Pergamon

Int. J. Multiphase Flow Vol. 23, No. 3, pp. 607–612, 1997

Printed in Great Britain
0301-9322/97 $17.00 + 0.00

PII: S0301-9322(96)00071-7

BRIEF COMMUNICATION

THE COMPUTATION OF PARTICLE SIZE IN EULERIAN–EULERIAN MODELS OF COAL COMBUSTION

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(Received 17 January 1996; in revised form 30 September 1996)

1. INTRODUCTION

The calculation of the particle size is one of the main ingredients in the simulation of coal-fired boilers. The particle size (or the specific surface-area) plays a major role in the interphase processes that are the driving force of coal combustion, such as particle drag and turbulent dispersion, heat-up (and hence pyrolysis) and heterogeneous combustion. The size of particles and fly-ash has also a clear influence on the radiative transfer of heat within the boiler.

The inability of Eulerian models of coal combustion to calculate the particle size has been one of their main disadvantages with respect to Lagrangian ones. The present contribution introduces a way of computing the average particle size in the framework of an Eulerian model, with allowance for size diminution due to mass transfer and for a 'phenomenological' representation of other mechanisms which may cause a particle-size change, such as devolatilization or particle breakup.

The method is first validated by comparison with a case which has an analytical solution; and then it is applied, in combination with an Eulerian–Eulerian model of coal combustion, to an actual power-production boiler.

2. THE EULERIAN–EULERIAN MODEL OF COAL COMBUSTION

Eulerian–Eulerian models use Eulerian conservation equations to describe the behaviour of the gas and particulate phases in a multiphase flow (Fueyo *et al.* 1995). The local share of space occupied by each phase is given by the phase volume-fraction $r_i(x, y, z, t)$, which is obtained from the conservation equation

$$\frac{\partial}{\partial t}(\rho_i r_i) + \nabla(\rho_i r_i \mathbf{V}_i) - \nabla(\Gamma_r \nabla r_i) = \dot{m}_{j\to i} \quad [1]$$

where $i = 1$ for gas and $i = 2$ for coal; ρ_i is the phase density; $\mathbf{V}_i$ is the phase velocity vector; Γ_{r_i} is a diffusion coefficient, accounting for the effect of turbulence on particle dispersion; and $\dot{m}_{j\to i}$ is the mass transferred from phase j into phase i per unit time and per unit volume, and encompasses all the mass-transferring processes (e.g. drying, volatilization, heterogeneous combustion).

The volume fractions r_1 and r_2 are further related to each other through the closure equation:

$$r_1(x, y, z, t) + r_2(x, y, z, t) = 1. \quad [2]$$

For any other coal or gas property ϕ_i, the corresponding (general) Eulerian conservation equation can be written as

$$\frac{\partial}{\partial t}(\rho_i r_i \phi_i) + \nabla(\rho_i r_i \mathbf{V}_i \phi_i) - \nabla(\Gamma_{\phi_i} r_i \nabla\phi_i) - \nabla(\Gamma_r \phi_i \nabla r_i) = \|\dot{m}_{j\to i}\|\phi_+ - \|\dot{m}_{i\to j}\|\phi_- + f_{j\to i}(\phi_j - \phi_i) + S_{\phi_i} \quad [3]$$

where Γ_{ϕ_i} is a (turbulent) diffusion coefficient of ϕ_i; ϕ_+ represents the value of property ϕ in the mass transferred into the phase, and ϕ_- has the corresponding meaning for the mass transferred out of the phase; the double bar indicates the maximum of zero and the quantity enclosed; $f_{j\to i}$ is a 'diffusive' interphase exchange of ϕ_i, such as heat conduction; S_{ϕ_i} represents other (non-interphase) sources. Two (turbulent) diffusion terms appear in this equation; one, $\nabla(\Gamma_r \phi_i \nabla r_i)$, is responsible for the exchange of ϕ_i through turbulent diffusion of phase (i.e. of r_i), and the other, $\nabla(\Gamma_{\phi_i} r_i \nabla\phi_i)$, is the (classical) within-phase turbulent diffusion of ϕ_i.

Equations like [3] are solved for a number of gas-phase variables, typically including: three velocity components, enthalpy, three composite radiation fluxes for a six-flux radiation model, turbulence kinetic energy and its dissipation rate, and the mass fractions of all the major chemical species but one (which is obtained from difference to one of all the other ones), and all the minor (e.g. pollutant) ones. For the coal phase, equations like [3] are solved for the three velocity components, enthalpy and the mass fractions of the particle components, namely (raw) coal, char and water, with the mass fraction of ash being obtained from difference to one.

3. THE SIZE-CALCULATION PROCEDURE

The present method is inspired by the 'shadow' technique of Spalding (1982), which calculates the particle size by solving for the volume fraction of an additional phase which behaves like (i.e. 'shadows') the particulate phase but does not participate in the transfer of mass. Unlike the original 'shadow' method, the present one allows for the selection of the mass-transfer processes which contribute to a size change.

In the current method, a special phase-2 variable ϕ_s is used instead. This variable represents the inverse of the fraction of phase (i.e. of the fraction of r_2) that has disappeared due to mass transfer. The new variable ϕ_s is obtained from the Eulerian transport-equation

$$\frac{\partial}{\partial t}(\rho_2 r_2 \phi_s) + \nabla(\rho_2 r_2 \mathbf{V}_2 \phi_s) - \nabla(\Gamma_{r_2} \nabla r_1) = S_{\phi_s}. \qquad [4]$$

In [4], S_{ϕ_s} includes the phase-2 mass sinks associated to all the processes which do not contribute to a diminution in particle size. Typically, the only mass-transfer process in coal combustion which is considered to contribute to a size change is heterogeneous (char) combustion.

It is important to remark that [4] is just a particular case of the general Eulerian equation [3], and hence can be solved using the general Eulerian-equation solver.

Once ϕ_s is computed, the local average diameter D can be retrieved from ϕ_s and the initial diameter D_i as

$$D = D_i \phi_s^{-1/3}. \qquad [5]$$

The boundary condition for ϕ_s at inlets, where fresh particulate phase enters the domain, is therefore $\phi_s = 1$, since no mass has evolved to the gas phase as a consequence of mass transfer.

The ϕ_s method described above has been implemented in an existing finite-volume Computational Fluid Dynamics code (PHOENICS). PHOENICS uses the IPSA method of Spalding (1981) to solve the coupling between pressure, velocities and volume fractions in a two-phase flow.

4. RESULTS

4.1. *A test case*

In this section, the proposed method is tested by comparison with an idealised one-dimensional problem for which an analytical solution has been proposed by Spalding (1982, 1987).

The problem considers the vaporization of droplets injected in a pipe as they move downstream. The constitutive equations are similar to [1]–[3], with the interphase mass-transfer given by

$$\dot{m}_{2\to 1} = \frac{0.5\ 10^5 r_1 r_2 \rho_1}{D^2} \qquad [6]$$

and the droplet drag by

$$f_{2\to 1} = -f_{1\to 2} = \frac{10^5\, r_1 r_2 (u_2 - u_1)\rho_1}{D^2}. \qquad [7]$$

The densities are taken as constant, with $\rho_1 = 10\ \mathrm{kg/m^3}$ and $\rho_2 = 10^4\ \mathrm{kg/m^3}$.

Spalding (1959) has shown that the problem has an analytical solution, which for the droplet size is given, using non-dimensional variables, by

$$\xi = \frac{1-\zeta^2}{2} - \frac{S}{5(S-3)}(1-\zeta^5) - \frac{\dfrac{\rho_1 u_{2_i}}{M_i} + \dfrac{3}{S-3}}{S+2}(1-\zeta^{S+2}) \qquad [8]$$

where ξ is a non-dimensional distance, given by

$$\xi = \frac{10^5}{6}\frac{x}{M}\frac{\rho_1^2}{\rho_2};$$

M is the mass flow rate per unit area; $\zeta = D/D_i$ is the non-dimensional diameter; S is a non-dimensional parameter depending upon the ratio of interphase friction to interphase mass-transfer,

$$S = 3\frac{f_{2\to 1}}{\dot{m}_{2\to 1}(u_2 - u_1)};$$

and the subscript i indicates values at the inlet.

Figure 1 compares the downstream evolution of the non-dimensional particle diameter D/D_i with the analytical solution, for $M_i = 1000$ kg/s and $u_{2_i} = 50$ m/s. The figure shows that the proposed method can predict the exact solution with sufficient accuracy.

4.2. Size calculation in a coal-fired boiler

The size-calculation method is now used to predict the evolution of the particle size in a tangentially-fired, coal boiler. The boiler is a 220 Mw(e) unit, burning a bituminous coal. The computational domain is sketched in figure 2. An Eulerian–Eulerian, three-dimensional model of coal combustion, as outlined in section 2 above is employed (Fueyo *et al.* 1995). The model includes three modes of mass transfer from coal to gas: coal drying, pyrolysis and heterogeneous

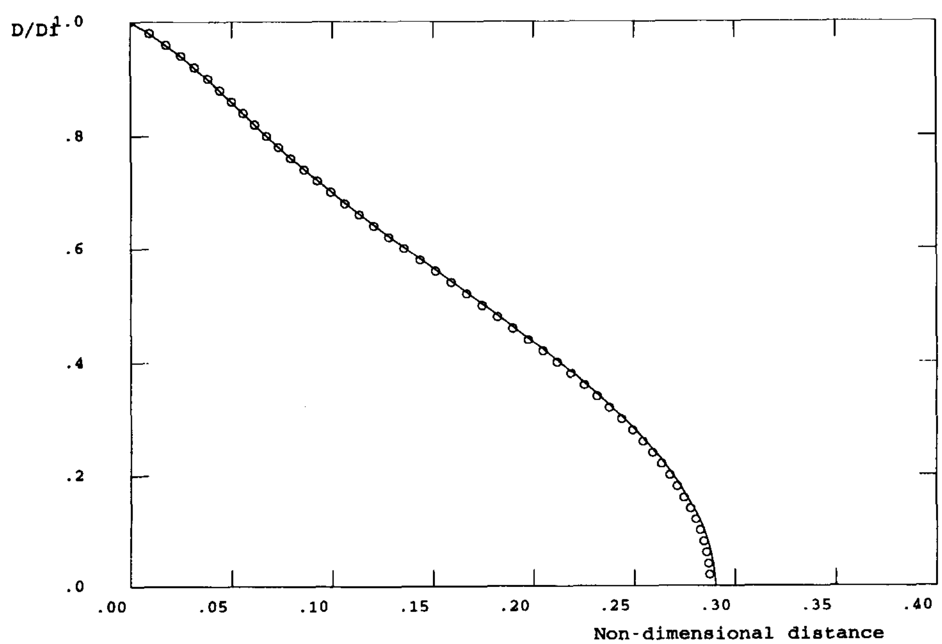

Figure 1. Comparison of the calculated downstream evolution of the non-dimensional particle diameter with the analytical solution. Line: analytical solution; symbols: present method.

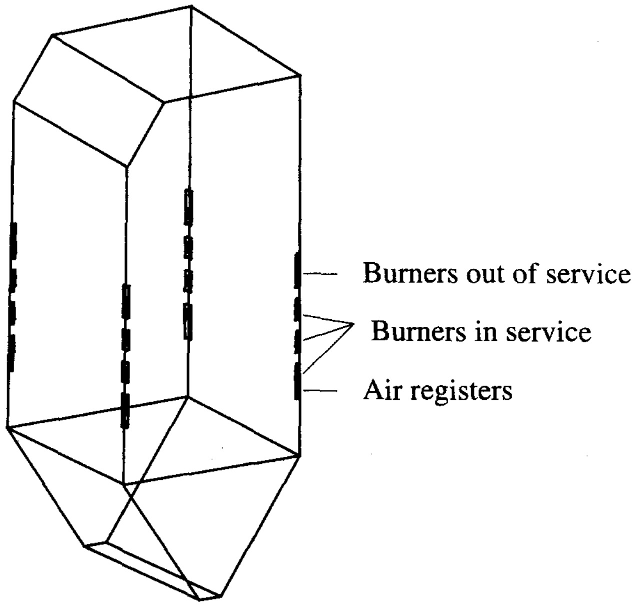

Figure 2. The computational domain for the boiler calculation.

combustion. The last two are often considered to lead to a particle-size change; the modelization of such change with the ϕ_s equation [4] is dealt with next.

Attention is first turned to heterogeneous combustion. Models of heterogeneous char combustion often presume that combustion takes place on the particle surface, causing the particle to shrink in size as combustion progresses. In the present method, such behaviour can be accounted for by omitting in the equation for ϕ_s ([4]) the mass source-term corresponding to heterogeneous combustion, and including those for drying and pyrolysis (assuming that these processes do not cause size changes).

Figure 3 shows the evolution of the particle size on a horizonal plane through the middle burner-level. (The figure shows also velocity vectors for completeness.) The plot shows how the

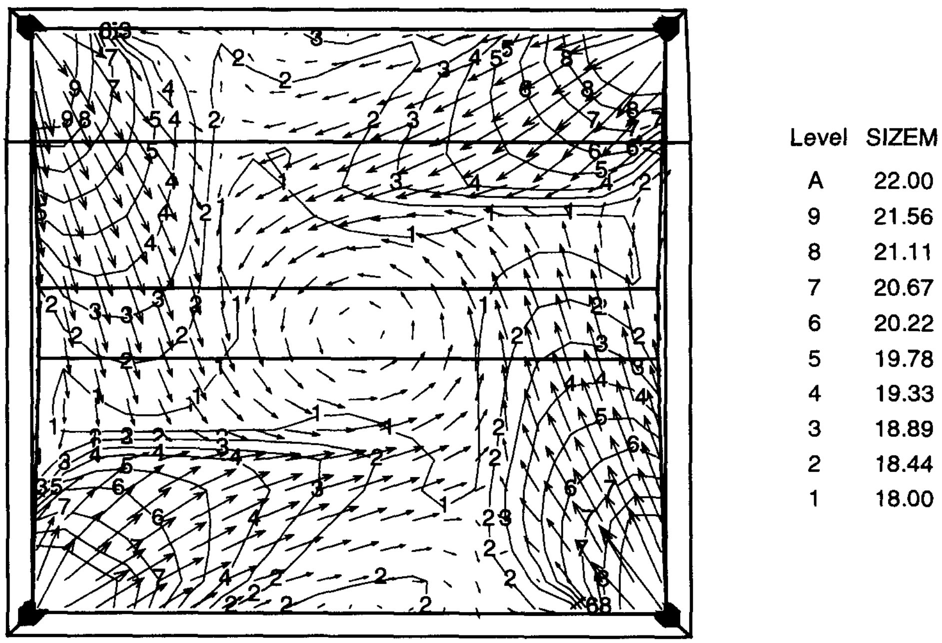

Figure 3. Particle-size decrease in a tangential boiler due to burnout (the legend is in μm).

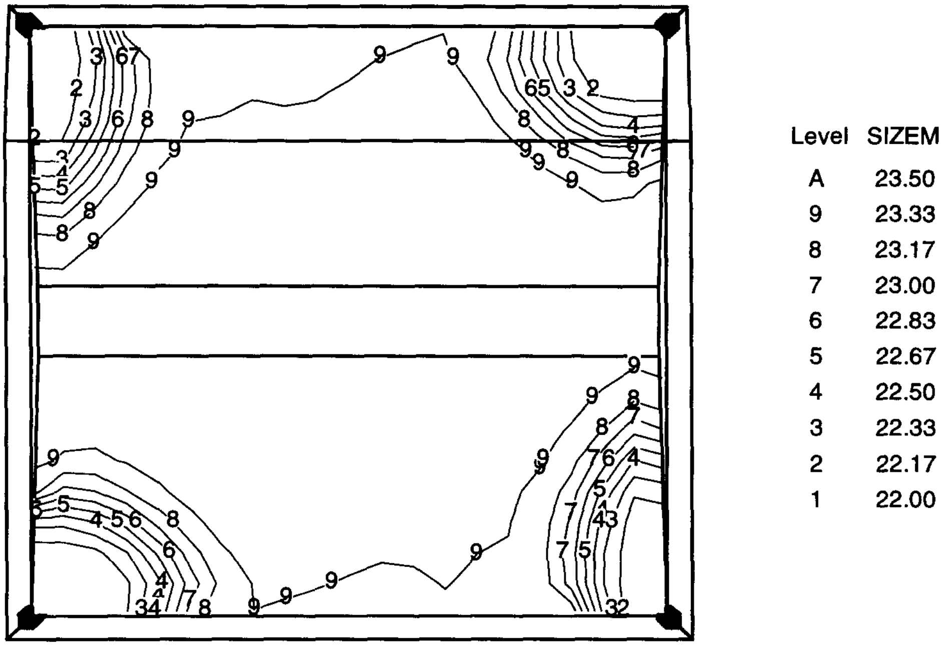

Figure 4. Particle-size increase in a tangential boiler due to volatilization (the legend is in μm).

mean particle size decreases from its initial value of 22 to 17.8 μm due to heterogeneous combustion.

Particle devolatilization is often considered to cause swelling (Smoot and Smith 1985). The proposed method can accommodate a size increase as well as a size decrease by simply reversing the sign of the source term associated to the process in question.

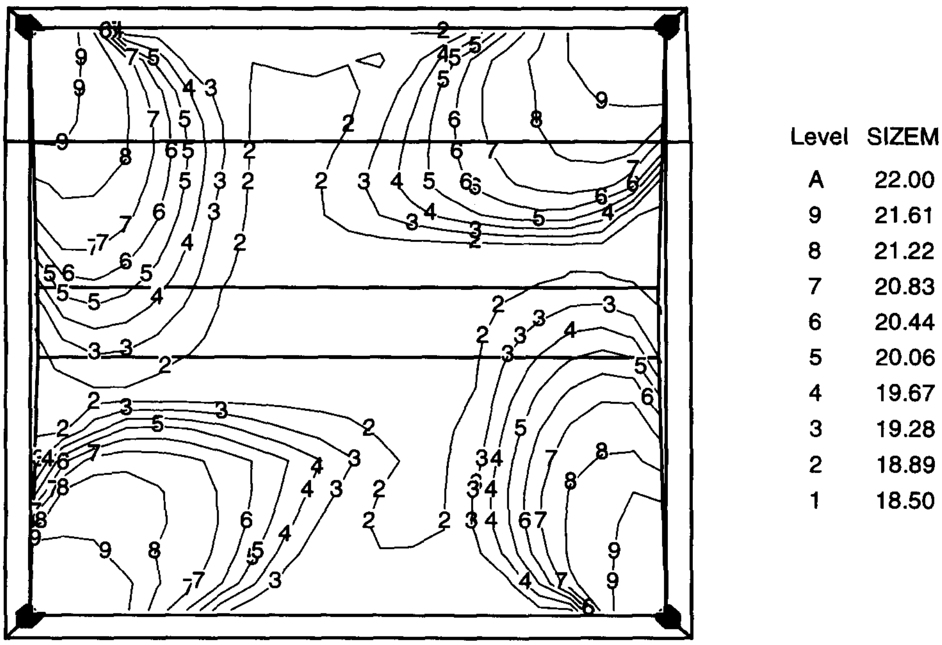

Figure 5. Particle-size evolution in a tangential boiler due to the combined effects of burnout and volatilization (the legend is in μm).

For devolatilization, for instance, the source term accounting for size decrease can be modelled as

$$S_{\phi_s} = -A_s \dot{m}_v \qquad [9]$$

or as

$$S_{\phi_s} = A_s(\phi_s^{\max} - \phi_s)\dot{m}_v \qquad [10]$$

where A_s is a swelling constant, $\dot{m}_v$ is the mass transferred due to volatilization and the (optional) factor $(\phi_s^{\max} - \phi_s)$ introduces a maximum size $D^{\max}$ attainable by particle swelling. This maximum size is that corresponding to $\phi_s = \phi_s^{\max} = (D_i/D^{\max})^3$. Since $D_i < D^{\max}$, then $\phi_s > \phi_s^{\max}$, and the source term in [10] is negative, causing, in [4] a decrease in ϕ_s and hence an increase (cf. [5]) in size.

Figure 4 shows the effect of the term [9] on particle size for the above-mentioned mid-burner plane of the tangential boiler for a value of $A_s = 0.1$. (In order to see the effect more clearly, the size decrease due to burnout which has been shown above has been switched off for this calculation.)

If it is regarded that a too vigorous devolatilization can cause particle breakup, the effect of this term [9] or [10] can be reversed as follows

$$S_{\phi_s} = A_s((\phi_s)^{-1} - (\phi_s^{\min})^{-1})\dot{m}_v \qquad [11]$$

where $\phi_s^{\min}$ introduces a minimum size in a similar manner as in [10], and the inverse of ϕ_s is taken so as to reflect the fact that larger particles are more likely to break up than smaller ones.

Finally, figure 5 shows the combined effect on particle size of particle swelling due to volatization and core-reduction due to heterogeneous combustion. This calculation can be therefore regarded as typical for the conditions prevailing in a coal-combustion computation.

5. FINAL REMARKS

The present contribution has shown how Eulerian–Eulerian models of coal combustion can be supplied with a method which allows the calculation of the evolution of the mean particle-size. The method has been tested by comparison with a simple case which has an analytical solution, and its use in an actual boiler calculation has exemplified. The effects of burnout in size diminution, and of volatilization in particle swelling and fragmentation have been shown. The method can readily incorporate further models of particle-size evolution, for instance those in which particle fragmentation is a function of particle temperature or composition, or is influenced by the local gas–particle velocity-difference or by the local values of the gas turbulent kinetic energy.

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