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Constructal method to optimize solar thermochemical reactor design

S. Tescari [a,*], N. Mazet [a], P. Neveu [a,b]

[a] PROMES-CNRS, Rambla de la Thermodynamique, Tecnosud, 66100 Perpignan, France
[b] Université de Perpignan Via Domitia, 52 Avenue Paul Alduy, 66860 Perpignan, France

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Abstract

The objective of this study is the geometrical optimization of a thermochemical reactor, which works simultaneously as solar collector and reactor. The heat (concentrated solar radiation) is supplied on a small peripheral surface and has to be dispersed in the entire reactive volume in order to activate the reaction all over the material. A similarity between this study and the point to volume problem analyzed by the constructal approach (Bejan, 2000) is evident. This approach was successfully applied to several domains, for example for the coupled mass and conductive heat transfer (Azoumah et al., 2004). Focusing on solar reactors, this work aims to apply constructal analysis to coupled conductive and radiative heat transfer. As a first step, the chemical reaction is represented by a uniform heat sink inside the material. The objective is to optimize the reactor geometry in order to maximize its efficiency. By using some hypothesis, a simplified solution is found. A parametric study provides the influence of different technical and operating parameters on the maximal efficiency and on the optimal shape. Different reactor designs (filled cylinder, cavity and honeycomb reactors) are compared, in order to determine the most efficient structure according to the operating conditions. Finally, these results are compared with a CFD model in order to validate the assumptions.

Keywords: Solar thermochemical reactor; Concentrated solar reactor; Cavity reactor; Constructal method; Geometrical optimization; Honeycomb

1. Introduction

Endothermic chemical processes involving solid and gas at high temperature are found in a wide range of industrial applications. The high amount of energy required by these processes can be supplied by concentrated solar energy, decreasing significantly greenhouse gases emissions. The industrial applications include extractive metallurgy, ceramic material processing and calcination (Lipinski and Steinfeld, 2004). Petrasch et al. (2009) classified some experimental solar chemical reactors for the production of fuels and material from 1990 onwards. The reactors are characterized by the irradiation mode: the incident solar energy can be used in an indirect heating configuration or be absorbed directly by a reactive solid leading to two reactor concepts. Indirect heating reactors are used for the carboreduction of ZnO (Wieckert et al., 2004, 2007) and for the steam-gasification of carbonaceous feedstock (Piatkowski et al., 2009). Directly irradiated reactors are used for C gasification (Z'graggen et al., 2006), $CaCO_4$ reduction (Meier et al., 2006) and thermochemical cycles based on metallic oxides such as ferrite (Roeb et al., 2006) and zinc oxide (Müller et al., 2006; Haueter et al., 1999; Abanades et al., 2007). This study focuses on the optimization of this kind of solar reactors, which operates simultaneously as solar collector and as chemical reactor. The shape and the design of the reactor strongly influence its efficiency. The best geometry is the one that at the same time minimizes the radiative losses towards the environment and maximizes the absorbed incident radiation. The optimal geometry depends on the constraints of the problem and on the operating parameters.

* Corresponding author. Tel.: +33 468 682 253; fax: +33 468 682 213.
E-mail address: stefania.tescari@univ-perp.fr (S. Tescari).

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Nomenclature

DNI	direct normal irradiance (W/m^2)
f_0	shape factor of single cavity or filled cylinder reactor (–)
f_1	shape factor of the whole honeycomb reactor (–)
F_{dj-k}	view factor between the infinitesimal surface δS_j and S_k (–)
F_{j-k}	view factor between S_j and S_k (–)
H_0	single cavity reactor radius (m)
H_1	honeycomb reactor radius (m)
i_0	solar incident radiation flux (W/m^2)
I_0	solar incident radiation power (W)
L_0	single cavity reactor length (m)
$L1$	honeycomb reactor length (m)
R_0	cavity radius (m)
r	radial coordinate (m)
S_0	enlightened surface (m^2)
S_1	lateral surface of the cavity (m^2)
S_2	bottom surface of the cavity (m^2)
T_{amb}	room temperature (K)
T_i	inversion temperature (K)
$T_{(j,k)}$	temperature at $r = j$ and $z = k$ (K)
$T_{Max(R0,0)}$	maximal temperature at $r = R_0$ and $z = 0$, calculated by neglecting the radiation toward S_1 and S_2 (K)
$T_{(R0,0)}$	temperature at $r = R_0$ and $z = 0$
$T_{(R0,L0)}$	temperature at $r = R_0$ and $z = L_0$: coldest point of the cavity surface
T_{Mean}	average cavity temperature (K)
V_m	reactive material volume (m^3)
z	axial coordinate (m)

Greek symbols

η	efficiency (–)
λ	thermal conductivity (W/m K)
σ_B	Stefan–Boltzmann constant (=5.67 × 10^{-8} W/m^2 K^4)
σ_q	uniform heat sink (W/m^3)
φ_0	void fraction of single cavity (–)

A new geometrical optimization method was proposed in 1997 by A. Bejan: the constructal approach (Bejan, 2000). This approach does not aim to simulate perfectly a real system. The objective is to predict the tendency of geometry variation, by solving a simplified problem. The results of this method cannot be used crudely to optimize the system but they can be used as a system pre-dimensioning.

The constructal theory is based on one general principle: for a flow system, the optimal geometry is the one that opposes the minimal resistance to the currents that flow through it. Studying solar chemical reactor, the optimal shape is the one that facilitates the heat propagation. The heat input is concentrated solar radiation. It lights a small surface (solar spot) and it has to be dispersed in the whole reactive volume in the most efficient way. This problem can be named "surface to volume" problem to highlight the similarity to the "point to volume" problem described by Bejan.

The strength of the constructal approach was shown through several examples, as heat transfer in electronic package (Bejan, 1997) or in porous media (Bejan, 2004), tree shaped flow structures (Lorente et al., 2002). An extension of this approach was applied successfully to a solid–gas reactor (Azoumah etal., 2004, 2006, 2007), by studying the effect of coupled heat transfer (conduction), mass transfer and chemical kinetics. A new extension, which consists in coupling radiative and conductive heat transfer, is the purpose of this study.

2. Definition of the problem

This study focuses on a solar thermochemical reactor, under concentrated solar radiation.

The chemical reaction is not fixed, in order to be able to adapt the study to various experiments. An example is the reduction of ZnO, performed in different cavity reactors, as shown in Fig. 1. The chemical reaction can be characterized by an inversion temperature T_i (the equilibrium temperature of the chemical reaction at standard pressure). The endothermic reaction occurs only for a temperature higher than this value. The volume of reactive material V_m is lighted by an incident solar power I_0. This energy is, for one part, lost by radiation towards the environment, and, for the other part, transferred by radiation and/or conduction to the reactive material to drive the endothermic reaction.

For given values of V_m and I_0 (global constraints), the *objective* of this optimization is to maximize the useful power delivered for the reaction in the reactive material.

Moreover, the temperature in all the reactive volume must be higher than the inversion temperature T_i, so that the endothermic reaction takes place in the whole material (T_i is the local constraint).

The *unknown* is the geometry of the reactor, defined by a shape factor.

For given constraints and operating parameters (V_m, I_0, T_i and λ), the optimal geometry is searched in order to maximize the heat provided to the reaction (σ_q).

The reactor efficiency (η) is defined as the useful power delivered for the reaction divided by the incident solar power (Eq. (1)).

$$\eta = (\sigma_q \cdot V_m)/I_0 \tag{1}$$

For given values of I_0 and V_m, Eq. (1) shows that the maximization of σ_q or η is equivalent.