

Introducing FIVER: An Open-Source Tool to Simulate Heat Transfer in Participating Media and Arbitrary Geometries

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Abstract. Decarbonization of industrial processes operating at above 1000 °C is a major challenge. A promising answer lies in concentrating solar thermal technologies, but current receivers operate at about 600 °C only. New concepts are needed to achieve the target temperatures with good efficiencies, thus enabling commercial deployments. Further advances require that researchers have access to simulation tools treating heat transfer problems in radiatively participating media accurately, which is seldom the case today. Here we present a first effort to bridge this gap, introducing FIVER (FInite VolumE Ray tracer), an open-source Matlab tool for solving transient radiative-conductive heat transfer problems in participating media with spectral properties and complex geometries. FIVER tackles the challenging simulations needed to design the solar receivers of the future, and we hope it will become a valuable tool for researchers investigating concentrating solar thermal receivers and other technologies needed to decarbonize high temperature processes.

Keywords: Ray Tracing, Radiation Heat Transfer, Participating Media, Volumetric Receiver

1. Introduction

Decarbonization of industrial processes operating at above 1000 °C – such as the production of cement, metals, and chemicals – poses a major challenge [1]. A promising answer lies in concentrating solar radiation, which can be directly converted to heat at temperatures as high as 3000 °C. Although the technology is already available, reduced costs and increased efficiencies are needed to enable commercial deployments of this renewable decarbonization pathway [1, 2]. Commercially deployed concentrating solar receivers feature directly exposed tube-walls and operate at about 600 °C. At higher temperatures, new concepts are required that abate reradiation losses which, being proportional to T^4 , rapidly jeopardises the receiver efficiency. One approach relies on the volumetric absorption of radiation into porous structures [3, 4, 5] or absorbing media [6]. To properly design and optimize these devices, detailed heat transfer simulations need to be performed, which are beyond the capabilities of the simulation tools commonly available to the community. Therefore, most of the literature on radiative absorption on porous structures is based on heavy approximations and in-house codes which are developed for specific research questions and are seldom made available.

We aim at bridging this gap with our FInite VolumE Ray tracer (FIVER), an open-source Matlab tool [7] conceived for solving 3D multi-mode heat transfer problems involving radiative transfer in spectral media and complex geometries, as encountered in high-T solar engineering.

2. Physical Modeling and Code Development

We consider a general unsteady problem involving radiation and conduction heat transfer, for which the energy balance equation can be written as

$$\rho c \frac{\partial T}{\partial t} = \nabla \cdot (k \nabla T) - \nabla \cdot \mathbf{q}_R \quad (1)$$

where ρ is the density, c is the specific heat, T is the temperature field, k is the thermal conductivity, and $\nabla \cdot \mathbf{q}_R$ is the divergence of the radiative heat flux.

With FIVER, this equation can be solved with a general Robin boundary condition. Radiative fluxes on the boundaries can be freely defined in terms of spectral power and direction to model, e.g., an incoming solar flux. FIVER is currently not solving convective heat transfer, but the framework and solvers allow for a seamless extension in this direction.

2.1 Solving Radiative Heat Transfer

Thermal radiation is modeled under the geometric optics framework – i.e., the wavelengths are small compared to the geometry – the assumption of local thermodynamic equilibrium.

Radiative heat transfer within the participating media is solved by using a collision-based Monte Carlo ray tracing method [8], and scattering effects are currently not modeled. The ray tracing method implemented in FIVER builds upon the voxelized algorithm recently proposed by Sas Brunser and Steinfeld [4], which was demonstrated to dramatically accelerate ray tracing by eliminating the need for ray-surface intersection calculations, which typically dominate computation time [9]. We extended the original algorithm to include spectral radiation in participating media. Spectrally varying properties – e.g., absorption coefficient, refractive index and radiative source power – are resolved using a gray band model approach [10].

To solve for the radiative flux divergence, the rays are first generated, with their emission locations distributed according to the spectral radiative emissive power at each location in the domain. A ray generated from an opaque voxel surface is assigned a direction according to a Lambertian distribution and the voxel's surface normal vector, which is estimated using the algorithm from Thurmer and Wulrich [11]. Surface normals are also used to estimate the surface areas of the voxels, following Flin et al. [12], and to resolve refractions at semitransparent interfaces. The generated rays are then traced in parallel using the voxel traversal algorithm from [13], modified to compute the distance traveled by rays in each voxel, which then allows for resolving absorption by participating media. After all rays have been traced, the radiative flux divergence for each voxel is calculated as

$$\nabla \cdot \mathbf{q}_R = \frac{P_{\text{ray}}}{V_{\text{vx}}} (N_{\text{emit}} - N_{\text{absorb}}) \quad (2)$$

where P_{ray} is the ray power, V_{vx} is the voxel volume, N_{emit} is the number of rays emitted by the voxel, and N_{absorb} is the number of rays absorbed by the voxel.

2.2 Coupling with Conduction

The energy equation (Eq. 1) is discretized and solved using the open-source finite-volume toolbox FVTool [14]. In doing so, the divergence of the radiative heat flux – determined by the ray tracer (Eq. 2) – can be treated as a constant or linearized source term. By default, the finite volume solver and the ray tracer use the same Cartesian grid, and so no interpolation is required, making for a simple and fast coupling. To cope with situations where the simulation domain features different geometrical scales of interest, the tool can be extended with the implementation of multigrid methods. For instance, the radiation term can be obtained at a finer grid and Eq. 2 is solved on a coarser grid.

3. Validation Cases

We validated FIVER against several classical radiative heat transfer benchmark solutions which, albeit not presented in this paper, are available as test cases in the distributed code. The two validation cases presented in the following were computed using a consumer laptop with an 8-core AMD Ryzen 7 4800H processor.

We first present the validation case of two spectral, semitransparent and conductive media enclosed between two infinite black parallel plates. The spectral properties of the model media –i.e., model A and model B– are defined according to Crosbie et al. [15]. The solution was computed on a $100 \times 2 \times 2$ grid, with specular reflecting boundary conditions applied to the y and z boundaries to enforce periodicity. Each plate was set to a fixed temperature with $T_1 = 2T_2$, and the optical depth set to $\tau_L = 1$. The equilibrium temperature distribution was computed, for each medium, for two values of the nondimensional conduction-to-radiation parameter N_c , defined as

$$N_c = \frac{\kappa\kappa}{n^2\sigma T_1^3} \quad (3)$$

where κ is the linear absorption coefficient, n is the refractive index, and σ is the Stefan-Boltzmann constant. The case $N_c = 0$ corresponds to pure radiation, while $N_c = 0.05$ corresponds to a case with coupled radiation and conduction.

The linear absorption coefficient was defined as τ_L/L , where L is the distance separating the two plates. The results obtained by FIVER, shown in Figure 1, agree closely with the reference data, with a maximum single-point error of 1.0% and a maximum root mean squared error of 0.5%. Solving all 4 cases required 100 seconds computation time.

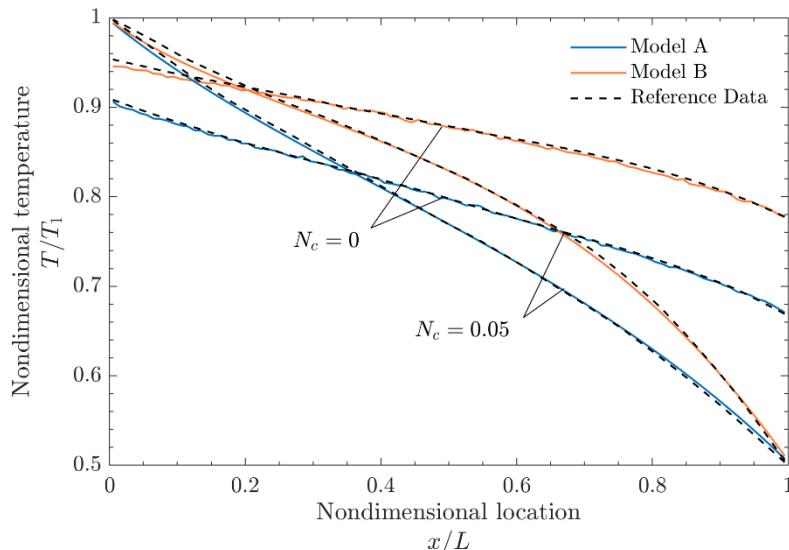


Figure 1. Nondimensional temperature profile of two spectral media at equilibrium between two infinite, black, isothermal parallel plates with internal conduction. Reference data extracted from Crosbie et al. [15]

As a second case, we present the results for a relevant problem in the field of high- T concentrating solar systems, i.e., the volumetric absorption of solar radiation by the hierarchically-ordered ceramic structure proposed by Sas-Brunser and Steinfeld [4]. A sample of this structure, made of cerium oxide with external dimensions 25x25x40 mm (Figure 2a), was tested in the ETHZ High Flux Solar Simulator [5]. The sample top surface was irradiated with a flux of 600 kW m^{-2} of simulated concentrated solar radiation, and three shielded thermocouples were inserted to measure the structure T at several locations.

The cerium oxide ceramic structure had dimensions 25x25x40 mm and was modeled as gray and opaque to radiation with emissivity $\epsilon = 0.7$ and with thermal conductivity $k = 5 \text{ W m}^{-1} \text{ K}^{-1}$. Radiation transfer was solved using a 202x202x324 grid and the combined radiation-conduction equation (Eq. 2) was solved on a coarser 101x101x162 grid. Radiation was free to exit the top and bottom boundaries of the domain, and the bottom boundary was treated as adiabatic to conduction. Figure 2 shows that FIVER predicts the temperature profile throughout the structure with reasonable accuracy, requiring a computation time of approximately 1 hour. As the solution does not account for losses from conduction through the bottom surface or from natural convection, the solution over-predicts the temperature.

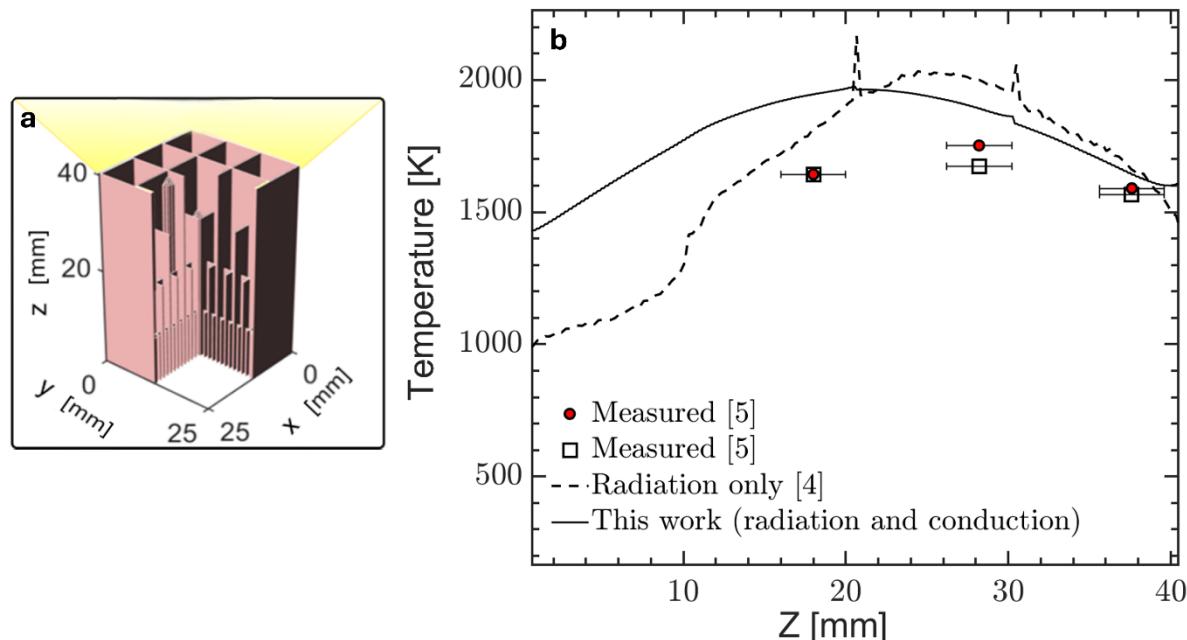


Figure 2. Hierarchically ordered ceramic structure solar irradiation. a) Digital representation of the voxelized domain [4]. b) Temperature profile along the z-axis of the structure as previously measured [5] and predicted [4], and as obtained by the FIVER model presented in this work. $z = 40 \text{ mm}$ is the top face of the structure, exposed to the radiative flux

4. Conclusion and Outlook

In this paper we introduce FIVER (FInite VolumE Ray tracer), an open-source computational tool to tackle multi-mode heat transfer problems involving radiative heat transfer. To summarize, the main strengths of FIVER are:

- Its ability to solve general 3D heat transfer problems, both steady and unsteady, on complex geometries.
- It can solve a variety of radiative heat transfer problems, including with surface-to-surface radiation, participating media, with gray or spectrally varying radiation and material properties, and with refractive interfaces.
- The coupling with a general-purpose finite volume toolbox allows for straightforward expansion to more complicated heat transfer problems.
- It is thoroughly validated by reference solutions.
- It is capable of simulating challenging cases relevant for the concentrated solar community, i.e., the volumetric absorption of solar radiation in porous ceramic structures, as discussed in this work.

- As an open-source Matlab tool, further improvements can be pursued collaboratively within the research community.

The main shortcomings of FIVER are:

- The flat voxelization of the domain means that problems with multiple length-scales are strongly memory-constrained.
- As a Matlab-based tool, it still requires the license of commercial programming language, which limits its availability. Future work could involve translation to another language such as Julia or C++.
- It lacks a graphical user interface.

The authors wish for FIVER to support the efforts of researchers and designers working to accelerate the science and technology needed to decarbonize thermal processes, and beyond.

Data availability statement

The data represented in Figure 1 are available in the FIVER repository [7]. The data represented in Figure 2 are available from the authors upon request.

Author contributions

C. Wetaski: Software, Validation, Visualization & Writing. S. Sas-Brunser: Software, Validation, Writing – review & editing. E. Casati: Conceptualization, Supervision & Writing.

Competing interests

The authors declare that they have no competing interests.

Acknowledgement

We thank Prof. Aldo Steinfeld, ETH Zurich, for providing the framework and resources to initiate the research work described in this paper.

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