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CIN4 : a multiphysics software for heterogeneous reactions at a reactor scale

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Abstract

A rigorous simulation of industrial reactors in the case of solid-gas reacting systems is a complicated task due to several difficulties linked to the kinetic problem at the scale of the solid grains and to the problem of gas and heat transfers within the powder bed. Firstly it requires the knowledge of the kinetic model for the calculation of the kinetic rate of reaction in one part of the reactor and for given conditions of temperature and gas composition, and secondly it necessitates solving the material and heat balance equations for the flow conditions settled in the reactor.

The first part of the article is devoted to the presentation of the kinetic models governing a population of grains transformed in the same conditions of temperature and gas composition. Then a short presentation of CIN4, a multiphysics software resulting from the collaboration between ASTEK and EMSE, shows the various scales of the calculations: CIN4 offers the resolution of the thermohydraulic equations combined with the kinetic laws which describe the heterogeneous reactions, including the diffusion aspects in the case of aggregates. Then two examples of application are given in order to illustrate the interest of this multiphysics modeling: the dehydroxylation of kaolinite and the carbonation of CaO by CO_2.

Keywords: kinetics, simulation, solid-gas reactions, reactor, aggregates

1. Introduction

The simulation of heterogeneous reactors has been done in the past using simplifying assumptions as regards to the law expressing the kinetic rate of reaction of a powder which transforms in conditions of constant temperature and gas composition. These assumptions are based on a kinetic law typically of the form:

$$\frac{d\alpha}{dt} = k(T)\, P\ f(\alpha) \qquad (1)$$

where k(T) usually follows the Arrhenius law, P is the pressure of the reacting gas and f(α) is a function of the fractional conversion α. The function f(α) most often corresponds to the core-shrinking model applied to various grain geometries. The order respective to the gas is chosen equal to 1. Such assumptions allow using the law of additive reaction times for solving numerically the problem of reacting porous media. However, as a result of about 20 years of experience in kinetic studies of solid-gas reactions in the Centre SPIN of EMSE, it must be recognized that most often, such assumptions are too much restrictive, so that the law of additive reaction times is not valid. Various reasons may be invoked such as a complex dependency of the kinetic rate with the temperature and pressure, several gases are involved in the reaction and influence the kinetics in different manners, the kinetic model equation does not vary according to a f(α) function, etc …

In order to overcome the difficulty due to the inadequacy of the law of additive reaction times, we decided to collaborate with ASTEK which previously developed the FLUX-EXPERT software tool applicable to homogeneous reactors, in order to solve the problem of gas-solid reactions in porous media for a large variety of kinetic models including those corresponding to equation (1).

In the following, we present first in section 2 the kinetic models based on a much more general equation such as equation (2):

$$\frac{d\alpha}{dt} = \phi\, S_m(t, \phi, \gamma, r_0) \tag{2}$$

in which:

ϕ (in units of mol m^{-2} s^{-1}) depends of the thermodynamic conditions only (temperature, partial pressures, etc…) and is called the "areic reactivity of growth",

$S_m(t, \phi, \gamma, r_0)$ is function of the initial and current morphology of the sample (r_0 represents a characteristic dimension of the initial grains) and therefore depends of time, whereas it also depends of ϕ, and according to the model, it may depend of the "areic frequency of nucleation" γ (in units of nb. of nuclei m^{-2} s^{-1}).

Then section 3 shortly describes the multiphysics CIN4 software structure, since the mass and heat balance equations and the assumptions settled for solving them were previously detailed by Favergeon et al. (2009). In a last part, section 4, we present examples of application of CIN4 and we discuss the results and the possible improvements to be done in the future before concluding.

2. The kinetic models at the grains[1] scale

2.1 The various scales for modeling

Several geometrical scales characterize all phenomena which occur in a reactor. A rigorous description of our modeling process requires a precise definition of these different scales. We have deliberately set these scales from the objects: mesh, grains, grains population, aggregates and reactor.

Four scales will be discussed in this work: grain, grains population, aggregate and reactor.

At the grains scale, in the case of solid-gas reactions, it is well admitted that the nuclei appear at the grain surface[1] and grow at the expense of the initial solid phase: the kinetics is governed by the shape of the grains, the type of growth, the localization of the rate determining-step of growth, and the direction of development of the new phase (inwards, outwards). Then a "micro" scale population is a set of grains in the same thermodynamic conditions, i.e. the gradients of temperature and gas partial pressure are extremely small inside the population. At the reactor scale, which corresponds here to the "macro" scale, the chemical reaction is coupled with mass and heat transfers (this case will be illustrated by the kaolinite dehydration reaction). An intermediate scale called "meso" has proven to be useful in the case of powders made of porous aggregates inside which the molecular diffusion of gases may not be neglected (this will be the case of the CaO carbonation reaction).

2. 2. The kinetic models for calculation of the rate at grains population scale

As shown by Pijolat et al. (2008, 2011), in order to model reactions which involve surface nucleation and growth of the nuclei, it is interesting to use equation (2) in which the rate is expressed as the product of two functions, ϕ and S_m, which means that the value of the rate at any time and thermodynamic conditions requires to know the expressions of these two functions. For constant temperature and gas composition, the S_m function can take various expressions calculated from assumptions on the growth type (isotropic or anisotropic), the development direction of the new phase (inwards or outwards), the localization of the rate determining step of growth (external interface, internal interface, diffusion) and the grains shape (spheres, cylinders, plates). Soustelle (2006) detailed the method for deriving the laws and the expressions of S_m for each model which result from the combination of the previous assumptions, which leads to more than 40 kinetic models. These models can be simulated using the free CIN3 software according to Pijolat et al. (2011). They have been incorporated in the part "micro" of CIN4. Moreover a numerical procedure allows fitting the experimental kinetic data in order to find the best values of ϕ and γ for any experiment done at constant temperature and gas composition.

These models can be divided in two families: those which involve only one process, surface nucleation or growth, and those which involve simultaneously both processes. In first case, if nucleation is

[1] The word "grain" represents an elementary dense particle.

[2] Avrami's laws cannot be used for solid-gas heterogeneous reactions involving powders since they are based on bulk nucleation in an infinite volume.

instantaneous, only growth is considered and all the grains behave similarly, so that the rate equation is exactly the same than for a single grain. If growth is instantaneous, a single law is obtained considering the behavior of a grains population. In both cases (first family), the rate equation follows the form of equation (2) in which $S_m(t,\phi,\gamma,r_0)$ is proportional to a function f(α) as in equation (1).

In the case of two processes family, the models are derived at the grains population scale: both surface nucleation and growth are taken into account, which leads to two kinds of models according to the growth type (isotropic or anisotropic). Two methods are used to calculate the fractional conversion and the rate of reaction:

- in the case of isotropic growth of the nuclei, we use a statistical approach based on the works of Johnson and Mehl (1939) and Mampel (1940), then developed by Delmon (1969).
- in the case of anisotropic growth, each grain starts its transformation at various times and the whole microscopic fractional conversion can be obtained from an integral over all the dates of nucleation, considering the nuclei appeared on each grain of the grains population.

For both types of nucleation and growth models, the rate equation involves the $S_m(t,\phi,\gamma,r_0)$ which cannot be expressed using a f(α) function. Such a difference in the rate equation between one process and two processes models explains why the classical approach (law of additivity reaction times) may be applied to one-process models while it cannot in the case of two-process models. In this last case, the kinetic rate of reaction depends both on γ and ϕ which vary independently with temperature and gas composition, so it will be necessary to numerically follow the behavior of all the grains populations vs. time in each part of the reacting bed. This method can be compared to a population balance but here there is no fluxes from a grain size class to another. The calculations corresponding to the kinetic models are available in the part of CIN4 called “micro”, which, in addition, enables to account for grain size distribution and successive reactions.

3. Mathematical modeling

3.1. The assumptions of the model

Six assumptions are done for the various scales of the modeling: the production and consummation of gas by the reaction do not disturb the total pressure distribution; the gases are diluted in a carrier gas; the gases flow rates are low; the gases are considered as ideal; the growth process can be written by a succession of elementary step and one of them controls the growth rate (rate-controlling step approximation); the grains population is supposed uniform in shape.

3.2 Heat and mass transport at reactor scale

The macroscopic scale is the center of heat and mass exchanges that are described by the thermal and hydrodynamic models, as well as by a mass transfer equation. The various equations corresponding to the thermal model, hydrodynamic and mass transport models can be found in a previous article (Favergeon et al. (2009)) so they will not be detailed here.

3.3 Coupling between the microscopic population scale and the reactor scale

At microscopic scale, the reaction fractional conversion is followed for a representative population of grains. By finite difference it is possible to evaluate the reaction rate $\frac{d\alpha}{dt}$. This rate allows to calculate heat and mass sources produced by the reaction. Thus the heat source density is equal to:

$$Q^T = \sum_{i=1}^{n_g} \nu_i M_A \frac{1-\varepsilon}{V_{mA}} \frac{d\alpha}{dt} \Delta H_i \tag{3}$$

And the mass (partial pressure) source density for a gas i is equal to:

$$Q_i^C = \nu_i \frac{1-\varepsilon}{V_{mA}} \frac{d\alpha}{dt} \tag{4}$$

So, using these sources terms, microscopic reactions have an impact on the spatial and temporal evolution of the thermodynamic processes at the reactor scale. Inversely since it modifies the areic frequency of

nucleation and the areic reactivity of growth, thermodynamics influences fractional conversion of the microscopic reaction.
As previously noted, the CIN4 software also allows to take into account an intermediate scale when grains are structured in aggregates. In this case, aggregates are considered spherical, with the same radius, and isotropic, which means that inside thin crowns of the aggregate, all the grains behave in the same way, with identical temperature and partial pressures at a given time. Furthermore, inside the aggregates, only diffusion accounts for heat and mass transfers (convection is neglected). The coupling is realized by the combination of the flow modeling at the aggregate scale based on the finite difference method, with the kinetics of heterogeneous grains population. A classical way is followed to obtain weak formulations for each state variable: temperature, charge and partial pressures. At the microscopic scale, the reaction fractional conversion is followed for a representative population of grains. It is thus possible to calculate the reaction rate for a given temperature and given partial pressures, and therefore to get heat and mass sources produced by the reaction.
It is worthwhile to notice that CIN4 allows to simulate the behavior of reactions for which the kinetic rate at time t (at the microscopic population scale) depends on the local thermodynamic conditions that were established between t=0 and t. CIN4 highly improves the previous approaches which were limited to kinetic model based at grain scale only, excluding the gas composition effects other than those with one gas with a first order, and the surface nucleation and growth models.
The equations used in CIN4 require numerous physical properties (porosity, viscosity, density, heat capacity, thermal conductivity, diffusivity). CIN4's user should be able to calculate these properties using empirical laws or mathematical models like for example those given by Bird et al. (2002).

3. 4. Numerical modeling

At grain and microscopic population scales, two types of modeling are envisaged according to the growth: anisotropic or isotropic. In the first case, the used method allows to calculate the evolution of the fractional conversion for all grains in each granulometric class. When the growth is isotropic, we used the Mampel's method (1940) for the three grain geometries: spheres, cylinders and plates.
At reactor scale, for heat, hydrodynamic and mass transport problems, two finite element formulations were built, depending on the system symmetry (cylindrical or Cartesian coordinates). A classical way was followed to obtain weak formulations for each state variable: temperature, charge and partial pressures.
For solving heat and mass transfers equations throughout the reactor by the finite elements method, a mesh is available by using Gmsh freeware application (Geuzaine et al. (2009)).

4. Applications

4.1. Kaolinite dehydroxylation

The dehydroxylation of kaolinite was followed by means of a SETARAM TAG16 balance. Isothermal and isobaric curves were first obtained by heating the powder samples in an alumina crucible (2 cm height, 1 cm diameter) at different temperatures in the range 420-460°C under water vapor pressure fixed in the range 0.25-2 kPa by means of SETARAM WETSYS. First, experiments were performed under with about 25 mg of powder. During the entire transformation, the sample weight was low enough to prevent any effect of pressure gradients in the powder layer. As expected, the reaction rate increases with temperature and decreases with water vapor pressure.
A second series of experiments was done with various heights of the powder bed. In the same crucible as previously, two distinct TGA experiments were performed at 450°C under a water vapor pressure of 7hPa: the first one with 50 mg of powder corresponding to a powder bed height of 3 mm; the second one with 300 mg corresponding to 10 mm. The kinetic curves and rates curves obtained with both bed heights are presented on Figure 2. One can see that the powder bed height has an important effect on the kinetic curves since the maximum reaction rate obtained for 3 mm is about twice more that obtained with 10 mm (and is about twice less than that obtained with 1 mm).
In order to interpret the experimental curves obtained with thin powder beds, we used a model involving random nucleation followed by anisotropic growth of the nuclei first proposed by Nahdi et al. (2002). Nucleation is supposed to occur at the surface of the individual particles with an areic frequency (γ). Once

a nucleus has been formed, the anisotropy of growth is such that the particle is instantaneously covered with a very thin layer of solid product. In this case the tangential component of the growth rate is very high compared to its radial component. The particles are considered as flat cylinders, as suggested by SEM characterizations, with a mean radius r_0 equal to 0.15 µm and a thickness h equal to 0.05 µm. The rate-determining step of growth is a diffusion step through the metakaolinite already present in the periphery of the particle. Moreover the growth of the metakaolinite is considered as occurring inwards (shrinking core type). With these assumptions and by considering the volumic expansion factor equal to 1 (i.e. kaolinite and metakaolinite have the same molar volume V_{mA} = 97.3 10^{-6} m^3 mol^{-1}), the reaction rate dα/dt for the powder can be determined by solving the following equations system:

$$\frac{d\alpha}{dt} = \frac{4\pi.h.\gamma.\phi.V_{m_A} l_0}{r_0} \int_{\varsigma}^{t} \exp(-2.\pi.h.r_0.\gamma.\tau).\ln(1-\beta).d\tau \qquad (5)$$

with β the fractional conversion for a single grain born at time τ, solution of the equation:

$$(1-\beta)[Ln(1-\beta)-1]+1 = 4\frac{\phi.V_{m_A}.l_0}{r_0^2}(t-\tau) \qquad (6)$$

where l_0 is equal to the length unity (l_0 = 1 m).

The optimization procedure of CIN4 provided the values of γ (in nb nuclei m^{-2} s^{-1}) and ϕ (in mol m^{-2} s^{-1}) for each experiment so the laws of variation of these quantities with temperature (T in K) and water vapor pressure could be expressed by:

$$\gamma = 10^{26} e^{-0.049T}\left(1-\frac{P}{P_{eq}}\right)^{3/2} \qquad (7)$$

$$\phi = 2\ 10^{-49} e^{0.1353T}\left(1-\frac{P}{P_{eq}}\right)^{1/2} \qquad (8)$$

Concerning the results obtained with thick powder beds, the "macro" part of CIN4 was used in order take into account the heat and mass transfers between all the various places inside the reactor (sample bed, crucible, gas flow). The first step consisted in defining the domains of calculation. The system being axi-symmetric, we used weak forms written in cylindrical coordinates.

Inside the granular medium, heat and mass sources were calculated simulating the reaction phenomena at the microscopic level. Figures 1 a and b show the gas flow rate obtained as well as temperature and fractional conversion fields at a given time for bed heights of 3 and 10 mm, respectively. Figure 2 presents a comparison of the whole rate of reaction versus fractional conversion between the experimental data and the simulation for both bed heights.

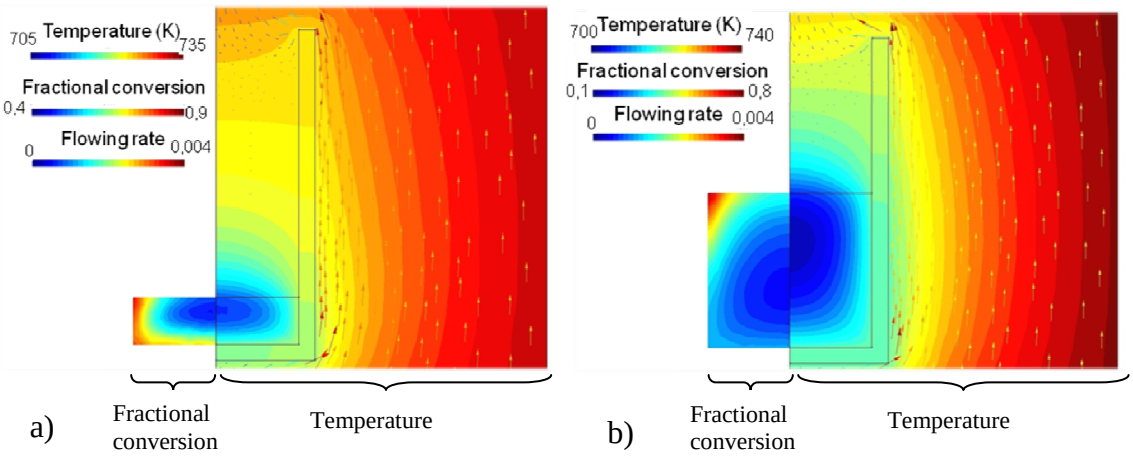

Figure 1: Representation of the temperature field, the fractional conversion and the flowing rate (arrows) at a given time for (a) 3 mm-height bed and (b) 10 mm-height bed.

Figure 2 shows that the CIN4 simulation is able to discriminate the height of the powder bed from 3 to 10 mm. It is important to notice that these results at reactor scale are obtained by means of numerical simulation without any adjustment of parameters. Nevertheless the calculated curves are not perfectly superimposed with the experimental ones. Some improvements should be done in order to get better simulations. For example several points could be improved: at the grains scale ("micro" optimization), the particles size distribution could be taken into account to obtain more precise values of γ and ϕ; at the reactor scale, the change in the physical properties of the granular medium (including the porosity) due to the transformation of kaolinite into metakaolinite should be considered using appropriate relationships between the physical properties of the granular medium and fractional conversion.

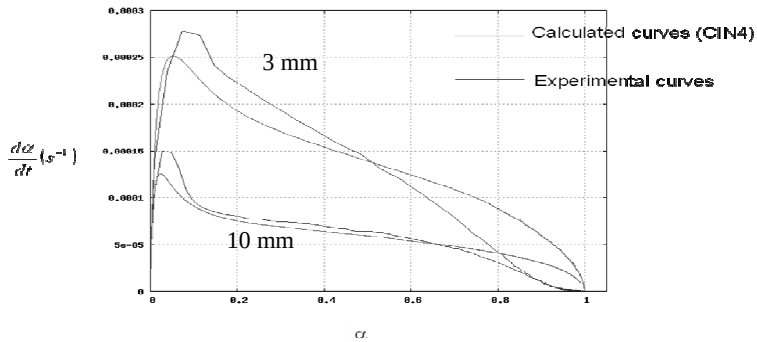

Figure 2: Reaction rate vs. fractional conversion from the experiment and from the simulation for 3 and 10 mm powder bed heights.

4.2. Calcium monoxide carbonation

CIN4 has been used to describe the kinetic behavior of CaO aggregates during the reaction of carbonation into $CaCO_3$ by CO_2 (5 kPa) at temperatures in the range 450-650°C. The experimental kinetic curves reveal two distinct features (cf. Figure 3a): first there exists an induction time which depends of the thermodynamic conditions (temperature and CO_2 partial pressure); secondly, it systematically appears a huge slowing down of the reaction kinetic rate linked to diffusion limitations in the aggregates (decrease in size of the pores during reaction due to a volumic expansion factor equal to 2.13). A typical shape of the CaO aggregates can be seen in Figure 3b. The kinetic modeling at the "micro" scale could be done due to the initial part of the experimental curves as shown by Rouchon et al. (2013). The model corresponds to a single nucleus appearing at the surface of the CaO grains (nucleation is supposed to be a sluggish process compared to the growth, in agreement with the existence of the induction period) which grows isotropically inside the grain until total consumption of the CaO phase. So all the grains behave in a similar manner, but begin to be transformed at distinct times between 0 to t. Thus in this case, we used for the "micro" kinetic model both functions describing the variations of the induction period τ and the areic growth reactivity ϕ with temperature and partial pressure as shown in Figure 4.

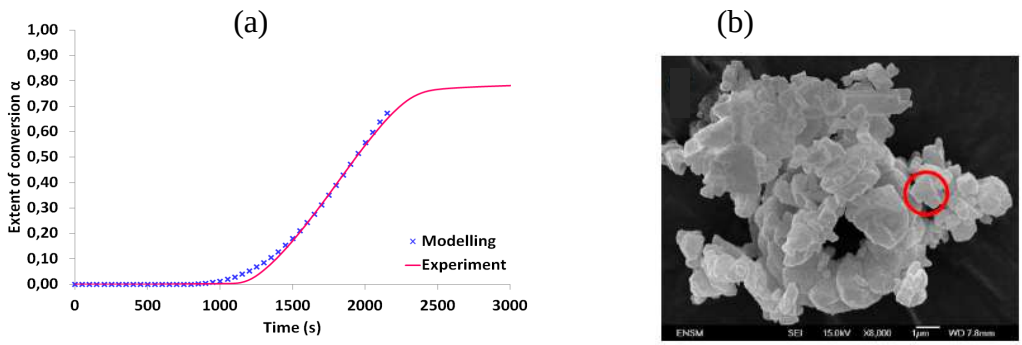

Figure 3: Experimental extent of conversion at 650°C compared to the CIN4 "micro-meso" scale simulation (a); SEM view of a CaO aggregate (b).

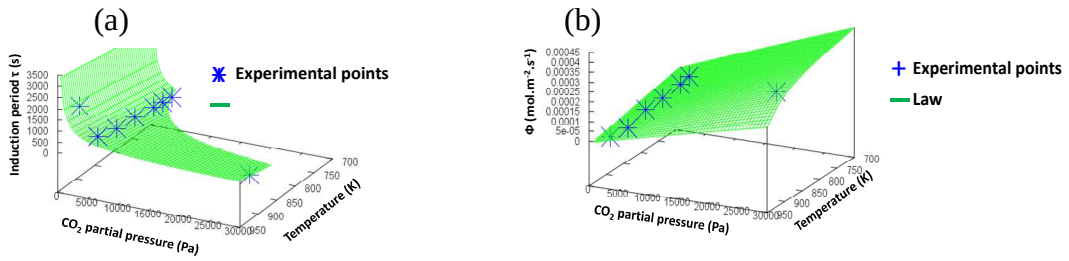

Figure 4: Variations of the induction period (a) and of the areic reactivity of growth (b) vs. temperature and CO_2 partial pressure for the CaO carbonation reaction.

CIN4 was used to describe the behavior of the aggregates, coupling the "micro" and "meso" scales, since it was assumed that at the reactor scale, all the aggregates in the powder bed are transformed with the same kinetics. This assumption is justified by the fact that the sample mass was very low, around 10 mg, and also due to a large pore size between aggregates, thus ensuring fast heat and mass transfers between aggregates. The simulation was realized considering the changes in the porous characteristics of the aggregates:

- an empirical law of variation of the pore size with the extent of conversion as shown in Figure 5, based on experimental characterizations of the porosity inside the aggregates,
- a physical law of variation of the porosity ε vs. the fractional conversion:

$$\varepsilon(\alpha)=1-(1-\varepsilon_0)[1+(z-1)\alpha] \qquad (9)$$

where ε_0 is the initial porosity and z is the volumic expansion factor (z=2.13).

A good agreement between the calculated and experimental curves can be observed in Figure 3a. The simulation stops when the diffusion of CO_2 molecules through the aggregates pores becomes impossible, i. e. when the pore size reaches that of the molecules size. Afterwards, when the periphery of the aggregates reaches a densified state, a solid state diffusion regime should be invoked (Rouchon et al. (2013)). However, real improvements could be done in the future for a better description of the changes in porosity, not only inside the aggregates, but also at the scale of the powder bed.

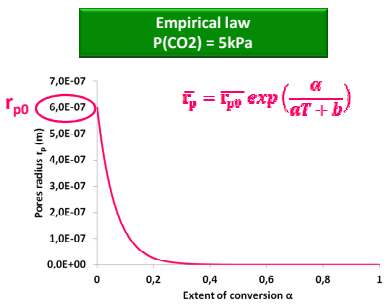

Figure 5: Variations of the mean average pore size in the aggregates vs. fractional conversion

6. Conclusions

CIN4 is a new software tool able to couple kinetics at grains population scale with both heat and mass transfers by means of the finite element method. Kinetic models are based on a general method agreeing with physical reality, offering the possibility to simulate more than 40 models depending on nucleation and growth processes, the shape of the grains, the growth type (isotropic or anisotropic), the development direction of the new phase and the localization of the rate determining step of growth (internal interface,

external interface or diffusion volume). Heat and mass transfers are governed by differential equations and solved by a finite element method. Powder beds consisting in separate individual grains (micro and macro scales) or aggregates (micro-meso-macro scales) may be considered. CIN4 allows simulating not only reactions at laboratory scales such as thermobalances, but also industrial reactors.

Notations

α Fractional conversion of the powder
β Fractional conversion of a grain
S_m Space function ($m^2.mol^{-1}$)
ε Porous medium porosity
ε_0 Initial porous medium porosity
ϕ Areic reactivity of growth ($mol.m^{-2}.s^{-1}$)
γ Areic frequency of nucleation (nuclei.m-2.s-1)
h Cylinder thickness (kaolinite particles)
M_i Molar mass for constituent i (kg mol^{-1})
ν_i Stoichiometric coefficient
P Total pressure (Pa)

P_i Partial pressure of reactive gas (Pa)
Q_T Heat sources density ($W.m^{-3}$)
Q_C Concentration sources density ($mol.m^{-3}.s^{-1}$)
r_0 Initial radius of the grain (m)
σ Stefan Boltzmann constant ($W.m^{-2}.K^{-4}$)
T Temperature (K)
τ (section 3.1) Nucleation date
τ (section 3.2) Induction period
V_{mA} Molar volume of A ($m^3.mol^{-1}$)
z expansion factor

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Résumé

La compréhension du comportement de réacteurs industriels est assez complexe dans le cas de réactions solide-gaz. En effet la phase solide est un milieu granulaire dans lequel circulent des réactifs et des produits gazeux. Les propriétés d'un tel milieu sont modifiées dans l'espace et le temps en raison des réactions se produisant à une échelle microscopique. Les conditions thermodynamiques sont fixées non seulement par les conditions de fonctionnement du réacteur, mais aussi par les transferts de chaleur et de matière dans le réacteur. Nous proposons de résoudre numériquement les équations régissant ces transferts en les combinant avec les lois cinétiques qui décrivent les réactions hétérogènes. L'avantage majeur de cette approche est la grande variété des modèles cinétiques de transformation de grains disponibles (~ 40) comparé à l'approche habituelle, notamment dans le cas de réactions impliquant la prise en compte de la germination à la surface suivie de leur croissance. Les termes sources de chaleur et de matière entrant dans les bilans à l'échelle macroscopique dépendent de la cinétique à l'échelle microscopique. La résolution numérique de ces équations par la méthode des éléments finis permet d'obtenir la température et les pressions partielles dans le réacteur, ainsi que le suivi de l'avancement local et global de la transformation. Deux exemples d'application sont décrits afin d'illustrer l'intérêt de CIN4 pour l'étude des transformations chimiques de solides divisés : la déshydroxylation de la kaolinite et la carbonatation du monoxyde de calcium.