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Large eddy simulation of polydisperse particles in turbulent coaxial jets using the direct quadrature method of moments

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ABSTRACT

Modeling coal particles in turbulent coal flames is a challenging but nonetheless critical step for predicting flame characteristics. Traditional approaches such as Reynolds-Averaged Navier-Stokes (RANS) coupled with Lagrangian solvers are unable to correctly predict particle concentrations and velocities in complex systems. This study shows how Large Eddy Simulations (LES) coupled with an Eulerian solver can address those issues. Previous Direct Numerical Simulations and Stokes number analysis suggest that LES has the capabilities to resolve all the turbulent length scales affecting coal particles in a coal flame and could therefore lead to more accurate simulation. The effects of fluid aerodynamics on the particle motion in the near field region of non-reacting coaxial particle-laden jets were simulated using LES. The Direct Quadrature Method of Moments (DQMOM) was used to track the particle phase in an Eulerian framework. Simulation results were compared to experimental data and accurately modeled a wide range of particle behaviors, such as particle jet waviness, spreading, break up, particle clustering and segregation, in different conditions. Simulations also predicted the mean axial velocity along the centerline for both the gas phase and the solid phase with a maximum error of 12% relative to experimental data. This study therefore provides a solid validation of the LES with DQMOM approach to model particles in turbulent flows and justifies its use for coal flame simulations.

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1. Introduction

Coal is an important and indispensable energy resource for electricity production as its reserves are far more abundant than those of other fossil fuels. As environmental regulations get stricter, coal thermal power plants need to control pollutants emissions such as NO_x, SO_x and ash particles. Coal also plays an important role in global CO_2 emissions, which will need to be reduced to limit the effects of climate change (Metz, 2005). In order to meet those requirements, understanding the pulverized-coal combustion mechanisms and developing advanced combustion technology is necessary. However, the combustion of pulverized-coal is a complex phenomenon compared with that of gaseous or liquid fuels, since dispersion of coal particles, devolitilization and oxidation reactions take place silmutaneously (Hwang et al., 2006; Tsuji et al., 2002). Moreover, experimental measurements of pulverized-coal flame characteristics are extremely difficult (Yin et al., 2002; Sabel et al., 2002; Seames, 2003; Spinti and Pershing, 2003; He et al., 2004; Wei et al., 2004; Wang et al., 2002). Accordingly, the development of new combustion furnaces and burners is still empirical and requires a significant amount of time and money.

In coal-combustion systems, finely pulverized coal particles are conveyed by a medium, air in general, that enters the combustor as a jet. The distribution of particles and its dispersion affect the local environment surrounding each particle and therefore its combustion kinetics (Smith et al., 2002). Although the reaction kinetics involved in coal combustion have been studied extensively, the fundamental mechanics of coal trajectories and of particle-laden jets in general are as yet poorly understood and have not been included in optimizing the design and operating flow condition for coal combustors. This issue can be addressed by using Computational Fluid Dynamics (CFD), which was shown to be a very useful and accurate modeling framework for the description of particulate systems, and for the description of turbulent flows in general (Ferrante and Elghobashi, 2003; Eaton and Fessler, 1994).

RANS (Reynolds-Averaged Navier-Stokes), LES (Large-Eddy Simulation) and DNS (Direct Numerical Simulation) are the three common CFD methods for turbulence modeling. DNS requires a very fine grid spacing and even though it has the highest numerical accuracy, its application to practical combustion systems is made impracticable by the high computer load required. RANS on the

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Nomenclature

ν	gas kinematic viscosity (m^2/s)	N_ξ	number of internal coordinates
d_p	particle diameter (m)	N	number of quadrature nodes
ϵ	turbulence energy dissipation rate (m^2/s^3)	Δ	Nyquist cut-off length (m)
ρ_g	gas density (kg/m^3)	$\boldsymbol{u_p}$	particle velocity in real space (m/s)
$\boldsymbol{u_g}$	gas velocity (m/s)	$\boldsymbol{v_p}$	particle velocity in internal coordinate space (m/s)
τ_p	particle relaxation time (s)	τ_f	fluid characteristic time (s)
ξ	internal coordinate vector	VR	inlet velocity ratio
κ	wave number (m^{-1})	w_α	weight for quadrature node α (number of particles/m^3)
η	Kolmogorov length scale (m)	$\langle \xi \rangle_\alpha$	abscissa for internal coodinate ξ and quadrature node α
n	number density function (number of particles/m^3/ internal coordinate)		

opposite end of the spectrum is widely used for practical applications. There is however evidence that RANS can be inaccurate in predicting particle-laden flows (Sommerfeld et al., 1992; Apte et al., 2003). As a result, interest for LES is growing, as it directly solves the transport equations for the large eddies and models only the smallest eddies. Unsteady turbulent motions are evaluated and the number of model parameters is greatly reduced. LES has been convincingly shown to be superior to RANS in accurately predicting turbulent mixing and combustion dynamics (Pierce and Moin, 1998; Kurose et al., 2009). Although LES requires a high computer load compared to RANS, its superiority in terms of prediction will likely make it the best choice for practical combustion applications as computational cost decreases.

In order to describe the evolution of the dispersed particulate phase, CFD must be coupled with a population-balance equation (PBE). Several numerical approaches can be used to solve this equation, such as classes methods (CM) or Monte-Carlo methods (MCM) (Ramkrishna, 2000). Classes methods, in which the internal coordinate (e.g., particle length or volume) is discretized into a finite series of bins, are the most popular, (Hounslow et al., 1988; Kumar and Ramkrishna, 1996, 1997) , whereas MCM (Bove et al., 2005) are well known for their ease of implementation. In order to get reasonable results, the CM method requires a large number of classes (e.g., 20-30), so it is a computationally expensive approach for CFD calculations. Although the Monte-Carlo method is theoretically applicable, especially for Lagrangian-Eulerian simulations, in order to reduce the statistical error, a very large number of particles must be used. Due to limitations on the computational resources, the number of particles which can possibly be tracked is often too low to get accurate particle statistics for applications such as coal boilers.

The method of moments (MOM) offers an attractive alternative where the PBE is tracked through its moments by integrating the internal coordinate (Hulburt and Katz, 1964). The main advantage of MOM is that the number of scalars required is very small (i.e., usually 4-6), which makes the implementation in CFD codes feasible. However, due to the difficulties related with expressing transport equations in terms of the moments themselves, the method has been scarcely applied until recently. The so-called closure problem (Wang et al., 2005; Upadhyay and Ezekoye, 2003; Marchisio et al., 2003b; Wright et al., 2001) has been reviewed (Diemer and Olson, 2002) and a new method known as quadrature method of moments (QMOM) has been proposed (McGraw, 1997) , validated (Marchisio et al., 2003a,, 1998) and applied for studying a wide range of practical problems (Wang et al., 2005; Upadhyay and Ezekoye, 2003; Marchisio et al., 2003b; Wright et al., 2000; Wright et al., 2001; Pyykonen and teknillinen tutkimuskeskus, 2002) . The main limitation of the classical QMOM is that it can treat only PBE tracking one property of the population of particles, such as particle mass, size, volume or area (that is, monovariate PBE). QMOM has then been extended to bivariate problems (Wright et al., 2001; Yoon and McGraw, 2004; Yoon and McGraw, 2004). However, in a number of practical cases it is interesting to describe the population of particles with multivariate PBE, where two or more properties of the population are simultaneously tracked. In order to address these issues, the direct quadrature method of moments (DQMOM) has been formulated and validated (Fan et al., 2004; Marchisio and Fox, 2005).

DQMOM is based on the direct solution of the transport equations for weights and abscissas of the quadrature approximation and presents the advantage of being directly applicable to multivariate PBE. It has been shown to be a powerful approach for describing polydispersed solids undergoing segregation, growth, aggregation and breakage processes in the context of CFD simulations (Fan et al., 2004; Fox et al., 2008; Marchisio and Fox, 2005). Pulverized coal flames are considered dilute systems as the volume of particles is less than 1% of the volume of the fluid. Aggregation and breakage phenomena are rare events and are therefore usually neglected. However, even in this context where drag is the main process affecting particles, the DQMOM equations are equivalent to the widely used Lagrangian particle method (Dukowicz, 1980), but it has the advantage of precisely controlling the statistical noise in the lower order moments (e.g. particle number density, mass density, Sauter radius). For a given desired accuracy, this greatly reduces the computational cost since it doesn't require a large number of particles (De Chaisemartin et al., 2007; Desjardins et al., 2008). In previous work, the advantages of using DQMOM for treating particle populations with low Stokes numbers (i.e., the dispersed-phase velocity follows closely the velocity of the continuous phase) have been clearly demonstrated (Marchisio et al., 2003a,; Wang et al., 2005; Zucca et al., 2007). However, coal particles, which typically range from 1 micrometer to 200 micrometers in pulverized coal flames, have a finite Stokes number and their velocity depends on the particle size. In quadrature methods, this dependency is accounted for by solving an Eulerian model where each quadrature node has its own velocity field. Fox et al. (Fox et al., 2008) have applied DQMOM to droplets spray with finite Stokes number and compared the results with the multi-fluid method and a classical Lagrangian solver. Results show that DQMOM can provide a comparable accuracy with a significantly lower computational cost, making it a very good candidate for more complex two-phase combustion applications.

The goal of this study is to show that DQMOM can be used in combination with LES to predict particle behavior in coal flames. The present approach combining LES and DQMOM has later been used to simulate coal flames and compare results with experimental data (Pedel et al., 2012, 2013). Since few data on particles in coal flames are available, experimental data of non-reacting turbulent flows with particles were chosen. The study presents LES simulations of coaxial particle-laden jets and compares the results to experimental data (Budilarto, 2003). Special interest is given to the following important characteristics of particle-laden jets: gas