

Modelling of gibbsite calcination in a fluidized bed reactor

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Abstract

A steady state, non-isothermal fluidized bed reactor model for co-current flow of gas and solids has been developed as a series of Continuous Stirred Tank Reactor (CSTR) compartments. For each CSTR compartment, mass and energy balances were coupled with a particle-scale gibbsite calcination kinetic model previously developed by the authors. The overall solids residence time distribution is captured by the compartment calcination model. The multi-scale model was solved numerically through an iterative procedure that alternated between solving particle-scale and reactor-scale parts of the model. Gas, water vapour and solids concentrations, as well as particle and gas temperatures and gibbsite conversion profiles, are predicted inside the calcination reactor. The developed model can be used to facilitate improvements in the operation and design of industrial-scale reactors.

Keywords: Gibbsite, Calcination, Fluidized bed, Reactor, Particle scale

Introduction

Particle-scale models are valuable for revealing kinetics from laboratory experiments of gas-solid reactions. In addition, investigation of a single reacting particle allows appropriate assumptions to be made about modelling the internal and external heat and mass transfer processes. However, engineers are often more interested in numerically-efficient, equipment-scale models that can predict the practical performance of large-scale units under different operating scenarios. For unit operations like Fluidized Bed Reactors (FBRs), this need can be more challenging to fulfil compared to reactors containing only fluids, because for the latter, process simulation software and models are well developed. For gas-solid reactions, therefore, validated micro-scale models must be connected to a comprehensive macro-scale model to address industrial end users' needs.

Because of their importance in many industries, the modelling and simulation of FBRs has increasingly received attention by researchers over the few last decades. Due to the wide range of physical and chemical mechanisms interacting in these reactors, modelling efforts are not always comprehensive enough to capture all their relevant features, including transport phenomena and reaction kinetics. Moreover, efforts for enhancement of current models tend to result in numerically complicated and costly models. A suitable compromise between model simplicity and capability should be central to any modelling endeavour.

A large number of modelling efforts for FBRs are based on considering two phases in the fluidized bed with exchange of mass and energy between them. In this approach, the gas can be in both bubble form and well mixed with the solids, forming an "emulsion", with the solid particles mainly existing in the emulsion phase. In other words, the gas bubbles are almost solid-free. Having solid-free bubbles is an idealistic assumption, as the existence of solids in the bubble phase has been

shown experimentally and theoretically (Mostoufi et al. 2001). In spite of these simplifications, the two-phase FBR model has been of interest due to its simplicity of model development and solution. In addition, the predictions of this model are precise enough and reasonably in agreement with practical data. The two-phase model is well presented by Kunii and Levenspiel (1991). Figure 1 shows conceptually how a two-phase fluidized bed model at the reactor scale could be linked with alternative particle-scale models to create a multi-scale model. At very high velocities, FBRs may show well-mixed properties in which it is very hard to distinguish between emulsion and gas bubbles. Under these conditions (Kunii and Levenspiel 1991), the gas and solid flows might be considered as pseudo-single-phase flow. Small bubble sizes and high interphase mass and energy transfer rates are embedded in this assumption. Therefore, temperature and concentration are approximately uniform throughout the bed (McAuley et al. 1994). This kind of model might be derived from a two-phase FBR model as a limiting case in which heat and mass transfer resistances are quite low.

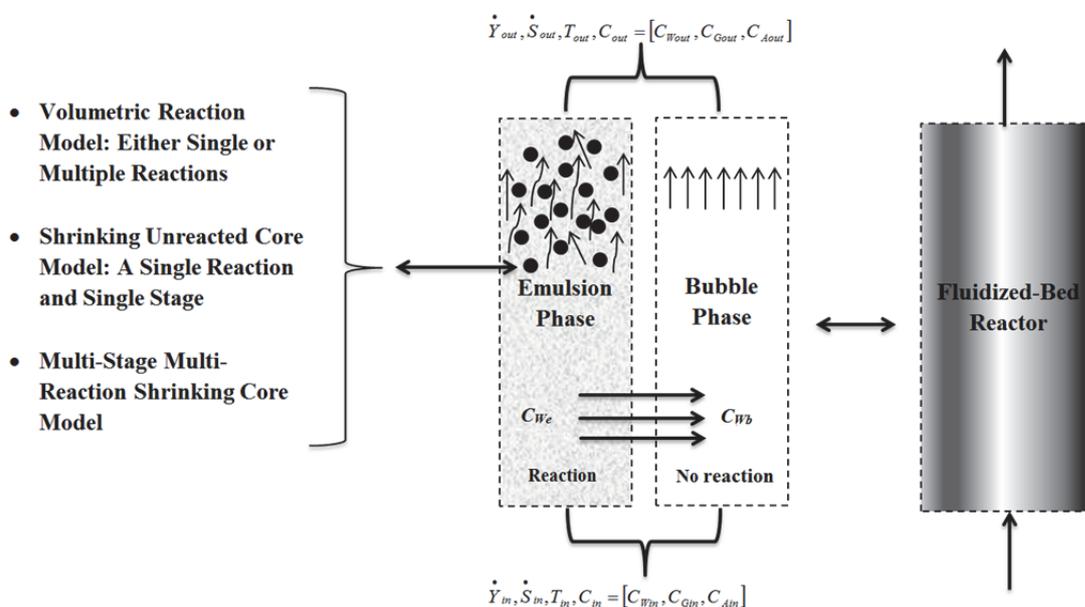


Figure 1. Schematic of a conceptual two-phase model for a FBR showing communication with alternative particle-scale models.

Due to the interaction of numerous mechanisms in a FBR, however, prediction and explanation of the behaviour of this system is complicated in its reactions and hydrodynamics. Multi-scale modelling has been found to be a useful approach to tackle some of these complexities, although it is still in its early stages. From a multi-scale point of view, investigations into the processes in FBRs might be classified as follows:

1. Qualitative (descriptive) research on the definition, application and importance of multi-scale modelling (Braatz et al. 2004);
2. Hydrodynamics of fluidized beds (Schmidt 1996; Curtis and van Wachem 2004; van der Hoef et al. 2005; Deen et al. 2007);
3. Multi-scale modelling of mass and heat transfer and reaction processes (Wang et al. 2005; Breault 2006; Behjat et al. 2008; Dong et al. 2008; Breault and Guenther, 2009).

This paper aims to present a simplified multi-scale model for gibbsite calcination in a FBR, as used in the production of alumina. A particle-scale gibbsite calcination model formerly developed by the authors (Amiri et al. 2013a) is integrated with a reactor-scale model in a case study.

The particle-scale model uses dynamic, radially distributed species balances and an energy balance to predict the concentration profiles of gibbsite, alumina and water vapour, and the temperature profile, inside a single reacting particle. The model accounts for internal and external resistances to mass and heat transfer, and for the solid-to-gas calcination reaction. The reaction rate depends on the local concentrations of gibbsite and water vapour, and the local temperature. Further details about the particle-scale model and its validation may be found in Amiri et al. (2013a).

A single-phase FBR might be approximated via ideal reactor models, such as the Plug Flow Reactor (PFR) or Continuous Stirred Tank Reactor (CSTR). However, due to its complex hydrodynamics, the behaviour of a real FBR may fall in between a PFR and a CSTR, or some network of them. A general model is needed to account for the non-ideal flow conditions. The tanks-in-series model is general enough to simulate both CSTR and PFR reactors. In addition, any kind of reactor performing between these two ideals could be simulated by adjusting the number of tanks. Therefore, this modelling approach is used in this paper as an illustration of how communication between particle-scale and reactor-scale models could be set up. Gas and solid temperature as well as gibbsite conversion profiles inside the reactor are captured through the integration of both particle-scale and reactor-scale models with a solids residence time distribution.

Multi-scale Model Development

Initially, the mass and energy balances over a single CSTR element, which will form part of the general model, are developed for co-current flow of gas and solids. Subsequently a MATLAB code was developed for the CSTR model solution and this interacts with codes previously developed for particle-scale models by the authors (Amiri et al. 2013a). The reactor code has been designed to be flexible so that it can employ different numbers of CSTRs in series and different Residence Time Distribution (RTD) functions. The communication between the codes at different scales was carefully established to ensure correct information transfer between the different scales.

Even though only the co-current flow regime is investigated in this paper, the model and corresponding codes could be applied to other flow configurations, including counter-current and cross-flow of gas and solid.

Modelling assumptions

- The model is steady state and non-isothermal.
- The reactor is oriented vertically with the gas and solid entering the base of the reactor and flowing co-currently upwards. The overall reactor is assumed to behave as a vertical collection of CSTRs connected in series.
- At each horizontal level, the gas and solid are well-mixed, showing pseudo-single-phase behaviour.
- All CSTRs are considered to have equal volume and the same residence time distribution. In particular, note that the solids residence time is assumed to be unaffected by any changes in the gas flow rate through the CSTRs.
- The temperature and species concentrations inside the particles exiting each CSTR are obtained by averaging the temperature and concentration profiles inside a single particle

with respect to radial position in the particle and over the solids residence time distribution for that CSTR.

- The voidage of the bed is constant throughout the reactor.
- Particles are assumed to have a constant size during the reaction.
- The particle scale reaction is the calcination of gibbsite into alumina and water vapour.
- The gas phase consists of air and water vapour, and the ideal gas law applies.
- The water vapour concentration inside the reactor has no significant influence on the reaction rate at the particle scale. The validity of this assumption has already been confirmed in Amiri et al. (2013a) for gibbsite calcination.
- A constant total pressure for the gas phase is assumed.
- The assumptions related to the solid's physical properties are the same as those reported in Amiri et al. (2013a).

Conservation and constitutive equations

The mass balances of a single CSTR with respect to the individual species involved in the calcination reaction are fairly straightforward. However, more attention must be paid to the energy balance, since the composition of the solid and gas mixture, local temperature and reaction rate are all changing. Table 1 summarises the governing conservation and constitutive equations of a single CSTR element (Figure 2) that will be utilised in a tanks-in-series model as the i^{th} element out of n .

Table 1. Conservation and constitutive equations at the reactor scale for CSTR i .

$\bar{X}_i = \int_0^\infty X(t)E(t)dt$	(1)
$\tau = \frac{V_R(1-\varepsilon)}{\dot{S}} = \frac{AH(1-\varepsilon)}{\dot{S}}$	(2)
$\tau_i = \tau / n$	(3)
$C_{G,i} = C_{G,i-1}(1 - \bar{X}_i)$	(4)
$C_{Al,i} = C_{Al,i-1} + \alpha C_{G,i-1} \bar{X}_i$	(5)
$C_{W,i} = \left(\frac{C_{W,i-1}Y_{i-1} + \omega C_{G,i-1} \bar{X}_i \dot{S}}{\dot{Y}_i} \right)$	(6)
$\dot{Y}_i = \left(\frac{T_i}{T_{i-1}} \right) \dot{Y}_{i-1} + \omega C_{G,i-1} \bar{X}_i \dot{S} \left(\frac{RT_i}{P} \right)$	(7)
$C_{Air,i} = \left(\frac{\dot{Y}_{i-1}}{\dot{Y}_i} \right) C_{Air,i-1}$	(8)
$T_i = \left[\dot{S} C_{G,i-1} C_{pG} + C_{Al,i-1} C_{pAl} T_{p,i-1} + \dot{Y}_{i-1} C_{W,i-1} C_{pW} + C_{Air,i-1} C_{pAir} T_{i-1} \right. \\ \left. - \dot{S} (C_{G,i} C_{pG} + C_{Al,i} C_{pAl}) T_{p,i} - \dot{S} C_{G,i-1} \bar{X}_i \Delta H \right] / \left[\dot{Y}_i C_{W,i} C_{pW} + C_{Air,i} C_{pAir} \right]$	(9)

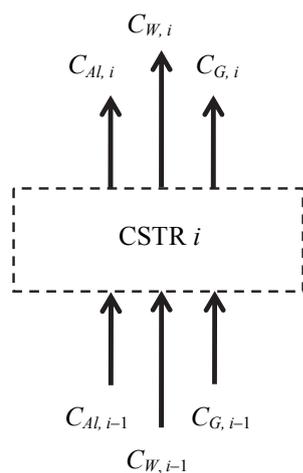


Figure 2. Schematic of a single CSTR element showing the inlet and outlet concentrations of gibbsite (G), water vapour (W) and alumina (Al).

Equation (1) uses the particle scale model via $X(t)$, and the solids residence time distribution $E(t)$, to determine the average gibbsite conversion in the i^{th} CSTR element. Equations (2) and (3) relate the mean solids residence time in each CSTR element to the solids mass flux, reactor size and the reactor voidage. Equation (4) is the gibbsite material balance, estimating the number of moles of gibbsite leaving the i^{th} element based on the difference between the inlet number of moles and the consumption due to conversion. Similarly, the material balances for the alumina and water vapour, Equations (5) and (6), respectively, can be determined from the inlet number of moles of both species, the gibbsite consumption and the appropriate stoichiometric coefficients. Even though air is inert in the calcination reaction, the local concentration of the air may change due to water vapour production and gas temperature changes. The total gas flow rate and the air concentration can be predicted by considering the water vapour production and temperature changes as shown in Equations (7) and (8).

The energy balance for the i^{th} element consists of different enthalpy terms. Gas and solid enthalpies for the inlet and outlet streams of the element, as well as the reaction enthalpy, must be considered in the energy balance. Due to changes in material compositions for both solid and gas phases, local mean values of the heat capacities are employed. Equation (9) shows the energy balance, rearranged for the outlet gas temperature. The first and third terms in the numerator are the enthalpy of the inlet and outlet solids. Similarly, the second and fourth terms of the numerator are the enthalpies of the inlet gas and the reaction, respectively. The denominator multiplied by T_i forms the enthalpy of the outlet gas.

In multi-scale modelling, establishing proper communication between the scales of interest is of vital importance. This issue was examined in Amiri et al. (2010) with the help of “multi-scale frameworks”. Here, data exchange between the reactor and particle scale is briefly described to exemplify the theoretical framework presented in the abovementioned study.

The reaction occurs in the solid at the particle scale. For a given particle size and surrounding gas temperature and pressure, a single-particle model can be solved to obtain radially distributed and dynamic temperature, pressure, and concentration profiles inside the particle. At any given time, the conversion of gibbsite can be calculated by integration of the gibbsite concentration over the radius of the particle. In this way, a prediction of conversion as a function of time, $X(t)$, is achieved. This function is used in combination with the solids RTD function to obtain the average conversion, \bar{X}_i , of

particles in reactor element i . It should be noted that the RTD is information that is passed from the reactor scale to the particle scale and \bar{X}_i is information exported to the reactor scale from the particle scale. The reactor scale also receives the temperature profile, as a function of the conversion, from the particle scale. This temperature profile is interpolated at the conversion value based on the inlet and outlet concentration of gibbsite at the reactor scale for element i to obtain the average solids temperature leaving the i^{th} reactor element. The calculation of temperature and concentration profiles at the reactor scale provides new input values at the particle scale for the surrounding gas temperature and pressure. Obviously, a new surrounding gas temperature affects all the information flows from the particle to the reactor scale. However, the water vapour pressure in the surrounding gas does not have a significant influence at the particle scale for reasons outlined previously (Amiri et al. 2013a). Nevertheless, iteration is needed to ensure convergence of the exit concentrations and temperature for each CSTR element.

Model solution and analysis

The reactor-scale and particle-scale models must be solved simultaneously to predict the overall performance of the reactor and also to update the parameters that the particle scale is receiving from the reactor scale. To implement this, the spatially distributed particle-scale model developed in Amiri et al. (2013a) is combined with the simplified CSTRs-in-series model developed in this paper. A distributed particle-scale model is used here in preference to the shrinking core models developed in Amiri et al. (2013b) and Amiri et al. (2014) for two main reasons. It has more flexibility for adding all the species involved in the gibbsite calcination process in the future, including boehmite and different alumina phases. In addition, water vapour pressure, which plays such a dominant role in phase formation, can be explained in more detail by using the distributed model.

However, use of shrinking core models in this multi-scale modelling formulation is also feasible and can proceed in a similar way to the distributed model. Further, the multi-stage, multi-reaction shrinking core model proposed in Amiri et al. (2013b) would permit the prediction of boehmite formation and consumption at the reactor scale, which is not the case in the current version of the distributed model. With regards to the shrinking core model developed in Amiri et al. (2014), the availability of an analytical solution at low temperatures could offer some advantages by shortening the model solution time.

The main outputs of the multi-scale model are the gibbsite, alumina and water vapour concentrations in addition to the gas and solid temperatures, all as functions of height in the reactor. A numerical solution has been created by developing a MATLAB code where the governing equations of the model were solved simultaneously along with the inlet boundary conditions.

The inputs of the first CSTR element are given: $C_{G,0}$, $C_{Al,0}$, $C_{W,0}$, $C_{Air,0}$, \dot{Y}_0 and T_0 . The surrounding gas temperature inside each CSTR must be calculated; it is a function of the reaction rate at the particle scale. On the other hand, the particle reaction rate is a strong function of surrounding gas temperature, which appears as a boundary condition in the particle-scale model. Therefore an iterative procedure has been employed, starting with an initial guess value for the surrounding gas temperature T_i . The initial guess for the temperature of element i was taken as the converged temperature of element $(i-1)$. The stopping point for these iterative calculations was set to be $|T_i^k - T_i^{k-1}| < 1$ K, where k is the iteration number. For each iteration, the particle-scale model must be called to provide an updated conversion value based on estimated surrounding gas temperature in that particular iteration. In addition, the particle temperature has been averaged by using the (T_p, X) data exported from the particle scale to the reactor scale during each iteration. The outputs from each element i provide the inputs, and also the initial guesses, for the next element $(i+1)$.

In the following sections, typical results and their interpretations are given for the multi-scale model predictions based on the reactor-scale parameters given in Table 2. The parameters of the particle-scale model are the same as those in Amiri et al. (2013a), unless noted otherwise.

Table 2. Reactor-scale model parameters.

Parameter	Value	Reference / comment
D_t	0.5 m	Typical value
H	1 m	Typical value
ΔH	147 kJ/mol	Beyer et al. (1989)
h	50 W/m ² K	As discussed in Amiri et al. (2013a)
n	20	See the discussion in the next section
P	3 atm	–
R	8.314 J/mol K	Ideal gas constant
\dot{S}	0.0004 m ³ /s	–
$\dot{S}\rho/A$	7.7 kg/m ² s	Solid inlet mass flux
T_0	2000 K	In the range of Marsh (2009)
T_{p0}	298 K	Inlet particles at ambient temperature
Y_0	4 m ³ /s	Typical value
ϵ	0.8	–

Comparison of modelling results of a single PFR and multiple CSTRs in series

The performance of the model with different numbers of CSTRs in series is tested against a single PFR. The results show a considerable deviation for $n < 20$, while for $n = 20$ and higher, the conversion profile is nearly the same for both reactor configurations (Figure 3). Accordingly, simulation of a single ideal CSTR, an ideal PFR and a flow regime between these two ideal patterns can be performed by using CSTRs in series with different n . Comparison of practical operating data with simulation results can help to estimate the appropriate n . For the remainder of the case studies in this paper, $n = 20$ will be used.

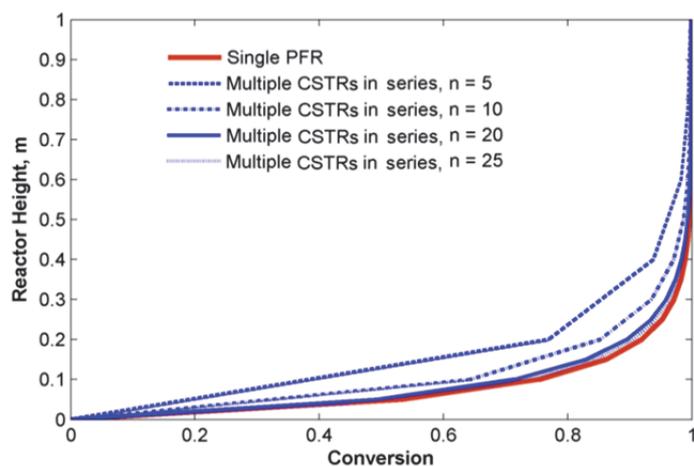


Figure 3. Conversion of gibbsite in a single PFR and multiple CSTRs in series.

Gas temperature, particle temperature and species profiles

The temperature profiles of the gas and reacting particles in a gibbsite calciner are of high interest for process control and the minimisation of energy consumption. The unsteady temperature profile inside a particle has already been discussed extensively in Amiri et al. (2013a,b). The temperature

profile inside a particle is strongly affected by the surrounding gas temperature, and the gas temperature changes through the reactor. One of the most important pieces of information that must be transferred from the particle scale to the reactor scale is the particle temperature.

Similarly, the surrounding gas temperature has to be transferred from the reactor scale to the particle scale. This interaction is essential, because assuming independent gas and particle temperature histories will certainly result in significant errors.

The particle-scale modelling work presented in Amiri et al. (2013b) shows that the temperature profile of a reacting particle consists of three stages (assuming only gibbsite to alumina conversion occurs). First is the initial warming stage during which the particle receives energy from the surrounding gas until its temperature is high enough to initiate the calcination reaction. After this stage, a temperature plateau during the reaction period can be seen, in which the environmental energy input is balanced by the endothermic reaction. Finally, another warm-up period will take place during which the particle temperature approaches the surrounding gas temperature.

Figure 4 shows the average particle and gas temperature profiles, and the overall conversion of the reactor at different heights, attained from the multi-scale model based on the parameters reported in Table 2. Similar temperature behaviour can be observed in Figure 4 at the reactor scale as was observed at the particle scale (Amiri et al. 2013a). In addition, the temperature drop of the gas at the inlet of the reactor suggests that more investigation into preheating the solids may have advantages.

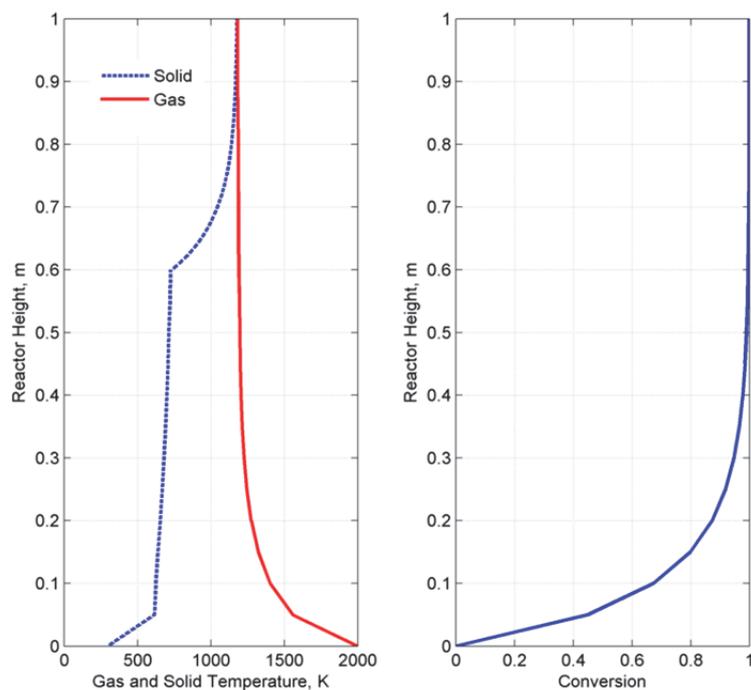


Figure 4. Average particle and gas temperature profiles (left), and overall conversion of the reactor (right), at different heights in the reactor.

It should be noted that particle temperature increases sharply when the conversion reaches close to 100% (Figure 4). Special attention needs to be paid to the numerical discretisation approach to be able to efficiently capture this sharp change.

The temperature histories for both gas and solid phases are strongly influenced by material flow rates, reaction rates and the heat transfer rate.

Similarly, the gibbsite and alumina concentrations may be estimated at different heights in the reactor as shown in Figure 5. This graph is consistent with the start of the post-reaction warm-up period in Figure 4 (left) at $H = 0.6$ m, as it shows the gibbsite concentration is almost zero at this point, causing the reaction to stop. Information of the type shown in Figures 4 and 5 is potentially of assistance in the design of alumina calciners. For the idealised reactor configuration and the conditions considered in this study, it can be clearly seen that conversion is essentially complete at $H = 0.6$ m, meaning that 40% of the reactor volume is not being used for reaction.

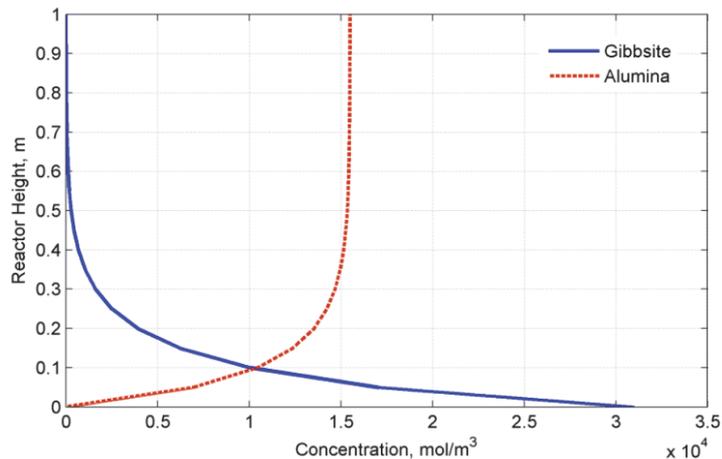


Figure 5. Gibbsite and alumina concentration profiles in the particle phase inside the reactor.

Effect of solid input rate on overall reactor conversion

Solid throughput considerably influences the residence time of the reacting particles. Consequently, different conversion profiles can be observed for different solid mass fluxes as displayed in Figure 6. As expected, a greater reactor volume is needed to fully convert a higher gibbsite feed rate. Information about the conversion profile as a function of reactor height (or volume) and the solid mass flux are valuable in optimisation of the reactor height and solids throughput.

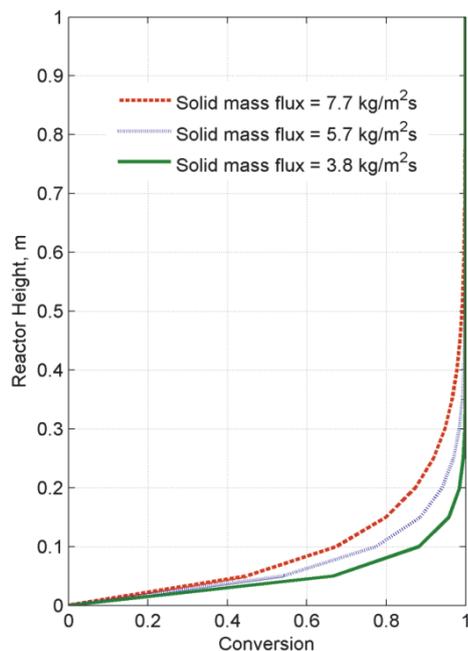


Figure 6. Effect of solid input rate on overall reactor conversion.

Water vapour and gas flow rate profiles inside the reactor

The role of water vapour pressure inside the particle and in the surrounding bulk gas on the progress of calcination has been studied previously by the authors (Amiri et al. 2013a, 2014). It was concluded that the effect of the surrounding vapour pressure on both the reaction progress and mechanism is insignificant as long as the water vapour pressure is less than 15 atm. However, the vapour content in a FBR is of interest for the treatment of the effluent gas and also for the heat balance inside the reactor. In addition, it could be worthwhile to estimate the maximum vapour pressure exerted by the water vapour under different operating conditions. A comprehensive model must involve the mass balance of the air and water vapour species along with the main reactant(s) and product(s). Figure 7 (left) shows how the water vapour builds up inside the reactor due to vapour production from the reacting particles. The profile of the total volumetric flow rate of the gas passing through the reactor, Figure 7 (right), shows a considerable decrease in the lower part of the FBR, which is due to the large temperature drop of the inlet gas (Figure 4). The production of water vapour due to the calcination reaction causes an increase in the overall molar gas flow rate inside the bed, and this counteracts the effect of the reduced temperature on the volumetric flow rate to some extent.

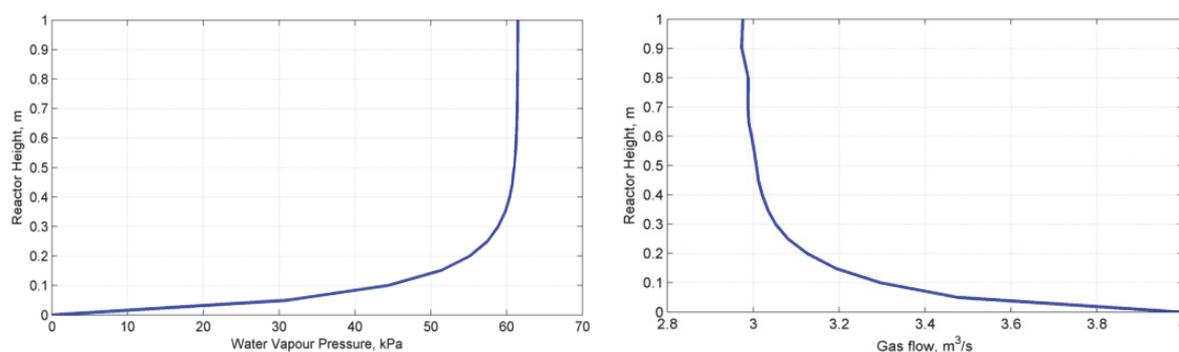


Figure 7. Water vapour pressure build-up inside the reactor (left) and overall gas (air + water vapour) volumetric flow rate inside the reactor (right).

Conclusions

In this paper, a simplified reactor-scale calcination model is presented and combined with a particle-scale calcination model to illustrate a multi-scale modelling methodology for FBRs. In spite of the simple structure of the proposed model, the main features of an alumina calciner are reasonably well captured. Gas and solids temperature profiles, trends in overall gas flow rate and water vapour pressure inside the bed, alumina and gibbsite concentration profiles within particles, and effects of the solids throughput rate on the reactor performance are predicted and explained based on the proposed model. The multi-scale model was solved numerically through an iterative procedure that alternated between solving particle-scale and reactor-scale models. An iterative method was chosen to enable solution of the model as the variables at the two different scales have complicated interactions. The key variable that complicates the model solution is the temperature of the gas at the reactor scale. It affects the conversion history at the particle scale by changing one of the boundary conditions and is in turn affected by the extent of particle reaction through the overall energy balance at the reactor scale.

Nomenclature

A	Reactor cross-sectional area [m^2]
C_{Air}	Air concentration [mol/m^3]
C_{Al}	Alumina concentration [mol/m^3]
C_G	Gibbsite concentration [mol/m^3]
C_p	Molar heat capacity [$\text{J}/\text{mol K}$]
C_W	Water vapour concentration [mol/m^3]
C_{Wb}	Water vapour concentration in bubble phase [mol/m^3]
C_{We}	Water vapour concentration in emulsion phase [mol/m^3]
D_t	Reactor diameter [m]
$E(t)$	Residence time distribution function [$1/\text{s}$]
h	Heat transfer coefficient [$\text{W}/\text{m}^2 \text{K}$]
H	Reactor height [m]
ΔH	Enthalpy of reaction [J/mol]
n	Number of CSTRs [–]
\dot{S}	Solids volumetric flow rate [m^3/s]
T	Gas temperature [K]
T_0	Inlet gas temperature [K]
T_p	Average particle temperature [K]
T_{p0}	Inlet particle temperature [K]
V_R	Reactor volume [m^3]
\bar{X}	Average solids conversion in a single CSTR [–]
$X(t)$	Conversion as a function of time in a single particle [–]
\dot{Y}	Gas volumetric flow rate [m^3/s]

Greek symbols

α	Stoichiometric coefficient: moles of alumina produced / moles of gibbsite consumed [–]
ε	Bed voidage [–]
ρ	Solid (gibbsite) density [kg/m^3]
τ	Average residence time [s]
τ_i	Average residence time in a single CSTR [s]
ω	Stoichiometric coefficient: moles of water produced / moles of gibbsite consumed [–]

Biography



Amirpiran Amiri (Presenter)

Amirpiran Amiri is a Postdoctoral Researcher and Sessional Lecturer in Chemical Engineering at Curtin University. His research interest is mainly in process modelling with a special focus on applied multi-scale modelling methodologies. As a PhD researcher, he investigated the multi-scale nature of the fluidized bed reactors by developing goal-oriented models at different scales. Currently he is working on development of a numerical tool for modelling and optimisation of fuel cell process plant through multi-scale approaches. He also has several years of experience in the teaching of process simulation and has worked as an engineer before commencing his PhD studies.

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