \quad (\text{E-4})$$

Where the constants are defined as:

$$C_1 = 1 + (\alpha^2 - 1)v_z^2 \quad C_2 = 2x_0v_x + 2y_0v_y + 2\alpha^2z_0v_z \quad C_3 = x_0^2 + y_0^2 + \alpha^2z_0^2 - c_r^2$$

DISTANCE LINE-CONE

On the one hand, the distance between a point of the line through which the ray travels, $P(t)$, and the OZ axis is:

$$dis(P(t), OZ) = \sqrt{(x_0 + t \cdot v_x)^2 + (y_0 + t \cdot v_y)^2} \quad (E-5)$$

On the other hand, the distance between a point of the cone, $M(x, y, z)$, and the OZ axis only depends on the z -coordinate and can be expressed as:

$$\begin{aligned} dis(M(x, y, z), OZ) &= \sqrt{x_1^2 + y_1^2} + \frac{z - z_1}{z_2 - z_1} \left[\sqrt{x_2^2 + y_2^2} - \sqrt{x_1^2 + y_1^2} \right] \\ &= R_1 + \frac{z - z_1}{z_2 - z_1} (R_2 - R_1) = R_1 - \frac{z_1}{z_2 - z_1} (R_2 - R_1) + \frac{(R_2 - R_1)}{z_2 - z_1} z \\ &= A + B z \end{aligned} \quad (E-6)$$

(x_1, y_1, z_1) are the Cartesian coordinates of any point of the cone at $z = z_1 = \min_{z \in \varepsilon} z$; and (x_2, y_2, z_2) are the Cartesian coordinates of any point of the cone at $z = z_2 = \max_{z \in \varepsilon} z$, where ε denotes the two-dimensional conical face.

The relation between z and t is:

$$z = z_0 + t \cdot v_z \quad (E-7)$$

Therefore, the distance to the intersection point can be calculated as:

$$t = \frac{-C_2 \pm \sqrt{C_2^2 - 4C_1C_3}}{2C_1} \quad (E-8)$$

Where:

$$\begin{aligned} C_1 &= B^2v_z^2 - v_x^2 - v_y^2 \\ C_2 &= 2AB \cdot v_z + 2B^2z_0v_z - 2x_0v_x - 2y_0v_y \\ C_3 &= A^2 + 2ABz_0 + B^2z_0^2 - x_0^2 - y_0^2 \end{aligned} \quad (E-9)$$

And:

$$A = R_1 - \frac{z_1}{z_2 - z_1}(R_2 - R_1) = \sqrt{x_1^2 + y_1^2} - \frac{z_1}{z_2 - z_1}(\sqrt{x_2^2 + y_2^2} - \sqrt{x_1^2 + y_1^2})$$

$$B = \frac{(R_2 - R_1)}{z_2 - z_1} = \frac{\sqrt{x_2^2 + y_2^2} - \sqrt{x_1^2 + y_1^2}}{z_2 - z_1} \quad (\text{E-10})$$

In the degenerated case of a cylinder (a particular case of a cone) the previous constants are simplified to $A = R$ and $B = 0$. In order to prevent unnecessary computations, a new subroutine for the particular case of cylindrical surfaces has been created.

It should be noted that for all the intersections described above (line-sphere, line-ellipsoid and line-cone), there exist there possible situations depending on the sign of the discriminant $C_2^2 - 4C_1C_3$:

$$1) C_2^2 - 4C_1C_3 < 0$$

The line does not intersect the surface. In this case the distance must be equaled to an arbitrarily big number (for modeling purposes) so that this is not the closest intersection of the ray with one of the cell faces.

$$2) C_2^2 - 4C_1C_3 = 0$$

The line is tangent to the surface. Since the ray does not enter the neighbor cell but rather it remains in the current cell, the distance is equaled to an arbitrarily big number so that this is not the closest intersection.

$$3) C_2^2 - 4C_1C_3 > 0$$

The line is secant to the surface and intersects is twice. The minimum positive root is to be chosen. If both roots are negative, there is no intersection in the positive direction and the distance should be equaled to an arbitrarily big number as in the previous two cases.

Note, finally, that only two intersections can exist for all the faces present in the Monte Carlo mesh since the mathematical surface is the boundary of a convex set (i.e. $K(\mathbf{x}) \geq 0$ where K is the Gaussian curvature or, in other words, $\det(\text{I}) \cdot \det(\text{II}) \geq 0$ for I and II the first and second fundamental forms, respectively.) Rare exceptions may appear when dealing with ruled surfaces (planes, cylinders and cones in the Monte Carlo mesh) if the line through which the ray travels happens to be part of the surface. In such unlikely situations the tracing of the ray is stopped without noticeable loss of accuracy in the numerical solution.

Appendix F

Validation of the Monte Carlo Software

TEST 1:

Description:

Surface to surface radiation heat transfer between two black, parallel, infinite plates at the same temperature.

Simulation conditions:

- Left and right plates are both blackbodies at 500 K.
- Distance between plates: 0.1 m.
- Nonparticipating medium between the plates.

Expected results:

- The net radiative balance between both plates must be exactly zero.
- The radiative heat flux should be approximately zero in all the cells. Nevertheless, small oscillations around zero are expected due to the statistical nature of the Monte Carlo method.

Simulation results:

Radial position (m)	Left Plate (W/m ²)			
	Angular Division #1	Angular Division #2	Angular Division #3	Angular Division #4
0.00-0.50	4.4465	-0.5644	-3.4587	1.4313
0.50-1.00	0.7680	-1.1116	-0.9158	0.8025
1.00-1.50	0.0092	-0.7303	0.9112	-1.1254
1.50-2.00	0.0930	0.4888	-1.0100	1.8032
2.00-2.50	0.7081	0.3705	-1.1596	-1.2364
2.50-3.00	0.1526	0.0594	-0.1141	-0.6296
3.00-3.50	0.3790	0.4413	-0.0970	0.4100
3.50-4.00	-0.0278	-0.2734	0.4212	0.4410
4.00-4.50	-0.7400	-0.1200	-0.1081	-0.7035
4.50-5.00	0.6095	0.0855	-0.5209	0.7497
TOTAL	0.000 W			

Right Plate (W/m ²)				
Radial position (m)	Angular Division #1	Angular Division #2	Angular Division #3	Angular Division #4
0.00-0.50	0.2765	0.5472	1.7538	-0.7315
0.50-1.00	0.6710	-1.4946	-0.7824	-2.2904
1.00-1.50	0.2436	0.7459	-0.0213	0.3980
1.50-2.00	0.2670	-0.0757	0.4481	1.7506
2.00-2.50	-0.6864	-0.5859	0.4070	-0.0445
2.50-3.00	0.1327	0.1319	-0.1775	0.5370
3.00-3.50	0.2133	0.1681	-0.2466	-0.1777
3.50-4.00	0.1839	-0.6443	-0.7800	0.7378
4.00-4.50	-0.0640	-0.3246	0.3498	-0.2036
4.50-5.00	0.1435	0.1338	-0.3077	0.0205
TOTAL	0.000 W			

Table 22 – Radiative heat flux through the left (top) and right (bottom) plates in Test #1 of the Monte Carlo method validation.

The greater uncertainty in the cells of the first radial division is expected since, on account of their smaller size, fewer rays contribute to their radiative heat flux, which in turn increases the variance of the solution. This result holds for the following tests as well.

TEST 2:

Description:

Surface to surface radiation heat transfer between two black, parallel, infinite plates at different temperatures.

Simulation conditions:

- Left plate: Blackbody at 800 K.
- Right plate: Blackbody at 500 K.
- Distance between plates: 0.1m
- Nonparticipating medium between the plates.

Analytical solution:

$$\dot{Q} = \left(\frac{1 - \varepsilon_1}{\varepsilon_1} + \frac{A_1 + A_2 - 2A_1F_{1-2}}{A_2 - A_1F_{1-2}^2} + \frac{1 - \varepsilon_2}{\varepsilon_2} \frac{A_1}{A_2} \right)^{-1} A_1 \sigma (T_1^4 - T_2^4) = 1,545,817.40 \text{ W}$$

$$\dot{q}_1 = -19,681.96 \text{ W/m}^2$$

$$\dot{q}_2 = 19,681.96 \text{ W/m}^2$$

Simulation results:

Left Plate (W/m²)				
Radial position (m)	Angular Division #1	Angular Division #2	Angular Division #3	Angular Division #4
0.00-0.50	-19682.10	-19680.41	-19687.90	-19683.71
0.50-1.00	-19679.68	-19680.82	-19683.26	-19680.45
1.00-1.50	-19683.30	-19680.54	-19682.33	-19682.80
1.50-2.00	-19684.13	-19682.79	-19682.58	-19679.65
2.00-2.50	-19681.48	-19681.30	-19682.27	-19681.14
2.50-3.00	-19682.97	-19682.14	-19682.26	-19682.08
3.00-3.50	-19680.66	-19683.61	-19680.48	-19680.66
3.50-4.00	-19680.14	-19681.45	-19683.56	-19681.41
4.00-4.50	-19683.43	-19682.55	-19681.20	-19683.02
4.50-5.00	-19681.80	-19681.30	-19682.70	-19681.88
TOTAL	-1,545,817.39W			

Right Plate (W/m²)				
Radial position (m)	Angular Division #1	Angular Division #2	Angular Division #3	Angular Division #4
0.00-0.50	19681.12	19662.00	19683.86	19660.16
0.50-1.00	19682.07	19684.50	19683.56	19687.26
1.00-1.50	19680.25	19672.94	19684.69	19683.48
1.50-2.00	19688.63	19685.45	19684.78	19688.30
2.00-2.50	19678.69	19679.33	19681.94	19677.86
2.50-3.00	19680.88	19682.29	19680.60	19682.27
3.00-3.50	19681.81	19682.36	19683.21	19686.49
3.50-4.00	19683.17	19678.29	19677.13	19686.08
4.00-4.50	19683.41	19683.63	19682.02	19678.97
4.50-5.00	19681.66	19681.88	19680.72	19682.75
TOTAL	1,545,817.39W			

Table 23 – Radiative heat flux through the left (top) and right (bottom) plates in Test #2 of the Monte Carlo method validation.

TEST 3:**Description:**

Surface to surface radiation heat transfer between two black, coaxial, infinite cylinders at the same temperature.

Simulation conditions:

- Inner cylinder: Blackbody at $T_1 = 500$ K and $R_1 = 0.1$ m.
- Outer cylinder: Blackbody at $T_2 = 500$ K and $R_2 = 0.2$ m.

- Nonparticipating medium between the cylinders.

Analytical solution:

$$\dot{Q} = 0 \text{ W} \quad \dot{q} = 0 \text{ W/m}^2$$

Small discrepancies between the analytical solution and the simulation results are expected not only for the local radiative heat flux on each cell (as in Tests #1 and #2) but also for the total radiative heat transfer: While in the radiation exchange between two parallel plates all the rays emitted by one of them reach the other, in the radiation heat exchange between coaxial cylinders (Test #3 and #4) not all the rays emitted by the outer cylinder reach the inlet cylinder. Actually, this ratio is a random variable of mean 0.50 (since the radius ratio is 2:1) and a certain uncertainty in the local radiative heat flux on each cell is expected.

Simulation results:

Inner Cylinder (W/m ²)				
Axial Position (m)	Angular Division #1	Angular Division #2	Angular Division #3	Angular Division #4
0.00-1.00	1.1537	-1.1875	-0.6566	-0.2259
1.00-2.00	-1.7959	-0.0516	1.0780	2.5878
2.00-3.00	-1.2885	4.2909	-0.0442	-2.4468
3.00-4.00	-1.2197	-0.7730	2.5764	1.6228
4.00-5.00	0.9576	-1.9244	-0.4725	0.1187
5.00-6.00	0.8968	1.3424	1.1870	1.4754
6.00-7.00	1.1141	-2.7484	-1.1061	2.3046
7.00-8.00	-0.6417	-0.3647	-0.4805	-0.9014
8.00-9.00	0.7288	3.3436	-0.0659	0.2643
9.00-10.00	0.5539	1.6423	1.4851	-1.0683
TOTAL	1.7688 W			

Outer Cylinder (W/m ²)				
Axial Position (m)	Angular Division #1	Angular Division #2	Angular Division #3	Angular Division #4
0.00-1.00	1.2472	-0.1568	0.1032	0.0324
1.00-2.00	-1.7681	0.7282	0.8885	-0.3461
2.00-3.00	-0.4275	-0.0077	0.1729	0.3033
3.00-4.00	-2.5010	0.5548	-0.2916	-0.3340
4.00-5.00	-0.6732	-0.6981	-1.1792	1.5938
5.00-6.00	0.0946	-0.4931	0.1089	-0.3079
6.00-7.00	-0.4923	1.6532	-0.2494	-0.8122
7.00-8.00	0.3383	1.5565	-0.0510	-1.2704
8.00-9.00	1.0577	0.5396	-2.1082	-0.4969

9.00-10.00	-0.4556	-0.0321	-0.4008	-1.0502
TOTAL	-1.7688 W			

Table 24 – Radiative heat flux through the inner (top) and outer (bottom) cylinders in Test #3 of the Monte Carlo method validation.

TEST 4:

Description:

Surface to surface radiation heat transfer between two black, coaxial, infinite cylinders at different temperatures.

Simulation conditions:

- Inner cylinder: Blackbody at $T_1 = 800$ K and $R_1 = 0.1$ m.
- Outer cylinder: Blackbody at $T_2 = 500$ K and $R_2 = 0.2$ m.
- Nonparticipating medium between the cylinders.

Analytical solution:

$$\dot{Q} = \left(\frac{1 - \varepsilon_1}{\varepsilon_1} + \frac{A_1 + A_2 - 2A_1F_{1-2}}{A_2 - A_1F_{1-2}^2} + \frac{1 - \varepsilon_2}{\varepsilon_2} \frac{A_1}{A_2} \right)^{-1} A_1 \sigma (T_1^4 - T_2^4) = 123,665.39 \text{ W}$$

$$\dot{q}_1 = -19,681.96 \text{ W/m}^2$$

$$\dot{q}_2 = 9,840.98 \text{ W/m}^2$$

Like in Test #3, small discrepancies between the analytical solution and the simulation results are expected for both the radiative heat flux and the total radiative heat transfer.

Simulation results:

Inner Cylinder (W/m²)				
Axial Position (m)	Angular Division #1	Angular Division #2	Angular Division #3	Angular Division #4
0.00-1.00	-19671.23	-19686.06	-19674.89	-19692.54
1.00-2.00	-19690.06	-19687.54	-19680.27	-19685.13
2.00-3.00	-19681.53	-19682.08	-19673.38	-19678.94
3.00-4.00	-19673.92	-19674.54	-19685.58	-19688.49
4.00-5.00	-19684.79	-19684.02	-19676.58	-19685.61
5.00-6.00	-19684.67	-19666.16	-19681.79	-19670.96
6.00-7.00	-19686.04	-19685.72	-19683.88	-19669.80
7.00-8.00	-19680.16	-19687.49	-19676.69	-19688.70
8.00-9.00	-19672.26	-19685.36	-19669.15	-19681.49
9.00-10.00	-19677.62	-19681.34	-19690.77	-19694.81
TOTAL	-123,661.26 W			

Outer Cylinder (W/m ²)				
Axial Position (m)	Angular Division #1	Angular Division #2	Angular Division #3	Angular Division #4
0.00-1.00	9842.10	9843.71	9839.16	9842.10
1.00-2.00	9836.38	9845.41	9842.06	9842.55
2.00-3.00	9844.32	9835.58	9841.87	9842.24
3.00-4.00	9838.48	9843.02	9834.37	9836.34
4.00-5.00	9850.09	9835.66	9846.07	9838.53
5.00-6.00	9839.26	9835.51	9835.15	9837.03
6.00-7.00	9846.92	9836.38	9838.38	9845.11
7.00-8.00	9834.70	9845.37	9838.57	9844.15
8.00-9.00	9835.89	9837.27	9842.62	9840.39
9.00-10.00	9843.48	9847.21	9840.01	9842.55
TOTAL	123,661.26 W			

Table 25 – Radiative heat flux through the inner (top) and outer (bottom) cylinders in Test #4 of the Monte Carlo method validation.

TEST 5:

Description:

Radiation heat transfer between two black, parallel, infinite plates at different temperatures surrounding a participating, gray medium [51].

Simulation conditions:

- Left plate: Blackbody at 800 K.
- Right plate: Blackbody at 500 K.
- Emission, absorption, non-scattering gray medium (optical thicknesses $\tau_L=0.5$ and 2.0 are tested.)
- The medium is in radiative equilibrium, i.e. $4\pi\kappa i_b - \kappa \int_{4\pi} i d\Omega = 0$.

Analytical solution:

$$\Phi_b(\tau) = \frac{1}{2} \left[E_2(\tau) + \int_0^{\tau_L} \Phi_b(\tau') E_1(|\tau - \tau'|) d\tau' \right] \quad (\text{F-1})$$

Where $\Phi_b(\tau) = \frac{T^4(\tau) - T_2^4}{T_1^4 - T_2^4}$ is the dimensionless emissive power and $E_n(\tau) = \int_1^\infty e^{-\tau t} \frac{dt}{t^n}$ is the exponential integral of order n .

Simulation results:

Figure 18 in Chapter 3 shows the dimensionless emissive power distribution for both the analytical solution and the in-house Monte Carlo method.

TEST 6:**Description:**

Radiation heat transfer between two black, coaxial, infinite cylinders at different temperatures surrounding a participating, gray medium [53].

Simulation conditions:

- Radius ratio 10:1.
- Inner cylinder: Blackbody at 800 K.
- Outer cylinder: Blackbody at 500 K.
- Emission, absorption, non-scattering gray medium (optical thicknesses $\tau_L=0.1, 2.0$ and 10.0 are tested.)
- The medium is in radiative equilibrium.

Analytical solution:

The analytical solution in cylindrical coordinates is rather involved and will not be reproduced here. The “exact” Monte Carlo solution was found by Perlmutter and Howell [53] and this is the solution with which the results of our in-house Monte Carlo method will be compared.

Simulation results:

Figure 33 shows the dimensionless emissive power distribution for both our in-house Monte Carlo method and the benchmark by Perlmutter and Howell [53].

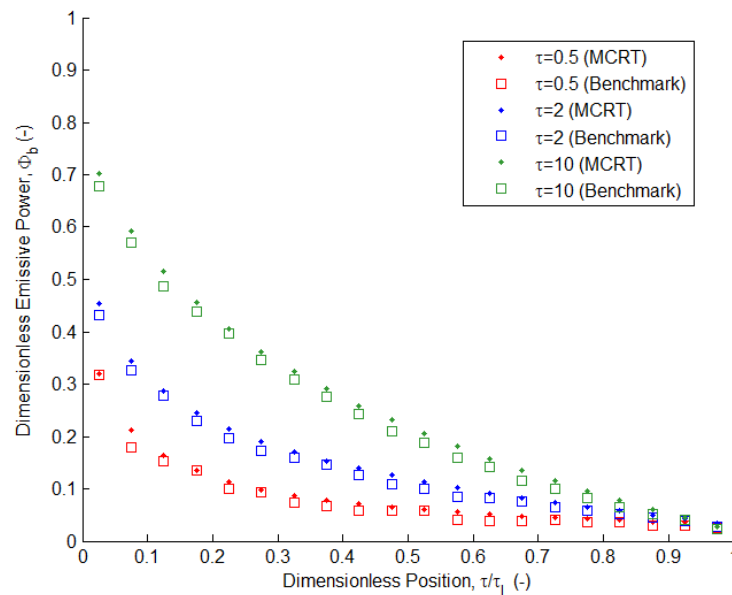


Figure 33 – Dimensionless emissive power distribution in the gas (Test #6 of the Monte Carlo method validation.)

Appendix G

Closure coefficients and auxiliary relations of the SST k- ω Turbulence Model

Generation of turbulence kinetic energy due to mean velocity gradients:

$$\begin{aligned}\tilde{P}_k &= \min(P_k, 10\beta^*\rho\omega k) \\ \tau_{ij} &= \mu_t \left(2S_{ij} - \frac{2}{3} \frac{\partial u_k}{\partial x_k} \delta_{ij} \right) - \frac{2}{3} \rho k \delta_{ij} & P_k &= \tau_{ij} \frac{\partial u_i}{\partial x_j} \\ S &= \sqrt{2S_{ij}S_{ij}} & S_{ij} &= \frac{1}{2} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)\end{aligned}\tag{G-1}$$

Turbulent eddy viscosity:

$$\mu_t = \frac{\rho k}{\omega} \frac{1}{\max\left(\frac{1}{\alpha^*}, \frac{SF_2}{a_1\omega}\right)}\tag{G-2}$$

Turbulent Prandtl number for k and ω :

$$\begin{aligned}\sigma_k &= \frac{1}{F_1/\sigma_{k,1} + (1-F_1)/\sigma_{k,2}} & \sigma_\omega &= \frac{1}{F_1/\sigma_{\omega,1} + (1-F_1)/\sigma_{\omega,2}} \\ F_1 &= \tanh(\Phi_1^4) & F_2 &= \tanh(\Phi_2^2)\end{aligned}\tag{G-3}$$

$$\begin{aligned}\Phi_1 &= \min \left[\max \left(\frac{\sqrt{k}}{\beta^*\omega y}, \frac{500\mu}{\rho y^2 \omega} \right), \frac{4\rho k}{\sigma_{\omega,2} D_\omega^+ y^2} \right] & \Phi_2 &= \max \left[\frac{2\sqrt{k}}{\beta^*\omega y}, \frac{500\mu}{\rho y^2 \omega} \right] \\ D_\omega^+ &= \max \left[2\rho \frac{1}{\sigma_{\omega,2}} \frac{1}{\omega} \frac{\partial k}{\partial x_j} \frac{\partial \omega}{\partial x_j}, 10^{-10} \right]\end{aligned}$$

On account of the high Reynolds number inside the Small Particle Solar Receiver, the low-Reynolds-number correction to damp the turbulent viscosity is not employed and $\alpha^* = 1$.

Model constants:

$$\begin{array}{llll}\sigma_{k,1} = 1.176 & \sigma_{k,2} = 1.0 & \sigma_{\omega,1} = 2.0 & \sigma_{\omega,2} = 1.168 \\ \beta_1 = 0.075 & \beta_2 = 0.0828 & \beta^* = 0.09 & \zeta^* = 1.5 \\ \alpha_1 = 0.31 & \alpha_\infty^* = 1 & \alpha_\infty = 0.52 & M_{t0} = 0.25\end{array}$$

Appendix H

Sensitivity analysis of the thermal absorption thickness of the walls

When electromagnetic waves reach opaque bodies, they only penetrate a few Å (metals) or μm (dielectrics) before they are completely absorbed. Similarly, only the radiation emitted by a very thin layer near the surface can actually go outside of the material. Therefore, all the radiation heat transfer between opaque bodies, like metals or ceramic, and their surroundings occurs in a very thin layer next to the surface. However, on account of the domain discretization in the CFD model, it is not possible to concentrate all the radiative heat transfer in an arbitrarily thin layer and the radiative heat flux computed by the Monte Carlo method needs to be distributed in a layer of thickness L , where L is greater than the mesh size.

Hence, the following question should be elucidated: *For a given net radiative heat flux on an opaque body and assuming it is uniformly distributed over a layer of thickness L , how exact is the average temperature in that layer compared to the exact solution (i.e. when the energy is concentrated in an arbitrarily thin layer, $L \rightarrow 0$)?*

This problem will be reduced to a one-dimensional heat transfer problem, which is appropriate for the goal pursued with this study. The total thermal resistance of the wall (including the insulation) can be split up into three serial thermal resistances:

1. R_1 : Thermal resistance due to exterior convection and conduction in the entire wall except the layer of thickness L in which the radiative heat flux is supposed to be uniformly distributed. Its equivalent convective heat transfer coefficient will be denoted by h_1 .
2. R_2 : Thermal resistance of the layer in which the radiative heat flux is supposed to be uniformly distributed (with thickness L).
3. R_3 : Thermal resistance due to interior convection. Its equivalent convective heat transfer coefficient will be denoted by h_3 .

Since only the temperature profile in the layer in which the radiative heat flux is supposed to be uniformly distributed needs to be known, the governing Ordinary Differential Equation will be only solved in the domain $x \in (0, L)$; while R_3 will be used to impose a proper boundary condition at $x = L$. Moreover, the cylindrical wall can be approximated by a plane wall since $L \ll D_{rec}/2$. Further assuming constant thermal

conductivity and neglecting the radiative heat transfer between the outer surface and the atmosphere, the problem can be written as:

$$\begin{aligned} k_w \frac{\partial^2 T}{\partial x^2} + q_v &= 0 \text{ for } x \in (0, L) \\ k_w \frac{\partial T}{\partial x} &= h_1(L)(T - T_{\infty, amb}) \text{ at } x = 0 \\ -k_w \frac{\partial T}{\partial x} &= h_3(T - T_{\infty, air}) \text{ at } x = L \end{aligned} \quad (\text{H-1})$$

Where $q_v = \frac{q_w}{L}$ and $\frac{1}{h_1(L)} = \frac{1}{h_1(0)} - \frac{L}{k_w}$.

The solution of the previous boundary value problem is:

$$\begin{aligned} T &= -\frac{1}{2} \frac{q_w}{k_w L} x^2 + Ax + B \\ A &= \frac{q_w + \frac{1}{2} h_3 \frac{q_w}{k} L + h_3(T_{\infty, air} - T_{\infty, amb})}{k_w \left(1 + \frac{h_3}{h_1(L)}\right) + h_3 L} \\ B &= T_{\infty, amb} + \frac{q_w k_w + \frac{1}{2} h_3 q_w L + h_3 k_w (T_{\infty, air} - T_{\infty, amb})}{k_w (h_1(L) + h_3) + h_1(L) h_3 L} \end{aligned} \quad (\text{H-2})$$

Therefore, the average temperature in $(0, L)$ –the value to be employed again by the Monte Carlo code– is:

$$\langle T \rangle(L) = \frac{\int_0^L T(x) dx}{\int_0^L dx} = -\frac{1}{6} \frac{q_w}{k_w} L + \frac{1}{2} AL + B \quad (\text{H-3})$$

The actual temperature of the inner surface of the wall can be readily calculated by taking the limit when L is arbitrarily small:

$$\begin{aligned} T_w &= \lim_{L \rightarrow 0} \langle T \rangle(L) = \lim_{L \rightarrow 0} \left(-\frac{1}{6} \frac{q_w}{k_w} L + \frac{1}{2} AL + B \right) \\ &= T_{\infty, amb} \frac{h_1(0)}{h_1(0) + h_3} + T_{\infty, air} \frac{h_3}{h_1(0) + h_3} + \frac{q_w}{h_1(0) + h_3} \end{aligned} \quad (\text{H-4})$$

The exact inner temperature T_w can also be easily obtained considering that, in the limit $L \rightarrow 0$, it is a serial heat transfer problem between a surface at $T = T_w$ and two media at temperatures $T_{\infty, amb}$ and $T_{\infty, air}$ with convective heat transfers h_1 and h_3 , respectively:

$$\begin{aligned}\dot{q} &= h_1(T_w - T_{\infty,amb}) + h_3(T_w - T_{\infty,air}) \xrightarrow{\text{yields}} T_w \\ &= T_{\infty,amb} \frac{h_1(0)}{h_1(0) + h_3} + T_{\infty,int} \frac{h_3}{h_1(0) + h_3} + \frac{q_w}{h_1(0) + h_3}\end{aligned}\quad (\text{H-5})$$

Finally, the ratio between the average temperature using a thickness L and the actual temperature of the inner surface of the wall, $r(L) = T(L)/\lim_{L \rightarrow 0} T(L)$, is:

$$\begin{aligned}r &= \frac{\langle T \rangle(L)}{\lim_{L \rightarrow 0} \langle T \rangle(L)} = \frac{h_1(0) + h_3}{T_{\infty,amb} h_1(0) + T_{\infty,air} h_3 + q_w} \left[-\frac{q_w L}{6k_w} \right. \\ &\quad + \frac{q_w L + \frac{1}{2} h_3 \frac{q_w}{k_w} L^2 + h_3 (T_{\infty,air} - T_{\infty,amb}) L}{2k_w \left(1 + \frac{h_3}{h_1(L)} \right) + 2h_3 L} + T_{\infty,amb} \\ &\quad \left. + \frac{q_w k_w + \frac{1}{2} h_3 q_w L + h_3 k_w (T_{\infty,air} - T_{\infty,amb})}{k_w (h_1(L) + h_3) + h_1(L) h_3 L} \right]\end{aligned}\quad (\text{H-6})$$

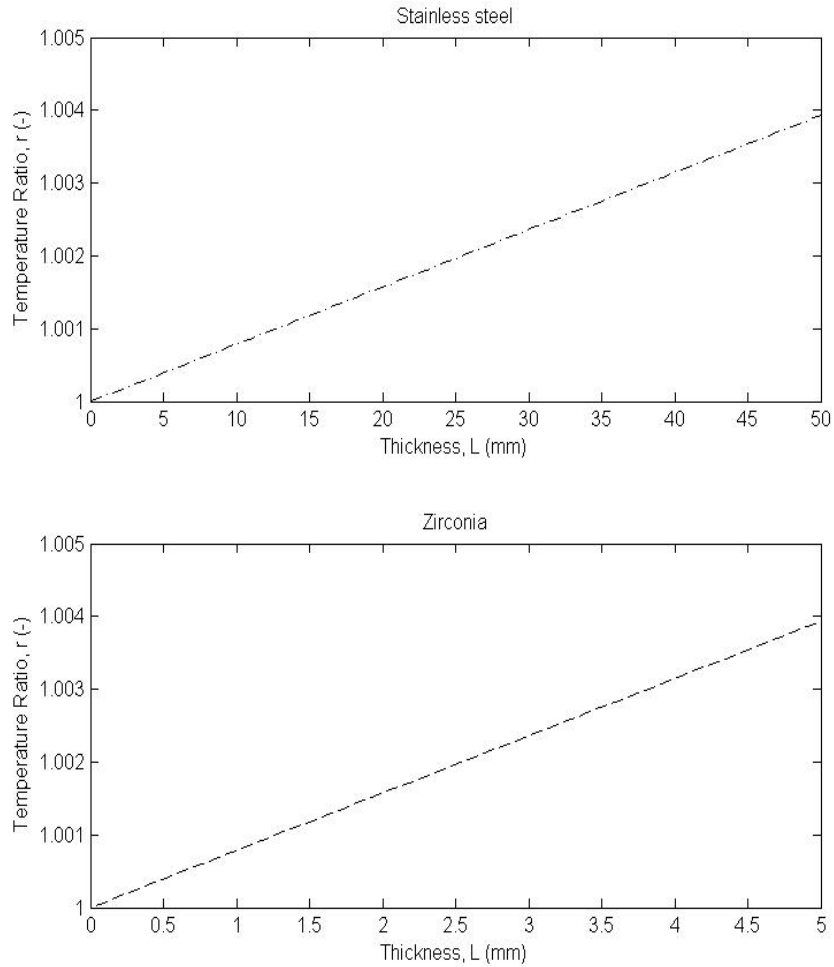


Figure 34 – Temperature ratio, $r(L) = T(L)/\lim_{L \rightarrow 0} T(L)$, in stainless steel walls (top) and zirconia walls (bottom). Note the different scale in the x-axis.

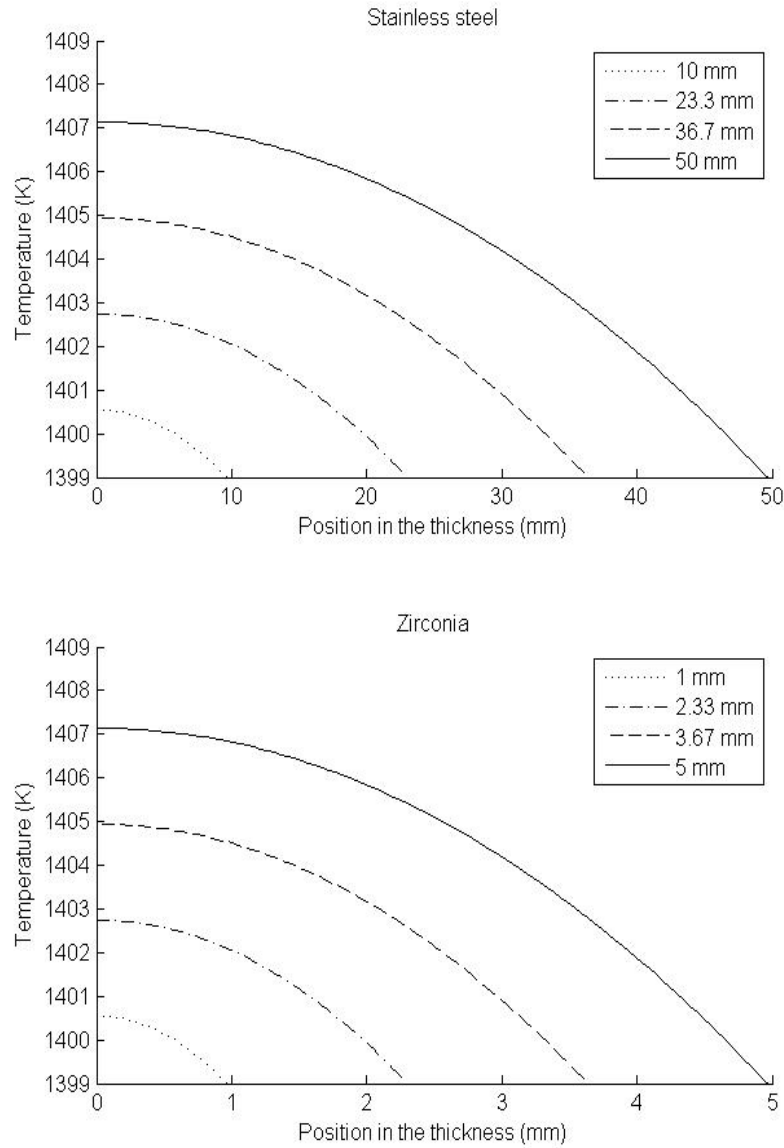


Figure 35 – Temperature profile throughout the layer of thickness L in stainless steel walls (top) and zirconia walls (bottom). Note the different scale in the x-axis and the different thicknesses shown.

It should also be noted that the value of $h_1(0)$, and therefore the thickness of insulation, can be selected to maintain the thermal losses through the wall of the receiver below a certain target level. Figure 34 shows the ratio $r(L)$ for stainless steel (top) and zirconia walls (bottom). For a maximum error of 1% in the estimate of the emissive power ($r \leq 1.0025$), the thickness of the layer should be not greater than 3 cm for stainless steel walls and not greater than 3 mm for zirconia walls.

Further analysis of the temperature profile in the layer of thickness L (Figure 35) reveals that the inner wall temperature is approximately equal to the exact solution regardless the

thickness. This, which occurs due to the fact that $h_1(L) \ll h_2$ for the range of L considered, implies that thicker layers are acceptable as long as only the CFD cells whose centroid is closer than a distance ε to the inner wall surface (around 1 cm for stainless steel and 1 mm for zirconia) are considered when averaging the temperature. Note, finally, that the CFD grid must be so that at least the centroid of the first row of wall cells is closer than a distance ε from the inner surface.

Appendix I

Mathematical Model of the Conservative Interpolation Scheme for the Source Term

The interpolation scheme employed is a multi-linear interpolation method, i.e., the radiative source term will be a hyperbolic paraboloid in $\mathbb{R}^4 = [z \times r \times \varphi \times S]$ that interpolates the eight neighbor Monte Carlo cells $-I_{1234}(z, r, \varphi)-$ multiplied by a proper constant $-K-$ so that the total interpolated source term exactly matches the actual value:

$$\Psi(z, r, \varphi) = K I_{1234}(z, r, \varphi) \quad (\text{I-1})$$

It is convenient to introduce the dimensionless variables shown in Table 26. This way, the resulting equations for cells Type 2 and 3 (recall the nomenclature for the fluid cells introduced in Section 3.4) can be expressed in the same (and more compact) manner.

Cells Type 2	Cells Type 3
$\tilde{z}(z) = \frac{z - z_1}{\Delta z}$	$\tilde{z}(z, r) = \frac{z - z_1(r)}{\Delta z(r)}$
$\tilde{\varphi}(\varphi) = \frac{\varphi - \varphi_1}{\Delta \varphi}$	$\tilde{\varphi}(\varphi) = \frac{\varphi - \varphi_1}{\Delta \varphi}$
$\tilde{r}(r, z) = \frac{r - r_1(z)}{\Delta r(z)}$	$\tilde{r}(r) = \frac{r - r_1}{\Delta r}$

Table 26 – Dimensionless variables employed for the interpolation function.

The interpolation function in dimensionless variables takes the same form for cells Type 1, 2 and 3:

$$\begin{aligned} \tilde{\Psi}(\tilde{z}, \tilde{\varphi}, \tilde{r}) = K[& S_1 + (S_5 - S_1)\tilde{\varphi} + (S_2 - S_1)\tilde{z} + (S_3 - S_1)\tilde{r} + (S_1 + S_6 - S_2 - S_5)\tilde{\varphi}\tilde{z} \\ & + (S_1 + S_7 - S_3 - S_5)\tilde{\varphi}\tilde{r} + (S_1 + S_4 - S_2 - S_3)\tilde{z}\tilde{r} \\ & + (S_2 + S_3 + S_5 + S_8 - S_1 - S_4 - S_6 - S_7)\tilde{z}\tilde{\varphi}\tilde{r}] \end{aligned} \quad (\text{I-2})$$

Where the value of the constant K is such that the total interpolated source term (energy) exactly matches the actual value. The total interpolated source term, $\mathbb{I}$, can be readily computed by integration:

- Cells Type 2:

$$\begin{aligned}
 \mathbb{I} &= \int_{\varphi_1}^{\varphi_2} \int_{z_1}^{z_2} \int_{r_1(z)}^{r_2(z)} \Psi(z, r, \varphi) r \, dr \, dz \, d\varphi \\
 &= \int_0^1 \int_0^1 \int_0^1 \tilde{\Psi}(\tilde{z}, \tilde{\varphi}, \tilde{r}) [r_{11} + (r_{21} - r_{11})\tilde{z} + (r_{12} - r_{11})\tilde{r} \\
 &\quad + (r_{11} - r_{12} - r_{21} + r_{22})\tilde{z}\tilde{r}] \left| \frac{\partial(r, z, \varphi)}{\partial(\tilde{z}, \tilde{\varphi}, \tilde{r})} \right| d\tilde{r} \, d\tilde{z} \, d\tilde{\varphi}
 \end{aligned} \tag{I-3}$$

- Cells Type 3:

$$\begin{aligned}
 \mathbb{I} &= \int_{\varphi_1}^{\varphi_2} \int_{r_1}^{r_2} \int_{z_1(r)}^{z_2(r)} \Psi(z, r, \varphi) r \, dr \, dz \, d\varphi \\
 &= \int_0^1 \int_0^1 \int_0^1 \tilde{\Psi}(\tilde{z}, \tilde{\varphi}, \tilde{r}) [r_1 + (r_2 - r_1)\tilde{r}] \left| \frac{\partial(r, z, \varphi)}{\partial(\tilde{z}, \tilde{\varphi}, \tilde{r})} \right| d\tilde{r} \, d\tilde{z} \, d\tilde{\varphi}
 \end{aligned} \tag{I-4}$$

For cells Type 1 either expression applies as they are just a particular case of both cells Type 2 and 3. The Jacobian of the transformation is:

- Cells Type 2:

$$\frac{\partial(z, \varphi, r)}{\partial(\tilde{z}, \tilde{\varphi}, \tilde{r})} = \begin{pmatrix} \Delta z & 0 & 0 \\ 0 & \Delta \varphi & 0 \\ (r_{21} - r_{11}) + (r_{11} - r_{12} - r_{21} + r_{22})\tilde{r} & 0 & (r_{12} - r_{11}) + (r_{11} - r_{12} - r_{21} + r_{22})\tilde{z} \end{pmatrix} \tag{I-5}$$

- Cells Type 3:

$$\frac{\partial(z, \varphi, r)}{\partial(\tilde{z}, \tilde{\varphi}, \tilde{r})} = \begin{pmatrix} (z_{21} - z_{11}) + (z_{11} - z_{12} - z_{21} + z_{22})\tilde{r} & 0 & (z_{12} - z_{11}) + (z_{11} - z_{12} - z_{21} + z_{22})\tilde{z} \\ 0 & \Delta \varphi & 0 \\ 0 & 0 & \Delta r \end{pmatrix} \tag{I-6}$$

And its determinant:

- Cells Type 2:

$$\left| \frac{\partial(r, z, \varphi)}{\partial(\tilde{z}, \tilde{\varphi}, \tilde{r})} \right| = [(r_{12} - r_{11}) + (r_{11} - r_{12} - r_{21} + r_{22})\tilde{z}]\Delta z \Delta \varphi > 0 \tag{I-7}$$

- Cells Type 3:

$$\left| \frac{\partial(r, z, \varphi)}{\partial(\tilde{z}, \tilde{\varphi}, \tilde{r})} \right| = [(z_{21} - z_{11}) + (z_{11} - z_{12} - z_{21} + z_{22})\tilde{r}]\Delta r \Delta \varphi > 0 \tag{I-8}$$

Therefore,

- Cells Type 2:

$$\begin{aligned} \mathbb{I} = \int_0^1 \int_0^1 \int_0^1 K [S_1 + (S_5 - S_1)\tilde{\varphi} + (S_2 - S_1)\tilde{z} + (S_3 - S_1)\tilde{r} + (S_1 + S_6 - S_2 - S_5)\tilde{\varphi}\tilde{z} \\ + (S_1 + S_7 - S_3 - S_5)\tilde{\varphi}\tilde{r} + (S_1 + S_4 - S_2 - S_3)\tilde{z}\tilde{r} \\ + (S_2 + S_3 + S_5 + S_8 - S_1 - S_4 - S_6 - S_7)\tilde{z}\tilde{\varphi}\tilde{r}] [r_{11} + (r_{21} - r_{11})\tilde{z} + (r_{12} - r_{11})\tilde{r} \\ + (r_{11} - r_{12} - r_{21} + r_{22})\tilde{z}\tilde{r}] [(r_{12} - r_{11}) + (r_{11} - r_{12} - r_{21} + r_{22})\tilde{z}] \Delta z \Delta \varphi d\tilde{r} d\tilde{z} d\tilde{\varphi} \end{aligned} \quad (\text{I-9})$$

- Cells Type 3:

$$\begin{aligned} \mathbb{I} = \int_0^1 \int_0^1 \int_0^1 K [S_1 + (S_5 - S_1)\tilde{\varphi} + (S_2 - S_1)\tilde{z} + (S_3 - S_1)\tilde{r} + (S_1 + S_6 - S_2 - S_5)\tilde{\varphi}\tilde{z} \\ + (S_1 + S_7 - S_3 - S_5)\tilde{\varphi}\tilde{r} + (S_1 + S_4 - S_2 - S_3)\tilde{z}\tilde{r} \\ + (S_2 + S_3 + S_5 + S_8 - S_1 - S_4 - S_6 - S_7)\tilde{z}\tilde{\varphi}\tilde{r}] [r_1 + (r_2 - r_1)\tilde{r}] [(z_{21} - z_{11}) \\ + (z_{11} - z_{12} - z_{21} + z_{22})\tilde{r}] \Delta r \Delta \varphi d\tilde{r} d\tilde{z} d\tilde{\varphi} \end{aligned} \quad (\text{I-10})$$

The previous two integrals take the form $\mathbb{I} = K C_1 \Delta z \Delta \varphi$, where the only difference is the expression of the constant C_1 :

- Cells Type 2:

$$\begin{aligned} C_1 = S_1 \left[-\frac{r_{11}^2}{24} + \frac{r_{12}^2}{48} - \frac{r_{21}^2}{72} + \frac{r_{22}^2}{144} + \frac{r_{11}r_{12}}{48} - \frac{r_{11}r_{21}}{36} + \frac{r_{11}r_{22}}{144} + \frac{r_{12}r_{21}}{144} + \frac{r_{12}r_{22}}{72} + \frac{r_{21}r_{22}}{144} \right] \\ + S_2 \left[-\frac{r_{11}^2}{72} + \frac{r_{12}^2}{144} - \frac{r_{21}^2}{24} + \frac{r_{22}^2}{48} + \frac{r_{11}r_{12}}{144} - \frac{r_{11}r_{21}}{36} + \frac{r_{11}r_{22}}{144} + \frac{r_{12}r_{21}}{144} + \frac{r_{12}r_{22}}{72} + \frac{r_{21}r_{22}}{48} \right] \\ + S_3 \left[-\frac{r_{11}^2}{48} + \frac{r_{12}^2}{24} - \frac{r_{21}^2}{144} + \frac{r_{22}^2}{72} - \frac{r_{11}r_{12}}{48} - \frac{r_{11}r_{21}}{72} - \frac{r_{11}r_{22}}{144} - \frac{r_{12}r_{21}}{144} + \frac{r_{12}r_{22}}{36} - \frac{r_{21}r_{22}}{144} \right] \\ + S_4 \left[-\frac{r_{11}^2}{144} + \frac{r_{12}^2}{72} - \frac{r_{21}^2}{48} + \frac{r_{22}^2}{24} - \frac{r_{11}r_{12}}{144} - \frac{r_{11}r_{21}}{72} - \frac{r_{11}r_{22}}{144} - \frac{r_{12}r_{21}}{144} + \frac{r_{12}r_{22}}{36} - \frac{r_{21}r_{22}}{48} \right] \\ + S_5 \left[-\frac{r_{11}^2}{24} + \frac{r_{12}^2}{48} - \frac{r_{21}^2}{72} + \frac{r_{22}^2}{144} + \frac{r_{11}r_{12}}{48} - \frac{r_{11}r_{21}}{36} + \frac{r_{11}r_{22}}{144} + \frac{r_{12}r_{21}}{144} + \frac{r_{12}r_{22}}{72} + \frac{r_{21}r_{22}}{144} \right] \\ + S_6 \left[-\frac{r_{11}^2}{72} + \frac{r_{12}^2}{144} - \frac{r_{21}^2}{24} + \frac{r_{22}^2}{48} + \frac{r_{11}r_{12}}{144} - \frac{r_{11}r_{21}}{36} + \frac{r_{11}r_{22}}{144} + \frac{r_{12}r_{21}}{144} + \frac{r_{12}r_{22}}{72} + \frac{r_{21}r_{22}}{48} \right] \\ + S_7 \left[-\frac{r_{11}^2}{48} + \frac{r_{12}^2}{24} - \frac{r_{21}^2}{144} + \frac{r_{22}^2}{72} - \frac{r_{11}r_{12}}{48} - \frac{r_{11}r_{21}}{72} - \frac{r_{11}r_{22}}{144} - \frac{r_{12}r_{21}}{144} + \frac{r_{12}r_{22}}{36} - \frac{r_{21}r_{22}}{144} \right] \\ + S_8 \left[-\frac{r_{11}^2}{144} + \frac{r_{12}^2}{72} - \frac{r_{21}^2}{48} + \frac{r_{22}^2}{24} - \frac{r_{11}r_{12}}{144} - \frac{r_{11}r_{21}}{72} - \frac{r_{11}r_{22}}{144} - \frac{r_{12}r_{21}}{144} + \frac{r_{12}r_{22}}{36} - \frac{r_{21}r_{22}}{48} \right] \end{aligned} \quad (\text{I-11})$$

And analogously for cells Type 3.

Finally, K is such that the integral of the interpolation function exactly matches the actual radiative source term in the interpolation zone:

$$K = \frac{\sum_{i=1}^8 S_i \check{V}_i}{C_1 \Delta z \Delta \varphi} \quad (\text{I-12})$$

With:

$$\begin{aligned}
\check{V}_1 &= \frac{1}{24} \Delta \varphi \Delta z_1 (r_\alpha^2 + r_\beta^2 + r_\alpha r_\beta - r_{11}^2 - r_\delta^2 - r_{11} r_\delta) \\
\check{V}_2 &= \frac{1}{24} \Delta \varphi \Delta z_2 (r_\beta^2 + r_\gamma^2 + r_\beta r_\gamma - r_\delta^2 - r_{21}^2 - r_\delta r_{21}) \\
\check{V}_3 &= \frac{1}{24} \Delta \varphi \Delta z_3 (r_{12}^2 + r_\varepsilon^2 + r_{12} r_\varepsilon - r_\alpha^2 - r_\beta^2 - r_\alpha r_\beta) \\
\check{V}_4 &= \frac{1}{24} \Delta \varphi \Delta z_4 (r_\varepsilon^2 + r_{22}^2 + r_\varepsilon r_{22} - r_\beta^2 - r_\gamma^2 - r_\beta r_\gamma) \\
\check{V}_5 &= \frac{1}{24} \Delta \varphi \Delta z_5 (r_\alpha^2 + r_\beta^2 + r_\alpha r_\beta - r_{11}^2 - r_\delta^2 - r_{11} r_\delta) \\
\check{V}_6 &= \frac{1}{24} \Delta \varphi \Delta z_6 (r_\beta^2 + r_\gamma^2 + r_\beta r_\gamma - r_\delta^2 - r_{21}^2 - r_\delta r_{21}) \\
\check{V}_7 &= \frac{1}{24} \Delta \varphi \Delta z_7 (r_{12}^2 + r_\varepsilon^2 + r_{12} r_\varepsilon - r_\alpha^2 - r_\beta^2 - r_\alpha r_\beta) \\
\check{V}_8 &= \frac{1}{24} \Delta \varphi \Delta z_8 (r_\varepsilon^2 + r_{22}^2 + r_\varepsilon r_{22} - r_\beta^2 - r_\gamma^2 - r_\beta r_\gamma)
\end{aligned} \tag{I-13}$$

Therefore, the interpolation function can be readily computed as:

$$\begin{aligned}
\Psi(z, r, \varphi) &= \frac{\sum_{i=1}^8 S_i \check{V}_i}{C_1 \Delta z \Delta \varphi} I_{1234}(z, r, \varphi) \\
&= \frac{\sum_{i=1}^8 S_i \check{V}_i}{C_1 \Delta z \Delta \varphi} \left[S_1 + \frac{S_5 - S_1}{\Delta \varphi} (\varphi - \varphi_1) + \frac{S_2 - S_1}{\Delta z} (z - z_1) + \frac{S_3 - S_1}{\Delta r(z)} (r - r_1(z)) \right. \\
&\quad + \frac{S_1 + S_6 - S_2 - S_5}{\Delta \varphi \Delta z} (\varphi - \varphi_1)(z - z_1) \\
&\quad + \frac{S_1 + S_7 - S_3 - S_5}{\Delta \varphi \Delta r(z)} (\varphi - \varphi_1)(r - r_1(z)) \\
&\quad + \frac{S_1 + S_4 - S_2 - S_3}{\Delta z \Delta r(z)} (z - z_1)(r - r_1(z)) \\
&\quad \left. + \frac{S_2 + S_3 + S_5 + S_8 - S_1 - S_4 - S_6 - S_7}{\Delta \varphi \Delta z \Delta r(z)} (\varphi - \varphi_1)(z - z_1)(r - r_1(z)) \right]
\end{aligned} \tag{I-14}$$

Or, in dimensionless variables:

$$\begin{aligned}
\tilde{\Psi}(\tilde{z}, \tilde{\varphi}, \tilde{r}) &= \frac{\sum_{i=1}^8 S_i \check{V}_i}{C_1 \Delta z \Delta \varphi} [S_1 + (S_5 - S_1) \tilde{\varphi} + (S_2 - S_1) \tilde{z} + (S_3 - S_1) \tilde{r} + (S_1 + S_6 - S_2 - S_5) \tilde{\varphi} \tilde{z} \\
&\quad + (S_1 + S_7 - S_3 - S_5) \tilde{\varphi} \tilde{r} + (S_1 + S_4 - S_2 - S_3) \tilde{z} \tilde{r} \\
&\quad + (S_2 + S_3 + S_5 + S_8 - S_1 - S_4 - S_6 - S_7) \tilde{z} \tilde{\varphi} \tilde{r}]
\end{aligned} \tag{I-15}$$