



Research Paper

Direct numerical simulation of the thermal dehydration reaction in a TGA experiment

Shuiquan Lan^{a,b,*}, Mohammadreza Gaeini^a, Herbert Zondag^{a,c}, Anton van Steenhoven^a, Camilo Rindt^a^a Department of Mechanical Engineering, Eindhoven University of Technology, Den Dolech 2, 5612AZ Eindhoven, The Netherlands^b China Resources Power Technology Research Institute, 518001 Shenzhen, China^c Energy Research Center of the Netherlands – ECN, P.O. Box 1, 1755ZG Petten, The Netherlands

HIGHLIGHTS

- A CFD model of the coupled mass and heat transfer processes is developed.
- The model is used to directly simulate the dehydration reaction of salt hydrates.
- Numerical results calculated by the CFD model are compared to experimental results.
- The influence of various parameters in a TGA experiment is studied.

ARTICLE INFO

Article history:

Received 11 December 2016

Accepted 11 August 2017

Available online 18 September 2017

Keywords:

Reaction kinetics

Direct numerical simulation

Nucleation and growth

TGA measurement

Thermochemical heat storage

Salt hydrate

ABSTRACT

This work presents a detailed mathematical model of the coupled mass and heat transfer processes in salt hydrate grains in a TGA experiment. The purpose of developing this numerical model is to get a more fundamental understanding of the influence of parameters like particle size, nucleation rate and vapor pressure on the dehydration reaction in a TGA experiment. Such a model needs a detailed description of the fluid flow and water vapor distribution between the particles. The dehydration reaction of grains of TCMS is described by the nucleation and nuclei growth model presented in our earlier work. The flow around grains is solved by means of the finite volume method using OpenFOAM including heat and mass transfer. Direct numerical simulations of TGA-experiments under various conditions are performed. Such simulations provide direct insight into the physics of mass and heat transport processes coupled with detailed reaction kinetics at grain scale. The numerical results are compared to the experimental results. The developed CFD model can be a promising tool to calculate the overall kinetics for dehydration reactions under realistic heat storage conditions. To that end, the effect of buoyancy should also be included in the model to get a more accurate description of convection within the sample.

© 2017 Elsevier Ltd. All rights reserved.

1. Introduction

Thermochemical heat storage materials (TCMs) are given more and more attention for the application in seasonal heat storage [1,2]. A number of salt hydrates have been identified as promising candidates such as $\text{MgSO}_4 \cdot 7\text{H}_2\text{O}$ [3], $\text{MgCl}_2 \cdot 6\text{H}_2\text{O}$ [4] and $\text{SrBr}_2 \cdot 6\text{H}_2\text{O}$ [5]. The main principle of thermochemical heat storage using salt hydrates is based on reversible reactions like:



where n is the number of water molecules per unit of species A. In this reaction, a thermochemical solid material (A) absorbs energy in

the form of heat and is converted chemically into two components (solid B and water vapor), which can be stored separately. The reverse reaction occurs when material B and water vapor are combined together and A is formed. Heat is released during this reaction and the storage system is ready for recharging.

Salt hydrates are most frequently characterized by thermoanalytical techniques like TGA-DSC [2]. Materials showing promising features like high energy storage density, fast reaction kinetics and good structural stability are used in reactor and system tests [6]. For better understanding and optimizing thermochemical heat storage systems using salt hydrates, several numerical models are developed to simulate the heat and mass transfer processes together with the gas-solid reactions at reactor- and system-scale [7–15]. In all these models, the reactive medium is treated as a continuum at macroscopic scale and the reaction kinetics is

* Corresponding author at: Department of Mechanical Engineering, Eindhoven University of Technology, Den Dolech 2, 5612AZ Eindhoven, The Netherlands.

E-mail address: lanshuiquan1@crpower.com.cn (S. Lan).

Nomenclature

A	interface area	g	acceleration due to gravity
D_T	thermal diffusivity	p	pressure
D_m	mass diffusivity	\mathbf{u}	flow velocity
ΔH	enthalpy of dehydration	t	time
M	molar mass	α	fractional conversion
R	universal gas constant	γ	nucleation rate
S	active interface between reactant and product	κ	thermal conductivity
T	temperature	ϕ	nuclei growth rate
V	volume	ρ	density
c	water vapor concentration	ν	kinematic viscosity
c_p	specific heat at constant pressure		

described by simplified kinetic models derived from thermal analytical experiments like TGA-DSC. It is clear that the reaction kinetics, as the root of such models, has a significant influence on the numerical predictions. It is necessary to implement more fundamental kinetic models to gain more detailed insight. Helbert et al. [16] presented a stochastic and deterministic model for nucleation and growth in powder transformation, which is applicable in non-isothermal and non-isobaric situations and is valid for all kinds of grain shapes. Favergeon et al. [17] used this model to study the dehydration reaction of $\text{Li}_2\text{SO}_4 \cdot \text{H}_2\text{O}$ single crystals under isothermal and isobaric conditions. With the assumption of constant parameter values, the rates of nucleation and growth were estimated by model-fitting of the corresponding TGA results. Our earlier work [18,19] characterized the rates of nucleation and growth under non-isothermal conditions and calculated the reaction kinetics in terms of the nucleation and nuclei growth processes.

Besides the importance of the reaction kinetics the thermal decomposition reactions derived from TGA-DSC also depend largely on the sample environment, particularly the atmosphere in the vicinity of the sample [20]. Unfortunately, such detailed information on the local atmosphere is not accessible in a TGA-DSC measurement. Moreover, thermal analysis most frequently focuses on the overall kinetic rates and the derivation of kinetic models, but less attention is paid to the local atmosphere around the sample particles. To take the influence of the sample environment into account, heat and mass transport processes in the void space between packed grains have to be included. A detailed numerical model of the TGA samples based on the actual packed bed geometry can be helpful to find out the physical phenomena taking place inside the TGA furnace.

In the present work, a traditional CFD method with body-fitted meshes is used to simulate the dehydration reaction of a powdery sample of $\text{Li}_2\text{SO}_4 \cdot \text{H}_2\text{O}$ grains in a TGA experiment. The nucleation and growth model developed earlier [18] is coupled to the mass and heat transfer processes between the $\text{Li}_2\text{SO}_4 \cdot \text{H}_2\text{O}$ grains. Direct numerical simulations using the CFD package OpenFOAM are performed to study the mass and heat transport processes during the dehydration reaction of multiple grains. The overall rate of the reaction is computed and compared to TGA results under various conditions. The influence of various parameters like particle size, nucleation rate and vapor pressure is then discussed.

2. Numerical model

The simulated configuration is schematically shown in Fig. 1. This is a typical TGA configuration in our lab (type: Netzsch STA 449 F3 Jupiter). It should be noted here that only a part of the furnace in the height direction is simulated. A humidified air flow

from top to bottom is used to control the humidity of the experimental environment. Temperature of all solid walls (T_s) including the side walls of the furnace and the crucible is set to a programmed temperature profile. All dehydration tests are performed under controlled temperature and humidity conditions. In the numerical model, a real-size 3D geometry of the TGA apparatus is implemented. The computational domain is divided into two regions. The first region is the powdery sample, which is composed of N spherical grains that are randomly packed. The second region is the flow region, which is a moist air flow at a low Reynolds number in the furnace chamber and in the void space between particles. These two regions are bounded by the solid walls of the crucible and the furnace. The reactions at grain level are described by the nucleation and nuclei growth models as presented in our earlier work [18]. Coupling of heat and mass transfer with chemical reaction is realized at the gas-solid boundary, where heat is extracted from the flow to the solid particles for the dehydration reaction and meanwhile water vapor generated during the reaction is released to the flow.

Assumptions for derivation of the model are as follows:

1. Each grain is considered to be spherical throughout the reaction. The shrinkage of the crystal grains is less than 10% and not taken into account in the present model.
2. A uniform temperature distribution in the grain is assumed, as the Biot number is in the order of 0.1.
3. Because of computational time, the effect of buoyancy around the grain is not considered. Also the influence of temperature on density and viscosity is neglected. This led to an acceptable computational time of several hours for the simulation of the dehydration experiment.
4. Water vapor is diluted in air. Water production by the reaction is assumed not to disturb the total pressure distribution of the flow around the particles. Also, the physical properties of the moist air are considered to be constant and are the same as those of dry air.
5. A quasi-steady flow is considered. In this coupled problem, the time scales of the fluid dynamics problem ($d/u = \vartheta$ (s)) and the solid reaction (ϑ (min)) are very different. Hence the temperature and vapor concentration in the flow domain are calculated at discrete moments in time based on an update of the particle boundary conditions.

2.1. Flow region

Based on these assumptions the governing equations for the quasi-steady flow problem can be written as follows:

$$\nabla \cdot \mathbf{u} = 0 \quad (2)$$

Download English Version:

<https://daneshyari.com/en/article/4990878>

Download Persian Version:

<https://daneshyari.com/article/4990878>

[Daneshyari.com](https://daneshyari.com)