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HeatTracer - A Novel Monte Carlo Radiative Heat Transfer Tool for Cavity Receivers Simulation

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Abstract. The development of new receivers for central receiver systems operating at high temperatures require the development of suitable tools able to accurately simulate heat and mass transfer processes.Such tools should be able to process complex receiver geometries with nongray and directionally nonideal surfaces. This work introduces the development of a new tool, HeatTracer, for the simulation of radiative heat transfer based on the Monte Carlo method, directed to the study of radiation exchange for arbitrary user-defined cavity geometries with spectral and/or directional nonidealities. The main characteristics of this tool are presented, including the main physical models as well as some of the more relevant mathematical and computational algorithms.

INTRODUCTION

The concentration of solar radiation can be used to power a wide range of thermodynamic and thermochemical processes operating at medium and high temperature levels (i.e. temperatures above 100°C). Its potential use encompasses diverse applications such as cooling and refrigeration, industrial process heat, electrical power generation, solar fuels and chemical production [1]. In order to fully tap this significant potential the development of improved and novel solutions able to achieve higher efficiencies and/or lower costs is required.

Central Receiver Systems (CRS) are considered to hold great cost reduction potential for solar thermal electricity (STE) applications [1, 2, 3]. Moreover, CRS can achieve high concentration ratios, being able to operate the solar receiver at higher temperatures (>550 °C), enabling the utilization of more efficient thermodynamic power cycles such as combined cycles, supercritical steam Rankine cycles or supercritical CO_2 Brayton cycles [1, 4, 5]. Additionally, long term development of CRS technologies for applications beyond STE is ongoing in areas such as high temperature thermochemical processes and high temperature industrial processes [6, 7].

Independently of the CRS' receiver/reactor technology (e.g.: molten salt, solid particles or gas receivers), one of the major research focus lies on the receiver design, namely the increase of its thermal efficiency at higher operation temperatures [8]. The development of a new generation of solar receivers for CRS plants require the development of advanced simulation tools able to accurately account for the heat and mass transfer processes occurring within the receiver. Moreover, considering the results from [9, 10], new receiver concepts might exploit the properties of nonideal surfaces or more complex geometries, requiring software tools able to cope with the accurate simulation of heat transfer under such nonideal conditions.

This work introduces a new software tool for detailed simulation of receiver's thermal radiation exchange, based on the Monte Carlo Radiative Heat Transfer method, able to model complex receiver geometries with nongray and directionally nonideal surfaces. The main characteristics of the method and the tool are presented, including the main physical models as well as the more relevant mathematical and computational algorithms.

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TOOL PURPOSE

The purpose of this software is to provide a general and flexible tool to simulate radiative heat transfer in cavity receivers with complex geometries and nonideal surfaces, enabling the study of radiation exchange for arbitrary user-defined cavity geometries with spectral and/or directional nonidealities.

The tool - nicknamed HeatTracer - can be used to study the impact of different geometries/surface optical properties in cavities' radiative heat transfer. Moreover it is being developed in order to allow integration with tools dealing with other heat transfer modes in order to enable integral simulation of cavity receiver's heat transfer. Additionally, it can also be used to compute view factors (including specular view factors) depending on the surface properties selected by the user.

MODELLING AND SIMULATION METHODOLOGY

Currently, many cavity receiver models use simplified approximations of surface properties such as gray, diffuse or specular reflectance and gray, diffuse absorptance and emittance. Also, the cavity geometries are usually relatively simple. However, some systems of interest may not be adequately described using these simplifications. In fact, there might be cases where more complex geometries and/or the utilization of surfaces with nonideal radiative properties could be explored to improve the receiver thermal efficiency, as can be hinted from [9, 10]. Such cases represent complex radiative heat transfer problems whose formulation and resolution is usually very heavy for traditional numerical methods (such as the net radiation method) but which may be more easily solved through a statistical approach by a Monte Carlo technique [11, 12].

The core of this computational tool is a solver for the cavities' radiative heat transfer problem, where the radiative heat transfer is modelled using a biased Monte Carlo approach able to process directionally nonideal surfaces as well as nongray surfaces. As a first approach only non-participating media are considered. The tool is being developed having in mind future coupling between radiative and other heat transfer mechanisms.

Incident solar radiation on the cavity apertures is taken into account through integration of the radiative heat transfer solver with the Tonatiuh software [13]. This is achieved by calling the Tonatiuh software at each time-step and running the ray-tracing simulation for the desired solar field/receiver geometry. This approach allows the simultaneous study of the solar field and receiver, enabling the combined optimization of both components.

Monte Carlo Method for Surface Exchange

When dealing with non-participating media it is possible to determine the radiative heat flux in a given surface by computing the difference between the amount of heat emitted by the surface through radiation and the amount of heat absorbed by the surface due to the incident radiation incoming from the cavity walls and apertures. For an enclosure surface divided in a set of J subsurfaces, the radiative heat flux at subsurface i may be written as [11]:

$$Q_i = \epsilon_i n_i^2 \sigma T_i^4 A_i - \sum_{j=1}^{J} \epsilon_j n_j^2 \sigma T_j^4 A_j \mathscr{F}_{A_j - A_i} - q_o A_o \mathscr{F}_{A_o - A_i} \tag{1}$$

where ϵ, n, T and A represent emittance, refraction index, temperature and area for a given surface. q_o represent the external energy entering the cavity through its aperture and A_o its area. $\mathscr{F}_{A_j - A_i}$ represents a generalized radiation exchange factor between surface A_j and A_i which may not be independent of surface temperatures (e.g.: nongray surfaces). Care must be taken to ensure the refraction index at the subsurface as well as its total hemispherical emittance and temperature are suitable average values for each subsurface, or mathematically:

$$\epsilon_i n_i^2 \sigma T_i^4 = \frac{1}{A_i} \int_{A_i} \epsilon n^2 \sigma T^4 dA. \tag{2}$$

Equation 1 can be solved using the Monte Carlo method by tracing the life of statistically meaningful random samples of photons throughout their lifetime in the cavity, i.e., from emission (or entrance in the enclosure of interest if openings exist) until absorption (or exit of the enclosure if openings are present). In order to have a statistically meaningful random sample of photon bundles it is necessary to determine its origin, direction of travel and wavelength as well as the effect on the bundle of eventual interactions with the enclosure surfaces. This can be achieved by considering the cumulative distribution functions for each parameter of interest (point of emission, direction of emission, wavelength of emission, reflectance, absorptance and transmittance) and relating them with random numbers. Given a large set of energy bundles emitted from surface i, (N_i), and counting the number of such bundles absorbed by surface j, (N_{ij}) then [11]:

$$\mathscr{F}_{A_i-A_j} \approx \left(\frac{N_{ij}}{N_i}\right)_{N_i>>1} \tag{3}$$

The use of a statistical technique implies the existence of a level of uncertainty in the solution due to statistical errors and fluctuations. Considering a division of the total number of bundles in a group of K subsets and computing the variance of the solution given by each subset it is possible to estimate the error associated with a solution. Assuming N_i bundles have been emitted from surface i and that $F_{ij}(N_i)$ is the solution obtained for the generalized exchange factor between surface i and j and dividing the N_i bundles in K subsets, the variance associated with the solution $F_{ij}(N_i)$ is given by

$$\sigma^2_{F_{ij}} = \frac{1}{K(K-1)} \sum_{k=1}^{K} \left(F_{ij}(N_k) - F_{ij}(N_i)\right)^2 \tag{4}$$

Following the central limit theorem, using large number of photon bundles, it is possible to state that with 95,5% of confidence the true solution lies within $F_{ij}(N_i) + 2\sigma_{F_{ij}}$ [11, 12, 14].

Description of the Receiver Geometry

The 3D cavity geometry is defined by a set of triangle-based tessellated surfaces, being each surface defined by the user through an STL (stereolithography) file. The STL format is one of the simplest CAD file formats, using triangular facets to describe 3D surfaces, each facet described by its three vertices' position and its outward pointing normal vector. Since STL is simple, vendor neutral Computer Aided Design (CAD) file, it is supported by the majority of CAD software. Moreover, using the STL file format ensures compatibility with the Tonatiuh ray-tracer, which also uses the STL file format for its CAD import tool. Not only HeatTrace is able to directly import surfaces designed using most common CAD tools but it also uses a format compatible with the Tonatiuh ray-tracer [15], avoiding the need to specify the same cavity geometry in different formats, thus contributing to simplify the users work flow.

At the moment it is not possible to define surfaces with multiple radiative properties, thus, each kind of surface, i.e., for each set of surface radiative properties, must have at least one STL file uploaded to the software.

Surface's Radiative Properties

This software is able to process several kinds of surfaces including black, grey and nongray surfaces, being capable of modelling anisotropic emission and nonideal reflection. The full list of available radiative properties can be viewed in table 1. Radiative properties with nonideal characteristics are defined for each surface according to user inputs provided in tabular form, being interpolated at a pre-processing stage. At the moment the cavity surfaces are restricted to opaque surfaces, thus no transmission effects are included, implying that semi-transparent surfaces cannot be used. Work is ongoing to relieve this limitation.

Incident Solar Radiation

In order to simulate the solar radiation incident on the cavity apertures, HeatTracer is being integrated with the open-source Tonatiuh ray-tracing software. The core for this integration is the ability to run and update Tonatiuh scripts and to process result files. For each Sun position/time step the Monte Carlo Radiative Heat Transfer (MCRHT) solver calls Tonatiuh, running a user-defined Tonatiuh script containing the optical system of interest. Tonatiuh's output files are automatically processed to determine the energy, position and direction vector of the rays at each aperture surface in the right coordinate system. This information is used to generate photon bundles that are propagated by the MCRHT solver.

Tracing the Life of Statistically Meaningful Random Samples of Photons

At the heart of the Monte Carlo method for radiative heat transfer lies the tracing of statistically meaningful random samples of photons. By convenience it is usual to consider bundles of photons of equal characteristics instead of single

TABLE 1. Available models for surface's radiative properties.

Property	Dependence	Type
Emissivity	Spectral	Black surface Gray surface Non-gray surface
	Directional	Diffuse Azimuthally isotropic and non-diffuse Anisotropic
Absorptance	Spectral	Black surface Gray surface Non-gray surface
	Directional	Diffuse Specular Bi-directional
Reflectance	Spectral	Gray surface Non-gray surface
	Directional	Diffuse Specular Bi-directional

photons. These bundles can correspond to radiation entering the cavity from external sources, in this case from the concentrated solar radiative flux incoming from the heliostat field, or radiation emitted by the cavity walls.

The statistical representativeness of the photon bundles and its interactions can be achieved by considering the relevant probability functions when dealing with an event, being it a photon bundle emission or an interaction with a surface. It is known that for a given variable the probability density function can be satisfied by casting random numbers and using the inverse cumulative distribution function to compute the variable values [11, 12, 14]. Currently the tool uses a Mersenne-Twister pseudo-random number generator [16]

Photon Emission

For each surface a user defined number of photon bundles is emitted (N_b). Since the surface is tesselated by N_t triangles, each triangular surface will emit $N_s = N_b/N_t$ bundles carrying energy equal to $\epsilon_s n^2 \sigma T_s^4 A_s/N_s$ per bundle.

The emission of a photon bundle requires the knowledge of the point of emission and the direction of emission. The determination of the point of emission can be perform independently from the surface radiative properties and the bundle wavelength as long as each triangular surface is small enough such that its temperature and radiative properties are constant throughout the surface. However, the direction of emission will be dependent on the surface temperature and radiative properties.

Considering a triangle of vertices A, B and C, any point P contained by the triangle surface can be described by using barycentric coordinates: $P = A + \beta(B - A) + \gamma(C - A)$. Assuming a surface of constant temperature and radiative properties, the emissive power of a triangular surface can be written as

$$E_s = \int_{A_s} \epsilon_s \sigma T_s^4 dA = 2\epsilon_s \sigma T_s^4 A_s \int_0^1 \int_0^{1-\gamma} d\beta\, d\gamma \quad (5)$$

From the above, it is possible to write a cumulative distribution function of the emissive power as a function of coordinate γ and its relation with random numbers, $R \in [0\,1]$:

$$R_\gamma = \frac{1}{E_s} \int_0^\gamma \int_0^{1-\gamma} 2\epsilon_s \sigma T_s^4 A_s\, d\beta = \frac{1}{E_s} \int_0^\gamma E_s^{'}\, d\gamma = 2\gamma - \gamma^2 \quad (6)$$

and the cumulative distribution function of the emissive power as a function of coordinate γ and its relation with random numbers of the interval [0 1] is given by

$$R_\beta = \frac{1}{E_s^{'}} \int_0^\beta 2\epsilon_s \sigma T_s^4 A_s\, d\beta \quad (7)$$

These relationships enable the computation of the photon bundle emission point in barycentric coordinates, β and γ, and 3D Cartesian coordinate system, P:

$$\gamma = 1 - \sqrt{(1 - R_\gamma)} \tag{8}$$

$$\beta = (1 - \gamma)R_\beta = \sqrt{(1 - R_\gamma} R_\beta \tag{9}$$

$$P = A + \sqrt{(1 - R_\gamma} R_\beta (B - A) + (1 - \sqrt{1 - R_\gamma})(C - A) \tag{10}$$

The relevant cumulative distribution function can be obtained considering the spectral emissive power, E_λ. Considering the spectral, directional emittance ϵ'_λ, the blackbody spectral radiative intensity $I_{b\lambda}$ and the blackbody emissive power $E_{b\lambda}$ it is possible to write

$$E_\lambda = \int_{2\pi} \epsilon'_\lambda I_{b\lambda} \cos\theta \, d\Omega = \frac{E_{b\lambda}}{\pi} \int_0^{2\pi} \int_0^{\pi/2} \epsilon'_\lambda \cos\theta \sin\theta \, d\theta \, d\psi \tag{11}$$

The cumulative distribution functions for the emissive power as a function of the emission azimuth, ψ, and zenith angle, θ and their relation with random numbers, R, of the interval [0 1] are respectively [11]

$$R_\psi = \frac{E_{b\lambda}}{\pi E_\lambda} \int_0^{\psi} \int_0^{\pi/2} \epsilon'_\lambda \cos\theta \sin\theta \, d\theta \, d\psi = \frac{1}{\pi \epsilon_\lambda} \int_0^{\psi} \int_0^{\pi/2} \epsilon'_\lambda \cos\theta \sin\theta \, d\theta \, d\psi \tag{12}$$

$$R_\theta = \frac{\int_0^{\theta} \epsilon'_\lambda \cos\theta \sin\theta \, d\theta}{\int_0^{\pi/2} \epsilon'_\lambda \cos\theta \sin\theta \, d\theta} \tag{13}$$

The determination of the azimuthal and zenithal angles of emission require the inversion of these equations. For surfaces with isotropic emission in the azimuthal angle $\psi = 2\pi R_\psi$. For surfaces with isotropic emission in the zenithal angle $\theta = \arcsin \sqrt{R_t heta}$. To account for surfaces with more complex behaviours the user can include the relevant relationships through a polynomial fit or in tabular format. Information presented in tabular format will be interpolated in a pre-processing step using cubic spline interpolation. Thus, the software is able to determine the relations between the desired emission angles and the random numbers for surfaces with directional non-ideal characteristics.

Photon-Surface Interaction

Once emitted by a surface or once entering the cavity from an aperture, the bundles are traced throughout the enclosure. At the base of the tracing process is the photon bundle - surface intersection algorithm, which determines were the bundle's next interaction with the cavity surfaces occur. Since the surfaces are described by triangular facets in HeatTracer, a suitable ray-triangle intersection algorithm was chosen. Taking advantage of the vast literature on ray-triangle intersection originated from the computer graphics field (since this is a critical operation for modern ray-tracing rendering), the Möller-Trumbore algorithm [17] was implemented, since it is considered to be one of the fastest ray-triangle intersection algorithm for both CPU and GPU implementations [18, 19].

The direct application of a ray-triangle intersection test results forces the test of all triangular surfaces for each photon bundle step, resulting in high computation times when the number of triangular facets is large. In order to avoid the test of all triangular facets and speed up the tracing process, a Bounding Volume Hierarchy (BVH) was implemented. BVHs are an hierarchical object partition structure consisting of a tree structure based on a root node with a bounding volume containing all the object geometry and a number of children nodes whith their corresponding bounding volumes containing a number of triangles [20]. This software uses binary trees with bounding volumes consisting of axis aligned bounding boxes. The BVH is built using a top-down approach: the root node contains all the triangular surfaces composing the cavity, and splits them in two child nodes following the Kay/Kajiya recursive top-down approach adapted from [20].

Photon bundle propagation throughout the cavity starts with the determination of the next intersection point with the surface. The implemented BVH traversal algorithm performs a top-down search in depth, testing the nodes of the binary tree. Ray-triangle intersection tests are only performed for the triangles contained in nodes whose bounding volumes are intersected by the photon bundle. If no intersection occurs with any of the triangles the photon bundle is terminated and its identity, exit position, direction and energy are registered.

Considering opaque surfaces only, when an intersection occurs it is necessary to determine if the bundle is absorbed or reflected. This software uses a energy partitioning method to increase the efficiency of the Monte Carlo method, implying that at each intersection if an absorption event occurs, only a fraction of the bundle's energy corresponding to the directional, spectral absorptance α'_λ is absorbed by the surface, being the bundle reflected with a fraction of its incoming energy equal to $1 - \alpha'_\lambda$. When the photon bundle energy drops below a given set point the ray is terminated. This type of energy partitioning scheme increases the convergence rate of the model by ensuring that each intersection event contributes to the computation of the generalized radiation exchange factor [11, 12].

The reflected ray's direction needs to be determined after each bundle-surface interaction in order to be traced once again. The reflection direction is dependent on the bidirectional reflection function of the intersected surface material, ρ''_λ. The cumulative distribution functions for the reflection angular direction and their relationship with a random number $R \in [0\ 1]$ are [11]

$$R_\phi = \frac{\int_0^\psi \int_0^{\pi/2} \rho''_\lambda \cos\theta \sin\theta \, d\theta \, d\psi}{\int_0^{2\pi} \int_0^{\pi/2} \rho''_\lambda \cos\theta \sin\theta \, d\theta \, d\psi} \tag{14}$$

$$R_\theta = \frac{\int_0^\theta \rho''_\lambda \cos\theta \sin\theta \, d\theta}{\int_0^{\pi/2} \rho''_\lambda \cos\theta \sin\theta \, d\theta} \tag{15}$$

For diffuse reflectors the reflected azimuthal and zenithal angles are given by $\psi = 2\pi R_\psi$ and $\theta = \arcsin\sqrt{R_\theta}$ respectively, while for purely specular reflectors the angles are given by $\psi = psi_i + \pi$ and $\theta = \theta_i$, where the subscript i represents the incoming beam. Similarly for the emission direction, it is necessary to invert the cumulative distribution functions in order to compute the required reflected angular direction, with the user having the option to provide the information in tabular format do be interpolated by the program or use a polynomial approximation.

Development Environment

The Monte Carlo radiative heat transfer computational model is being developed in Fortran 2008 using the Eclipse IDE and the GFortran compiler under a Linux operative system. The User inputs and program outputs are passed through text files processed using scripts developed by the user (e.g. in Python, Matlab, Mathematica, etc.). Current development is focused on the MCRHT engine being the improvement of the user interface a secondary objective to be developed in future work. The model can be called by external software, as long as they can execute a shell command, enabling the integration of the model in other codes/programs.

CONCLUSIONS AND FUTURE WORK

The first version of HeatTracer is being developed with the goal of simulating the radiative heat transfer processes in user-defined cavity receivers with non-participating media and generalized surface properties, using a Monte Carlo approach. The model deals only with radiative heat transfer, not accounting for convection or conduction phenomena. Further development is required in order to couple the radiation heat transfer mode with other heat transfer mechanisms.

Currently the model is only able to simulate surface exchange being unfit for the treatment of receivers with participating media. The development of future version will focus on expanding the tool to allow the treatment of participative media. This will be a significant improvement, enabling the study of a wider range of receivers and thermochemical reactors.

A validation process is currently under definition and will be performed in the near future, consisting on comparing results from the HeatTracer tool for generalized view factors with analytical results for typical geometries and result comparison with other tools.

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