4th Int. Conf. on Multiphase Flow (ICMF-2001) May 27 - June 1, 2001, New Orleans (LA) USA

CFB reactors, CFD and particle/turbulence interactions

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Abstract

The design of furnaces and boilers for solid fuels is supported increasingly by powerful softwares and ever faster computers. A round-robin over the most important CFD (computational fluid mechanics) models and softwares currently available shows, however, that numerical procedures for particle/turbulence interactions are not (yet) very advanced. Particle/fluid interphase slip is considered, but turbulent velocity fluctuations are largely ignored. Particle trajectories can be calculated with reasonable accuracy, but realistic calculations involving gas/solid mass and heat transfer and gas/solid chemistry are impossible.

Here, the influence of particle/turbulence interactions on circulating fluidised bed (CFB) combustor riser chemistry is discussed, based on multi-phase mixing by turbulent dispersion of solid particles in a dilute suspension. After a short discussion on CFB hydrodynamics modelling, commercial CFD codes are analysed. Thereafter, an approach for taking into account the effect of particle/turbulence interactions and gas/solid mass transfer on gas/solid conversion is given, illustrated by a typical example.

1. Introduction

The development work on improved furnace and boiler designs for solid fuels is supported more and more by powerful softwares and ever faster computers. By combining commercial and/or user-specific codes for computational fluid dynamics (CFD), detailed chemistry and thermodynamics (*i.e.* Gibbs' energy minimisation) it is, in principle, possible to optimise the design and performance of furnaces and boilers based on first principles. This is refered to as "comprehensive combustion modelling" (Eaton et al., 1999).

At the same time, a round-robin over the most important commercial CFD softwares currently on the market shows that numerical procedures for particle/turbulence interactions are not (yet) very advanced (Zevenhoven, 2000). Deterministic-separated flow (DSF) models are current state of the art in commercial CFD, i.e. interphase slip between particles and the surrounding continuum are considered, but the effects of turbulent velocity fluctuations are ignored or simulated by a random number generator. Hence, particle trajectories can be calculated with reasonable accuracy, but realistic calculations involving gas/solid mass transfer, heat transfer and heterogeneous chemistry are impossible. This would require a more advanced approach based on a physically sound stochastic-separated flow (SSF) - type model.

The dispersion and trajectories of solid particles in a turbulent gas stream are determined by particle/turbulence interactions in the form of a slip velocity between the particle and the

surrounding gas, and the interaction with fluctuating velocity components of the turbulence. Particle/turbulence interactions influence the mixing of the "phases" (every particle size can be considered a separate phase) with the gas phase and the contacting of the phases. High slip velocities result in thin boundary layers, which benefits mass transfer, and a high degree of particle dispersion is required for the necessary gas/solid contact. When a chemical reaction occurs between the solid and the gas, or with a solid catalyst particle, multi-phase mixing over the full scale of turbulence is needed: particles that are unable to follow all turbulent oscillations of the flow are effectively non-available for chemical interactions with gas molecules transported by the smallest eddies.

As will be shown below, this is far beyond the state-of-the-art of commercial CFD codes that are currently available on the market. Therefore, in parallel with widespread use of CFD as a tool for consulting and semi-quantitative design work, many scientists are involved in development work on stretching and expanding the possibilities of CFD in, e.g. comprehensive combustion modelling. A very good example is a circulating fluidised bed (CFB) combustor or gasifier for solid fuels, as shown in Figure 1.

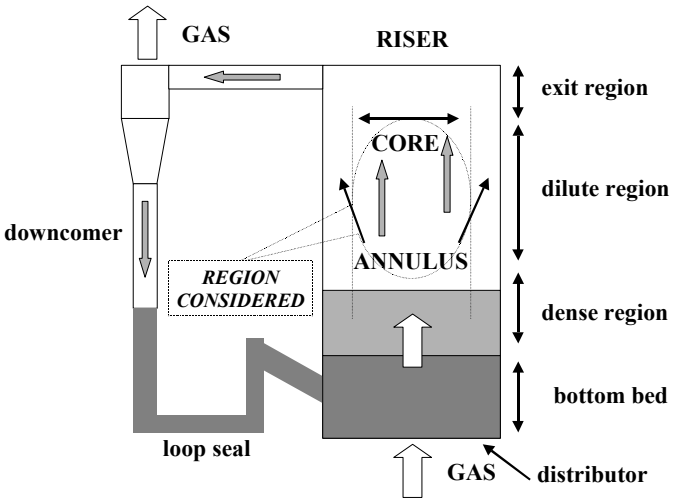

Fig. 1 Typical lay-out of a circulating fluidised bed reactor (after Grace et al., 1997)

The purpose of this work is to consider options for CFD-based modelling of the reacting multi-phase system in the dilute upper zone of a CFB combustor riser. As a typical yet highly relevant gas/solid reaction the heterogeneous reaction between NO and CO, catalysed by char particles, is considered:

$$CO + NO + \text{char} \rightarrow CO_2 + \tfrac{1}{2} N_2 + \text{char} \qquad \textbf{(R1)}$$

At FB combustion temperatures (750-950°C), the gas phase reaction between CO and NO is too slow to play any role. An effective reaction rate for reaction (R1) will be calculated based on the chemistry for (R1), the gas/solid mass transfer limitations and multi-phase mixing limitations due to particle/turbulence interactions:

reaction rate in CFBC riser = chemical rate ´ efficiency of gas/solid mass transfer ´ ´ efficiency of multi-phase mixing by particulate dispersion **(1)**

A particle's eddy dispersion determines its degree of mixing with the gas phase. The last mentioned efficiency factor in Eq. (1) has also been referred to as "gas-solid contact efficiency" in relation to CFB combustion (Dry and La Nauze, 1990).

Below, first a short review on CFD and hydrodynamics modelling of CFB reactors is given. This is followed by reporting the results of a round-robin amongst commercial CFD software providers on several issues related to multi-phase flow modelling, aiming at CFB combustion and gasification reactors as the application. Thereafter, a procedure for calculating the effective rate of reaction (R1) in a CFBC upper riser is briefly presented, including some results. The procedure is based on 1) independent fixed bed reactor measurements on the chemistry for reaction (R1) for chars from several solid fuels, without mass transfer limitations or turbulence effects, 2) a model for heat / mass transfer to and from a sphere emerged at a fixed position in a turbulent gas stream in a CFB riser, i.e. without turbulent eddy dispersion effects, and 3) a description of CFBC riser turbulence based on a Lagrangian eddy frequency spectrum combined with the Tchen/Hinze model for spherical particle dispersion in homogeneous, dilute multi-phase turbulence, which defines the degree of multi-phase mixing. This approach is easily implemented in CFD models via a formulation as a k-ε-k_p model.

2. CFB riser hydrodynamics modelling

From a hydrodynamics point of view, the multi-phase flow can be modelled as an Eulerian-Eulerian ("two-fluid") or Eulerian-Lagrangian system, which implies that in combination with an Eulerian description of the fluid flow, the behaviour of the particulates is described by an Eulerian or Lagrangian approach. Both alternatives are being used in a wide field of applications, Eulerian models being, in general, more versatile for dense multi-phase flows, whilst Lagrangian models appear better suitable for dilute systems. (Gouesbet and Berlemont, 1999, Shirolkar et al., 1996). Boemer et al. (1995) state that "....in case of extremely low solid concentrations the Eulerian approach is questionable in general".

Increasing computational power and capacity appears to benefit mostly the Lagrangian models. When the composition, size and/or shape of solid particles is changing with time by chemical reaction or mechanical effects (attrition etc.), it is most natural to apply a Lagrangian approach that follows the particle and its characteristics along its trajectory.

For CFB reactor systems as shown in Figure 1, the riser reactor can be divided in a dense bottom bed, a dense region and a dilute upper zone with typical voidages, ϕ, of ~ 0.4, 0.7 ~ 0.99 and > 0.99, respectively, the dilute zone occupying the largest volume. Apart from 1-way coupling (the fluid flow turbulence effects the particulates but not vice versa), also 2-way coupling (turbulence moduation by the particles) and even 4-way coupling (hydrodynamic interactions between the particles and particle collisions) become increasingly important when going downwards. According to Elgobashi, 1-way coupling holds up to a particulate volume fraction $\phi_p \sim 10^{-6}$, ($\phi + \phi_p = 1$) while the transition from dilute to dense suspensions lies at $\phi_p \sim$ 0.001- see Figure 2. Often, only 1-way coupling is considered in dilute suspensions, if $\phi_p \ll 0.01$.

Particles respond to a turbulent flow through their concentration (i.e. ϕ_p) and particle size. Small particles may follow all velocity fluctuations of the fluid flow; acceleration of these particles in turbulent eddies suppresses the turbulence. Large particles, however, may enhance the turbulence due to the wake of the particles or the vortex shedding by the particles (Hetsroni, 1989, Gore and Crowe, 1989). This can be quantified by the ratio of the kinetic particle response time, τ_P, to the Kolmogorov time scale of the turbulence, τ_K, as shown in Figure 2.

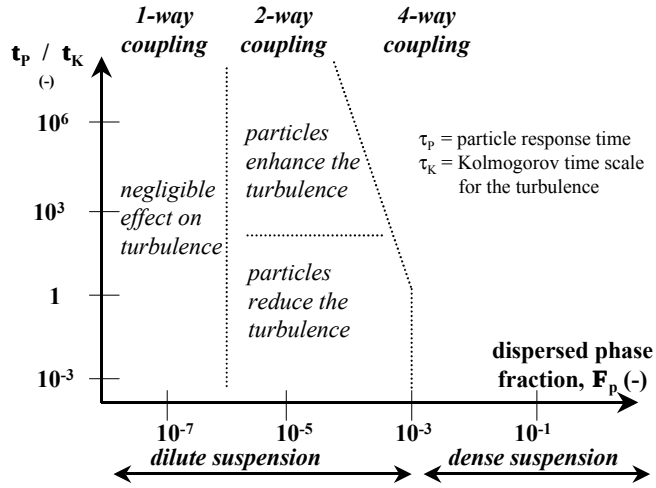

Fig. 2 Map of flow regimes in turbulent particle-laden flows (after Elgobashi, in: Sirignano, 1999)

According to many researchers, Eulerian-Eulerian modelling of CFB reactors, has many benefits over Eulerian-Lagrangian approaches (e.g. Mathiesen et al., 2000). A recent overview by Sinclair (in: Grace et al., 1997) on CFB hydrodynamics considers mainly the Eulerian approach. In most cases the particulate phase is modelled through the concept of "granular temperature" as part of kinetic theory formulations (Gidaspow, 1994). This suffers from the questionable inherent assumption that particle velocity fluctuations follow a Maxwell distribution, which remains to be verified for CFB reactors. In addition, "granular temperature" considers particle motion as a result of particle/particle collisions. For dilute systems this leads to the problem of describing the particle/turbulence interactions as well.

The team of Hjertager produced promising results with an Eulerian-Eulerian model, although the calculated particle velocity fluctuations were underpredicted (Samuelsen and Hjertager, 1996) and the calculated small scale turbulence was found significantly too small (Mathiesen et al., 2000). Likewise, the group of Simonin combines Eulerian modelling with the concept of granular temperature, including a correction for the interstitial gas. The fluid/particle fluctuation velocity is calculated from an eddy viscosity model and a (Lagrangian !) Langevin-type stochastic equation for a fluid velocity along a particle trajectory (e.g. Balzer and Simonin, 1997). In more recent work simulations with this model are compared with numerical simulation results of discrete particles in a homogeneous, stationary turbulent flow, using (Lagangian) particle tracking in a 3-dimensional turbulent flow that is computed using large eddy simulation (LES) (Gourdel et al., 1999). A more careful approach to LES is needed considering sub-grid scale (SGS) turbulence modelling when the kinetic particle response time, τ_p, of the particles is smaller than the SGS scale of the turbulence, or when 2-way coupling effects are included (Boivin et al., 2000). Very promising results obtained on this approach to Eulerian modelling with corrections for turbulence/particle interactions were presented by Flour and Balzer (1999) for a full scale CFB combustor. Computing time is still a serious drawback, though.

A description of interactions between dispersed particles and turbulence requires some particle/eddy interaction model. The model of Gosman and Ioannides (1981) is very powerful but suffers from the assumption that the turbulent eddy remains unchanged during the interaction time. More advanced models were presented by the group of Graham (e.g. Graham 1998, Graham and James, 1996) and Hennick and Lightstone (2000), based on the actual time-

correlated gas-phase velocities that are actually "seen" by a particle, and crossing trajectory effects (i.e. the interaction time is shortened as a result of particle motion in the direction of an external field). These advanced eddy lifetime concepts have not been applied to CFB reactors.

3. Commercial CFD codes

The increasing versatility and power of commercial CFD software codes that are readily avialable on the open market has resulted in their widespread and straightforward use in industrial equipment design. R&D institutes and academia, however, typically operate outside the range of possibilities offered by these products and are often involved in improving or developing certain sub-models - see the previous section. This certainly holds for CFB reactors involving a complex situation of multi-phase flow and chemistry. For CFB combustion or gasification reactors homogeneous (gas phase) as well as heterogeneous (gas/solid) turbulence/chemistry interactions must be considered.

Aiming at CFD-based modelling of CFB reactors a round-robin was made over several commercial CFD codes considering their use in multi-phase flow system calculations. The results are collected in Tables 1 and 2 for six CFD softwares.

Table 1 General characteristics of six commercial CFD codes considering multi-phase flow

CFD code	Turbulence models, besides k- ε*	Sub-model for particle/turbulence interaction
#1	k-ε+RNG, RSM, advanced k-ε, advanced RNG, wall methods, one-equation, full RSM, enhanced LES	1-way Lagrangian, random walk
#2	Prandtl models, k-ε+RNG, RSM, various special k-ε, k-ω, Smagorsky SGS, low Re method	"Extended k-ε" based on turbulence modulation by "additional volume sources"**
#3	low Re k-ε, k-ε+RNG, various RSM	Lagrangian particle tracking, full 2-way coupling
#4	k-ε+RNG, k-length, non linear k-ε, wall methods, LES	Euler-Lagrange (1-way), random walk / Monte Carlo
#5	k-ε+RNG, LES	1-way coupling
#6	-	Lagrangian particle tracking

* RNG = renormalisation group model, RSM = Reynolds' stress model, LES = large eddy simulation, SGS = sub-grid scale

** Chen and Wood, 1985; Mostafa and Mongia, 1988

Table 1 shows that the codes are mainly based on a k-ε model for turbulence model closure, in most cases in combination with an RNG approach to non-isotropic turbulence and LES for more rapid simulations of complex systems (see e.g. Wilcox, 1994 for more detail). Considering multi-phase systems, all codes contain a procedure for particle tracking based on gas/solid slip (Eulerian-Lagrangian), or a "two fluid" approach (Eulerian-Eulerian). Typical is the use of random number generators or a Monte Carlo approach, followed by averaging over a

large number of particles in order to take into account the influence of turbulent velocity oscillations on particle motion. A second typical feature is that 1-way coupling is assumed valid up to very high volume fractions of the dispersed phase, typically up to $\phi_p = 0.1$. Finally it is noted that models other than standard k-ε, for example LES, are not an option for multi-phase flows.

More detailed characteristics considering particulate dispersions are collected in Table 2. Two of the six codes offer no means of including 2-way or 4–way coupling, whilst an Eulerian-Eulerian approach is applied when this coupling is to be considered. Two CFD codes offer some sort of particle/eddy interaction concept, in one case based on the well-known eddy interaction model by Gosman and Ioannides (1981).

Table 2 More detailed characteristics of six commercial CFD codes considering multi-phase flow

CFD code	Concepts, besides standard particle-fluid slip velocity	Turbulence modulation (2-way coupling), particle/particle interaction (4-way coupling)
#1	"Stochastic tracking" based on Gaussian distribution, "discrete random walk model" /eddy lifetime concept *	Eulerian granular multi-phase flows
#2	see Table 1	see Table 1
#3	Particle tracking as post-processing	Full coupling (Euler-Euler)
#4	see Table 1	4-way coupling (Euler-Euler)
#5	-	-
#6	Eddy interaction model **	-

* Litchford and Jeng, 1991, Baxter and Smith 1993
** Gosman and Ioannides, 1981

From Tables 1 and 2 it is concluded that comprehensive modelling of multi-phase reacting systems such as encountered in a CFBC riser with a commercial CFD code will not be straightforward when a Eulerian-Langrangian method is preferred, motivated by the need to follow individual, reacting particles along their path. Very much will depend on the use and the quality of user-defined sub-models that are to be linked with the commercial software.

A procedure for dealing with a gas/solid reaction in a CFB combustor upper riser is given in the next section.

4. Gas/solid chemistry in the upper CFB riser

For a numerical simulation of a gas/solid reaction in the upper part of a CFB riser, sub-models are needed for the turbulence in the riser, the particle/turbulence interaction in the riser, the gas/solid mass transfer and the gas/solid chemistry. Here, a Lagrangian description of the two-phase turbulence is used. The dispersion is considered dilute, at particulate volume fraction of the order $\phi_p = 0.001 \sim 0.01$, typically 0.005 (Palchonok, 1998, Palchonok et al., 1996, Rizk and Elgobashi, 1989). Only 1-way coupling is considered.

4.1 CFB riser turbulence

A model by Palchonok, (1998), Palchonok et al. (1996), Peirano et al. (1996) based on estimates by Beér et al. (1984) was used here to describe the CFB riser turbulence. With fluidisation velocity U_F and bed voidage N, the turbulent energy dissipation per kg gas, ε, can be approximated by

$$e = gU_F \frac{r_p(1-f)}{r_F f} \qquad \textbf{(2)}$$

which allows for estimating the Kolmogorov microscales of length, time and velocity of the turbulence. Following Palchonok et al. (1996), Peirano et al. (1996) the integral length scale for the gas phase turbulence in a CFB riser equals 0.005 m < L_t < 0.5 m. Here, for a riser with diameter scale L, L_t is estimated as L_t = 0.1 L. (E.g. Risk and Elgobashi, 1989). The relation between the fluid velocity fluctuation u_F' and the energy dissipation ε is taken as (e.g. Risk and Elgobashi, 1989):

$$e = O\left(\frac{\overline{u'_F{}^3}}{L_t}\right) = C_m{}^{3/4} \frac{\left(\frac{3}{2}\overline{u'_F}\right)^3}{L_t}, \qquad C_m = 0.09 \qquad \textbf{(3)}$$

A Lagrangian description of the turbulent energy spectrum is used. Based on an autocorrelation function $R_L(\tau)$ for the turbulent fluctuations (with frequency f) in the gas flow, the Lagrangian energy spectrum is found as the Fourier transform of $R_L(\tau)$ (e.g. Hinze, 1975):

$$E_L(f) = 4\overline{u'_F{}^2}\int_0^\infty R_L(t)\cos(2pft)dt \qquad \textbf{(4)}$$

Here, a exp-cos Frenkiel correlation for R_L(J) is used (Frenkiel, 1953), giving

$$R_L(t) = \exp\left(-\frac{t}{(m^2+1)t_L}\right)\cos\left(\frac{mt}{(m^2+1)t_L}\right) \quad \Rightarrow, \quad \text{with} \quad t_L = \frac{L_t}{\overline{u'_F}},$$
$$E_L(f) = 2\overline{u'_F{}^2}(m^2+1)t_L\left(\frac{1}{1+(m+2pf(m^2+1)t_L)^2} + \frac{1}{1+(m-2pf(m^2+1)t_L)^2}\right) \qquad \textbf{(5)}$$

with Lagrangian integral turbulence time scale τ_L. The value m=1 describes decay of velocity correlation in a tube flow most closely and is used here (Gouesbet and Berlemont, 1999).

4.2 Particle turbulent dispersion

Based on a Lagrangian flow analysis, eddy diffusivity for fluid elements, $Ð_F$, can be defined as

$$Ð_F = \overline{u_F{}^2}t_L \qquad \textbf{(6)}$$

For particles smaller than the dimensions of the Kolmogorov eddies the eddy diffusivity of fluid elements and discrete particles in a turbulent flow can be evaluated from the Basset-Boussinesq-Oseen ("BBO") equations for the motion of a particle in a turbulent flow. As derived by Tchen (1947, see also Hinze, 1975, 1972):

$$m_p \frac{d\underline{u}_p}{dt} = 3\pi\eta_F d_p(\underline{u}_F - \underline{u}_p) + \tfrac{1}{2}V_p\rho_F \frac{d}{dt}(\underline{u}_F - \underline{u}_p) + V_p\rho_F \frac{d\underline{u}_F}{dt}$$
$$+ 1\tfrac{1}{2}d_p^{\,2}\sqrt{\pi\rho_F\eta_F}\int_{t_o}^{t}\left(\frac{d\dfrac{(\underline{u}_F - \underline{u}_p)}{dt}}{\sqrt{t-t}}\right)dt + \sum \underline{F} \qquad \textbf{(7)}$$

Here, m_p represents particle mass, η_F dynamic fluid viscosity, V_p particle volume, ρ_P and ρ_F density of particle and fluid, respectively, external force F and time t. This expression implies that the acceleration force on the particle equals the sum of Stokes' drag, surrounding medium acceleration, virtual mass effect, the Basset force (i.e. resistance to acceleration) and external forces, $\underline{F}$. By writing the velocities of the fluid and dispersed particulate phases,u_F and u_P, as a set of Fourier integrals, a solution was derived by Tchen that leads to an amplitude ratio η_A, which is the ratio of the amplitude of the oscillation of the particle and that of the surrounding turbulent eddy as function of turbulent fluctuation frequency f :

$$\eta_A = \sqrt{1 + f_1(f,k_1,k_2,k_3)^2 + f_2(f,k_1,k_2,k_3)^2} \qquad \textbf{(8)}$$

where k_1, k_2, k_3 are contants defined by d_p, ρ_p, ρ_F and η_F: note further that $k_1 = 1/\tau_p$. This amplitude ratio relates the particle and fluid eddy diffusivities after integrating over the spectrum $E_L(f)$ given in Eq. (5), defining a particle turbulent Schmidt number, $Sc_{t,p}$:

$$Sc_{t,p} = \frac{Đ_p}{Đ_F} = \frac{\overline{u'_p{}^2}}{\overline{u'_F{}^2}} = \frac{\int_0^\infty \eta_A^{\,2} E_L(f)df}{\int_0^\infty E_L(f)df} = \frac{k_p}{k} \approx \frac{t_L}{t_L + t_p} \qquad \textbf{(9)}$$

which relates the turbulent kinetic energy for gas, k, and particles, k_p. For η_A=1 the particle motion equals that of the fluid, following every oscillation, for η_A= 0 the particle motion is determined only by the mean flow. The ratio $Đ_p/Đ_F$ determines the degree of mixing of the multi-phase system. Particles that are unable to follow all turbulent oscillations of the flow are effectively non-available for chemical interactions with gas molecules transported by the smallest eddies.

For particle/gas dispersions with $\rho_p \gg \rho_F$, the Basset term and virtual mass term in the BBO equations can often be neglected, giving the last right hand side estimation given in Eq (9). In this work, the full equations were integrated, however.

Although the Tchen/Hinze model suffers from several imperfections it is identical to the later, more generalised formulation by Maxey and Riley (1983) when uniform unsteady flow is considered (Gouesbet, and Berlemont, 1999). A discussion on solutions of the BBO equations was given by Michaelides and Feng (1996).

4.3 Mass transfer to a single particle in a CFB riser

Following Palchonok (1998), Palchonok et al. (1998) the mass transfer to a single particle, with diameter d_p, in a CFB riser can be quantified by the Sherwood number, Sh, as

$$Sh = \frac{k_{mt}d_p}{D_{mol}} = 2f + 0.89\,\mathrm{Re}_p^{\,0.5}\,Sc^{0.33} = \frac{d_p}{d} \qquad \textbf{(10)}$$

with mass transfer boundary layer thickness, δ, particle Reynolds' number Re_p, and Schmidt number Sc. This yields the mass transfer coefficient k_{mt}.

The slip velocity in Re_p was calculated as $(U_F - u_p) = u_{p,t}\ \phi^{n-1} = \tau_p g$, with gravity g, particle terminal velocity $u_{p,t}$, particle mechanical relaxation time τ_p, riser voidage ϕ and Richardson-Zaki parameter n. (e.g. Horio in: Grace et al., 1997). For $Re_p < 0.2$, n=4.65; for $Re_p > 0.2$ the value for n varies with Re_p, which was solved by a few interations.

4.4 Gas/solid chemistry

For the heterogeneous reaction (R1), recent experimental data from Zevenhoven and Hupa (1998) was used. This gives the reaction rate r_{NO} (mol /m³s) for 1 %-vol CO and 100 ppm-vol NO in N_2 for the temperature range 750-950EC:

$$r_{NO} = k_{het} c_{NO,surf} c_{CO,surf} = 18.31\,\mathrm{FR}\exp(-\frac{FR}{0.349})\exp(-\frac{48730}{RT})c_{char} \qquad \textbf{(11)}$$

Here, c_{char} is the char particle concentration (g/m³) and FR is the fuel ratio FR (= proximate fixed carbon/ volatiles) of the parent fuel ranging from 0.08 to 1.6, (chars from wood, peat and coal). Eq. (11) defines heterogeneous reaction rate constant k_{het} (m^3/mol.s).

4.5 The effective gas/solid conversion rate

The effective conversion rate, $r_{NO,eff}$, in a reactor combines the gas/solid reaction kinetics, the gas/solid mass transfer and the turbulent particle dispersion. The concentration of NO at the particle surface, $c_{NO,surf}$ is determined by the bulk gas concentration, $c_{NO,bulk}$, mass transfer coefficient, k_{mt}, and the heterogeneous reaction rate constant k_{het}, defining a mass transfer efficiency factor, η_{mt} , for total particle outer surface A_p per unit gas volume. For simplicity, and since $c_{CO} >> c_{NO}$, the boundary layer diffusion limitations for CO are neglected: $c_{CO,surf} \approx c_{CO,bulk}$.

Since the diffusive velocity ~ √Đ, an efficiency, η_{mix}, for mixing by particulate eddy dispersion can be defined from (eq. 9) and thus the effective heterogeneous rate in the CFBC can be calculated as:

$$r_{NO,eff} = r_{NO}\frac{c_{NO,surf}}{c_{NO,bulk}}\sqrt{\frac{Đ_p}{Đ_F}} = r_{NO}\eta_{mt}\eta_{mix} \quad \text{where} \quad \frac{c_{NO,surf}}{c_{NO,bulk}} = \frac{k_{mt}A_p}{k_{het}c_{CO,bulk} + k_{mt}A_p} = \eta_{mt} \qquad \textbf{(12)}$$

For small particles the turbulent mixing efficiency η_{mix} is close to 1, whilst fast mass transfer is characterised by thin boundary layers, ($\delta / d_p \sim 1/\mathrm{Sh}$, *viz*. eq. 10). However, note that for a given mass concentration of particles, small particle sizes correspond to many particles, resulting in large gas-solid interfacial areas, A_p.

Char particle concentration is calculated from the voidage in the riser, ϕ, and the fraction *f*(-) of the solids particles that are char particles, amongst bed material:

$$c_{char}(g/m^3) = 1000 f(1-f)\, r_{char} \qquad \textbf{(13)}$$

Here, ρ_{char} = 500 kg/m³ was used for char particle density, and *f*= 0.01.

4.6 Results of effective gas/solid rate calculations

All calculations were made for a gas phase composed of 1 %-vol CO, 100 ppmv NO, 300 ppmv CO_2 and (the rest) N_2 (as during the experiments on which eq.(11) is based). More detail on the model calculations is given in Zevenhoven and Järvinen, 2001.

Figure 3 shows the influence of particle size on the effective rate for reation (R1) in a CFBC riser, based on the other process parameters as indicated. It is found that the mass transfer and eddy dispersion mixing both become much less efficient than 100% with increasing particle size. This has a large effect on the effective rate of the heterogeneous conversion (R1): for a 100 μm char particle the effective conversion rate in the CFBC riser is less than 20 % of the rate under chemical kinetics control, for a 1 mm char particle this is less than 1%.

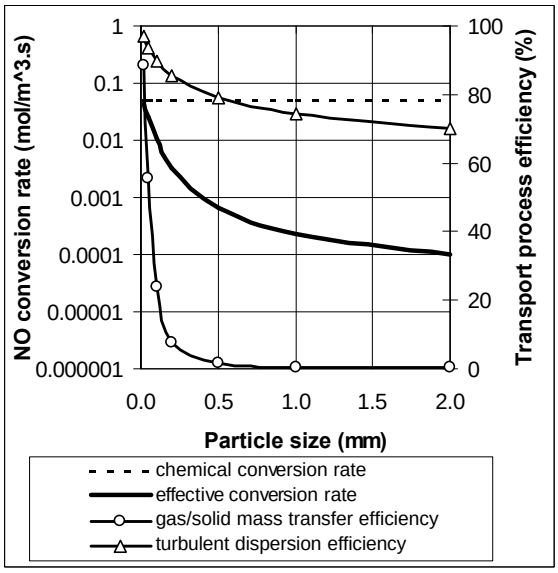

Fig. 3 Heterogeneous chemistry rate, effective heterogeneous conversion rate (*left*) and the efficiency of the transport mechanisms, η_{mt} and η_{mix} (*right*) *vs.* char particle diameter. (Temperature 1123 K, fuel fuel ratio 1.5, CFB riser voidage 0.995, gas velocity 8 m/s, reactor diameter 5 m).

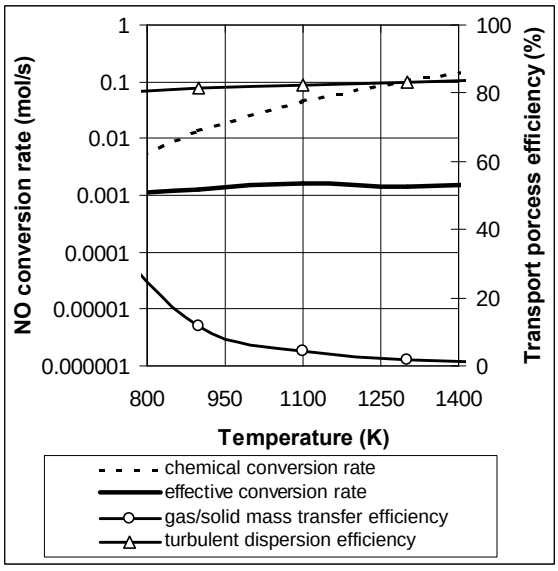

Fig. 4 Heterogeneous chemistry rate, effective heterogeneous conversion rate (*left*) and the efficiency of the transport mechanisms, η_{mt} and η_{mix} (*right*) *vs.* temperature.
(Char particle diameter 0.3 mm, fuel fuel ratio 1.5, CFB riser voidage 0.995, gas velocity 8 m/s, reactor diameter 5 m).

Fig. 4 shows that the effective conversion rate is typically less than 10 % of the chemical rate for temperatures above 900 K. With increasing temperature the eddy diffusivity of the particles is closer to that for the gas but the mass transfer becomes more strongly limiting.

Calculated turbulence characteristics agree well with recent data from CFB reactors of various sizes (Caloz et al., 1999). More detail and results (e.g. the effect of voidage, reactor diameter, fluidisation velocity) are given elsewhere (Zevenhoven and Järvinen, 2001).

5. Conclusions

CFD-based modelling of CFB reactors was addressed. Most current models are based on an Eulerian-Eulerian / "two fluids" approach with the "granular temperature" concept for the particulate phase. For dilute suspensions such as found in the upper part of a CFB riser reactor, a Eulerian/ Lagrangian approach that includes particle/turbulence interactions appears better applicable. Significant progress is being made, though, to combine the best of both approaches. Commercial codes for CFD, though, follow the developments at a time lag of at least 10 years. A procedure is presented for integrating gas/solid chemistry with CFB hydrodynamics via a k-ε-k_p -like approach, based on the Tchen/Hinze turbulent particle dispersion model and a simple description for CFB riser turbulence. Future work will address anisotropic turbulence, 2-way and 4-way coupling, particle size distribution, eddy interaction time, and more complex chemistry.

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