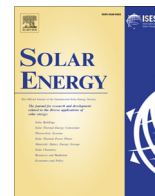




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Modelling of solar thermochemical reaction systems

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ABSTRACT

This article reviews the progress, challenges and opportunities in numerical modelling of thermal transport, thermochemical reactions and thermomechanics in high-temperature solar thermochemical systems. Continuum-scale models are presented in mathematical detail while highlighting the literature that uses them. The discussion is enhanced by selected examples of numerical studies of solar thermochemical systems for solar fuels and commodity material production. Property predictions necessary for the modelling of solar thermochemical reaction systems are covered.

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1. Introduction

Thermochemical reaction systems driven by concentrated solar irradiation hold great potential as environmentally benign alternatives to traditionally fossil-fuel-intensive industrial processes, including the production of transportation and stationary-application fuels as well as material commodities such as lime, metals, and ammonia (Bader and Lipiński, 2016a; Romero and Steinfeld, 2012). Solar thermochemical applications usually target highly endothermic, large-scale processes that require high-temperatures to proceed spontaneously (Bader and Lipiński, 2016b). Point-focusing solar concentrators can provide heat for the required high-temperatures. However, the long-term operation of processes at temperatures beyond the operating temperature limits of steel-based components remains a technical challenge. In hybrid processes, the high temperature requirements are alleviated with the aid of an electric energy input or a reaction agent, although usually at the expense of added process complexity, costs, or CO₂ emissions. There are also many industrial processes that can be supplemented with solar energy as a generic source of dispatchable process heat. Solar thermochemical processes can be grouped according to the feedstocks and energy sources used: solar-thermal H₂O/CO₂ splitting processes; hybrid (solar-

electrothermal or solar-carbothermal) processes; and processes for the solar-thermal conversion, upgrade, and de-carbonisation of carbonaceous feedstocks (e.g. coal, natural gas, biomass). Solar thermochemical fuel production processes generally aim at producing synthesis gas (CO and H₂), which can be further processed to conventional liquid fuels (e.g. diesel, kerosene, ethanol, dimethyl ether). Material and commodity related processes can be further grouped per the process type: production of lime for the cement industry; production of ammonia as a fertiliser or energy carrier; production of metals, metal oxides, carbides, and nitrides from ore or from waste materials for manufacturing; capture of CO₂ from flue gases or from the atmosphere to mitigate climate change and as a feedstock to produce carbon-neutral fuels; and conversion of bulk materials into nanostructures used as advanced materials. A recent comprehensive review and discussion of solar thermochemical processes can be found in (Bader and Lipiński, 2016a).

Introducing high-flux solar heat into high-temperature industrial processes in a controlled, efficient, and non-destructive way poses a thermal engineering challenge. Computational models can be powerful tools to evaluate and optimise the design and performance of solar thermochemical reaction systems (STRSs) and guide the engineering process, thus reducing the need for costly and time-consuming repetitive prototype development and experimental testing. However, computational modelling of STRSs can be challenging. First, these systems typically utilise solid-gas heterogeneous media at temperatures ranging from several hundred to more than 2000°C. Second, the full engineering scope of

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Nomenclature

<i>Latin</i>		μ'	effective viscosity for a porous material (N s m^{-2})
a	interfacial surface area per unit volume (m^{-1})	ρ	density (kg m^{-3})
A	reaction rate constant (s^{-1})	σ_s	(effective) linear scattering coefficient (m^{-1})
c	speed of light (m s^{-1})	$\bar{\tau}$	stress tensor (N m^{-2})
c_T	thermophoretic velocity (m s^{-1})	Φ	(effective) scattering phase function (sr^{-1})
D	Brownian diffusion coefficient (m^2s^{-1})	Ω	solid angle (sr)
E_a	activation energy (J)	<i>Subscripts</i>	
f	external force per unit volume (N m^{-3}) or reaction model (–)	0	initial
F	Dupuit–Forchheimer coefficient (m^{-1})	∞	final
g	acceleration due to gravity, (m s^{-2})	b	blackbody
Gr	Grashof number (–)	B	Brownian diffusion
h	specific enthalpy (J kg^{-1})	d	diffusion
h_{sf}	volumetric heat transfer coefficient ($\text{W m}^{-2}\text{K}^{-1}$)	D	Darcy
I	radiative intensity ($\text{W m}^{-2}\mu\text{m}^{-1}\text{sr}^{-1}$)	DF	Dupuit–Forchheimer
k	thermal conductivity ($\text{W m}^{-1}\text{K}^{-1}$)	e	enthalpy change due to mass diffusion
\bar{K}	permeability tensor (m^2s^{-1})	h	convection
m	mass (kg)	j	index over species
\dot{m}	mass flux ($\text{kg m}^{-2}\text{s}^{-1}$)	k	index over mass/momentum/energy transfer mechanism
p	pressure (Pa)	r	radiative
q	heat flux (W m^{-2})	s	mass/enthalpy transfer by adsorption or desorption
\dot{q}	heat rate per unit volume (W m^{-3})	sf	solid–fluid
r	mass source or sink (kg s^{-1})	T	thermophoretic
R	gas constant (J K^{-1})	v	viscous drag
Re	Reynolds number (–)	<i>Superscripts</i>	
\hat{s}	propagation direction of radiation (–)	f	fluid phase
Sc	Schmidt number (–)	s	solid phase
St	Stokes number (–)	ξ	arbitrary phase
St_{th}	thermal Stokes number (–)	<i>Abbreviations</i>	
t	time (s)	D–F	Dupuit–Forchheimer
T	temperature (K)	DO	discrete ordinate method
v	velocity vector (m s^{-1})	FV	finite volume method
w	species mass fraction (kg kg^{-1})	LTE	local thermal equilibrium
x	location (m)	LTNE	local thermal non-equilibrium
\dot{W}	work per unit volume (W m^{-3})	MC	Monte Carlo
<i>Greek</i>		N–S	Navier–Stokes
α	conversion coefficient (kg kg^{-1})	RD	Rosseland diffusion approximation
β	coefficient for interface force ($\text{kg m}^{-3}\text{s}^{-1}$)	RTE	radiative transfer equation
ε	phase volume fraction (m^3m^{-3})	STRS	solar thermochemical reaction system
κ	(effective) linear absorption coefficient (m^{-1})		
λ	wavelength (μm)		
μ	dynamic viscosity (N s m^{-2})		

STRSs includes considerations that span kilometres—such as power grid integration, optical concentrator field design, and plant process design—down to the scale of nanometres when considering the chemical and morphological design of the reactive materials. Third, conditions in and around STRSs fluctuate due to many time-dependent phenomena ranging from seasonal solar flux variations to rapid chemical kinetics occurring on microsecond time scales. Finally, STRSs are generally highly multi-physical; radiative, conductive, and convective heat transfer, momentum transfer, and complex mass transfer involving multiple phases, species, and chemical reactions all play key roles in the operation of reactor systems. In addition, thermally induced mechanical stresses are often critical. Such high temperatures, variations in length scales, temporal scales and physical complexity represent significant challenges when numerically modelling STRSs. A recent perspective by Floudas et al. (2016) highlights the challenges of multi-scale phenomena for the energy sector as a whole.

In this review, we will focus on the numerical modelling of the complex thermophysical phenomena occurring inside STRSs. Important features that require modelling attention include: (i) chemically reacting solid–gas interfaces, (ii) multi-component, often multiphase, mass transport, (iii) high-flux solar irradiation and its interaction with complex reacting media at high temperatures and (iv) the transient nature of solar energy leading to a time-varying process heat input to the STRS. Items (i) and (ii) together constitute a “classical” chemical reactor system where the dominant heat transfer mechanisms are conduction and/or convection. The tome by Jakobsen (2014) is an excellent resource for modelling considerations in these areas. The addition of highly directional, transient, intense irradiation is the defining feature of STRSs. Interactions between thermal radiation and active materials are of keen interest since the conversion of incident solar irradiation to the creation or destruction of chemical bonds is the fundamental process that defines the efficiency of STRSs. Characterisation and simulation techniques that accurately, but

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