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Hybrid radiation modeling for multi-phase solar-thermal reactor systems operated at high-temperature

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ABSTRACT

This work presents a method to couple ray-tracing and finite-volume radiation models at an arbitrary surface via both spatial and angular discretization. The interfacing algorithm is validated by comparing its results with full ray-tracing simulations of a compound parabolic concentrator as well as a large-scale solar-thermal reactor. The validated model is employed to investigate effects of silicon carbide tube radius on efficiency of ceria particle reduction for such applications as water or carbon dioxide splitting. Decreasing reactor tube radius from 25 to 5 cm reduced the total oxygen vacancy production rate from 3.7 to 0.3 kmol/h but nearly doubled the extent of ceria conversion when the particle bed velocity was maintained.

1. Introduction

The objective of the present work is to facilitate the use of concentrated solar-thermal energy for such applications as gasification of carbonaceous solids (Piatkowski et al., 2011), carbothermal reduction of metal oxides (Murray et al., 1995), and water (Muhich et al., 2016) or carbon dioxide splitting by active redox particles, among others. At high temperatures required for these processes (>1000 K), radiation becomes an important heat transfer mechanism. Therefore, a computational model for solar-thermal reactor design and scale-up needs to interface radiative, convective and conductive heat transfer processes.

1.1. Methods for simulating radiation

Typical radiation models for engineering applications can be classified into Monte-Carlo/ray-tracing (MC/RT) and finite-volume (FV) based approaches. RT radiation models are based on tracing the paths of individual rays from a given source. By increasing the number of rays, the statistical error can be reduced below an arbitrary precision. Therefore, RT results are often considered as reference solutions for other methods (Howell, 1998). Due to the high computational cost of tracing sufficient numbers of rays (10^5–10^8), however, RT models are usually employed to solve radiation in static systems where effects of scattering, absorption and emission caused by moving particles or gases can be neglected as well as temperature-dependent and anisotropic material properties. In contrast, these effects are readily accounted for in FV-based radiation models that are per iteration computationally more efficient (Joseph et al., 2009). The accuracy obtained with FV-models is limited by the number of employed discrete solid angles as well as computational cells which result in ray-effect and false scattering errors, respectively (Martinek and Weimer, 2013b). Above mentioned features makes RT methods suitable for heliostat fields while FV models are used mostly for chemical reactors and combustion chambers where iterative coupling with conductive and convective heat transfer is required.

Previously, He et al. (2011) coupled RT and FV models to obtain 3-dimensional flow fields and temperature distributions for an absorbing tube used in a parabolic trough solar-thermal power generator. The MC simulated surface heat flux through the outer surface of the absorber tube was then used as the input for the FV simulations. The model predicted tube outlet temperature agreed within 2% of experimental results.

Wirz et al. (2012) used an in-house MC code to compute the incident solar radiation for a parabolic trough solar concentrator. The temperature distributions at all relevant receiver surfaces were calculated by applying FV model for conduction as well as convection, and MC for thermal radiation, iteratively. Model predictions of heat losses, glass window temperatures and thermal efficiencies were consistent with experimental data.

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Nomenclature

α	volume fraction
a	absorption coefficient
A_{red}	pre-exponential factor for ceria reduction (720,000 1/s)
A_{ox}	pre-exponential factor for ceria oxidation ($82\ s^{-1}$ - $bar^{-0.218}$)
δ	moles of oxygen vacancies per mole of cerium
E_{red}	activation energy for ceria reduction (232 kJ/mol)
E_{ox}	activation energy for ceria oxidation (36 kJ/mol)
γ	lookout angle (°)
Φ	phase function
$\vec{g}$	gravitational acceleration (9.81 m^2/s)
h	specific species enthalpy (kJ/kg)
I	radiation intensity (energy per area of emitting surface per unit solid angle)
J	diffusion mass flux ($kg\ m^{-2}\ s^{-1}$)
K	interphase momentum exchange coefficient
$\dot{m}$	mass flow rate (kg/s)
n	refractive index
Ω'	solid angle
p	pressure (Pa)
$\vec{q}$	heat flux (W/m^2)
Q	interphase heat exchange coefficient
ρ	density (kg/m^3)
$\vec{r}$	position vector

R	reaction rate ($kmol\ m^{-3}\ s^{-1}$)
R_G	universal gas constant ($8.314\ J\ K^{-1}\ mol^{-1}$)
σ	Stefan-Boltzmann constant ($5.669 \cdot 10^{-8}\ W\ m^{-2}\ K^{-4}$)
σ_s	scattering coefficient
s	path length
$\vec{s}$	direction vector
S	enthalpy source term due to reaction (kJ/m^3)
Θ	acceptance angle (°)
$\bar{\tau}$	stress tensor (Pa)
t	time (s)
T	temperature (K)
$\vec{v}$	velocity vector (m/s)
x	maximum extent of ceria conversion (0.35)
Y	local mass fraction

Subscripts

Ce	cerium
i	species i
g	gaseous phase
p	phase p
q	phase q
s	solid phase
vac	oxygen vacancies

To reduce computational cost without compromising the accuracy, a hybrid RT-FV radiation modeling scheme was suggested for a solar-thermal process by Martinek and Weimer (2013b). In this approach, the incoming specular reflections were solved with a RT code while a FV model was applied for the diffusive re-radiation away from the reactor walls. FV solutions were found to be least accurate when the reactor cavity was highly specular or the absorber area was minimized.

Recently, Moghimi et al. (2015) compared FV and MC predictions of solar heat flux at an absorber tube surface for a linear Fresnel collector cavity receiver. Good agreement (error <0.4%) between the methods was obtained by sufficient mesh refinement and angular discretization accuracy.

Here, a method to couple RT and FV radiation models at an arbitrary surface by spatial and angular discretization of the RT input data is presented. The accuracy and optimal discretization level are evaluated by comparing the hybrid model predictions with those of the well-established and validated RT code SolTrace (Wendelin et al., 2013) for a secondary compound parabolic concentrator (CPC) as well as an industrial-scale reactor.

1.2. Methods for simulating multi-phase flows

If reactive and moving particles are present in the solar-thermal reactor, the process model needs to account for heat, mass and momentum transfer within, as well as between, the fluid and solid phases. More information about heat transfer processes in particle beds can be found in the systematic review by Özgümüş et al. (2013). The particles can be modelled either as discrete points (Lagrangian-approach) or as a continuum (Eulerian-approach) (Subramaniam, 2013). In general, the discrete particle model is more accurate since the particle-particle interactions can be solved directly e.g. by discrete element methods. However, the source terms due to the particles at point locations can attain very high values causing non-linear behavior in the numerical solver (ANSYS, 2015). The Eulerian approach is numerically more stable and efficient as only few additional transport equations need to be solved to account for the solid-phase. Its disadvantage is the need for closure models to describe the particle-particle interactions (ANSYS, 2015).

Meier (1999) investigated thermal decomposition of limestone ($CaCO_3$) in a solar-thermal falling particle receiver. The multi-phase flow and convective heat transfer were solved by computational fluid dynamics (CFD) while a MC-method was employed to calculate particle heating by radiation. The Lagrangian particle transport model omitted effects of absorption and emission as well as chemical reactions. The falling particles could be heated up to 1200 K, though particles smaller than 300 μm were found to leave the reaction zone due to entrainment by convective air streams or contaminate the transparent window if one is used to enclose the reactor.

Chen et al. (2006) conducted 3-D CFD simulations of multi-phase flow and heat transfer inside a falling particle solar receiver. Particles were modelled by a two-way-coupled Lagrangian method while a two-band FV-radiation model was employed to account for radiative heat transfer within the particles as well as their interaction with the receiver surfaces. Recirculation of hot exhaust gases was suggested to increase the absorber cavity efficiency.

Abanades et al. (2007) developed a CFD model to simulate the reduction of metal oxides for solar-thermal water splitting. The simulations accounted for multi-phase fluid flow, heat and mass transfer as well as zinc oxide dissociation. Lagrangian description was used for the particle-phase while the incoming solar flux was represented by a boundary condition in the CFD simulations. The model predicted increased zinc metal production rate as the absorber cavity diameter was decreased, consistent with experiments.

Thermal decomposition of ZnO was simulated also by Perkins and Weimer (2007) who solved the governing partial differential equations for momentum, energy, and mass transfer in a tubular solar receiver reactor using a finite element method. Uniform temperature profiles were attained regardless of the absorber tube diameter for the investigated small-scale systems. Increased oxidation rates near the tube walls suggested that novel methods need to be developed to increase material oxidation resistance at very high temperatures.