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Consistency issues of Lagrangian particle tracking applied to a spray jet in crossflow

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Abstract

Numerical simulations are performed for multiphase jets in crossflow. The flow solver uses an Eulerian/Lagrangian approach. Turbulence in the gas phase is modeled in the framework of large eddy simulation. The dispersed phase is handled using Lagrangian particle tracking. The model assumptions of solvers for Lagrangian particle tracking are critically assessed for typical flow conditions of spray jets in crossflow. The droplets are assumed to be spherical and isolated. It is shown that several model assumptions are apparently inconsistent in larger portions of the flow field. Firstly, average Weber numbers can be so large that the model assumption to regard droplets as spherical is questionable, not only near the nozzle, but also in the far-field. Secondly, the average droplet spacing can be so low that droplets directly interact with each other, again also in the far-field. Thirdly, the average Stokes numbers in the jet region can be so large that the phase coupling between the dispersed and continuous phase is weak. Some remedies to these deficiencies are proposed.

Keywords: Lagrangian particle tracking; Euler/Lagrange; Spray; Particle interaction; Droplet deformation; Phase coupling

1. Introduction

Spray jets in crossflow (JICF) are of interest for application as fuel injection systems in low NO_x burners operating in the lean premixed prevaporized (LPP) combustion mode. A liquid fuel jet is injected into a crossflow of preheated air flow. The liquid jet atomizes to fine droplets which disperse and evaporate quickly. The evaporated fuel mixes with air ideally prior to combustion. Premixed flames are preferable to diffusion flames as they offer the opportunity to chose the equivalence ratio well below or above stoichiometric conditions and thereby reduce local temperatures and NO_x formation rates. While NO_x emissions for gas turbines operating with gaseous fuel are down to single-digit ppm levels (Caraeni et al., 2000), the emissions are significantly higher if liquid fuels are used. This is due to local intermittent non-mixedness which leads to hot spots with

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excessive production of thermal NO_x. Fuel injection systems for LPP gas turbine combustors are therefore required to steadily provide a homogeneous mixture of fuel and air with an adjusted equivalence ratio profile. A spray JICF is advantageous as fuel injection system since atomization offers the opportunity to disintegrate the liquid fuel jet to fine droplets, which evaporate fast, while the momentum ratio, the injection angle, or swirl can be used to tailor various equivalence ratio profiles.

The Lagrange/Euler description is often applied for simulation of droplet- or particle-laden gas flows. The Eulerian description of the continuous phase handles the turbulence by large eddy simulation (LES). With respect to Lagrangian particle tracking (LPT) this has the distinct advantage that the large scale motions, on which dispersion of the droplets mainly depends (Yeh and Lei, 1981), are simulated while only the small scales are modeled. Turbulence models based on Reynolds-averaged Navier–Stokes (RANS) equations, on the other hand, require also modeling of the large scales. Consequently, the leading effects on droplets dispersion also have to be modeled with RANS-based turbulence models. LPT implies among other things that one assumes that the droplets are spherical, the drag-coefficient is known, and that no inter-particle interaction takes place. The accuracy of these assumptions can be assessed *a posteriori* by examining characteristic parameters of two-phase droplet flows, i.e. the average Weber- and the Stokes numbers as well as the average inter-particle spacing.

The local average inter-particle spacing may vary largely, by more than an order of magnitude. In very dilute flow one-way coupling is enough, in less dilute flow two-way coupling is required. Even smaller inter-particle distances imply that so-called four-way interaction is important (Elghobashi, 1994). Four-way interaction can be divided into direct (collision) and indirect (aerodynamic) interaction. For in-line droplets the aerodynamic inter-droplet coupling has noticeable impacts up to many droplet diameters in the wake of a preceding droplet (Holländer and Zaripov, 2005). The drag coefficient of the second of two in-line particles decreases by 30% for an inter-particle spacing $L/D_{\mathrm{p}} \sim 6$ (Prahl et al., 2006). L is the distance between two particles and D_{p} the particle diameter. While direct interaction is routinely treated through collision models, aerodynamic interaction in fully coupled multiphase flow computation of turbulent flow is always neglected to present date. Isolated droplets are further assumed in current models for evaporation (Torres et al., 2003) and droplet breakup (Reitz and Diwakar, 1987). Secondly, large Weber numbers imply that the droplets do deform which may mean that modifications in the lift and the drag coefficients are required (Helenbrook and Edwards, 2002; Prahl et al., 2006). This droplet deformation is usually neglected in computations, e.g. in Khosla and Crocker (2004), Becker and Hassa (2002), or Ghosh and Hunt (1998). In recent years some attempts are being made to incorporate the effect of droplet deformation, e.g. Madabhushi (2003). Additionally, the assumption of a spherical droplet is not only used in the computation of the trajectory, but also in recently improved submodels for collision (Schmidt and Rutland, 2000), evaporation (Torres et al., 2003), and breakup (Reitz and Diwakar, 1987). Lastly, large Stokes numbers suggest that the droplets do not follow the continuous phase and the mutual interaction between continuous and dispersed phases is weak.

To give *a posteriori* estimates of these frequently used model assumptions, average Weber numbers, average Stokes numbers, and the average droplet spacing are plotted in this work. The sensitivity to the injection droplet radius, momentum flux ratio, collision, evaporation, and breakup models is assessed. Regions are identified in which the model premises are inconsistent with the results, suggesting that no consistent solution can be obtained. Model inconsistency may therefore be regarded as as strong a driver towards development of new models as dissonance between measurement and computation. In addition to the flow-dependent inconsistencies, there is an inherent inconsistency in the Eulerian/Lagrangian description of any problem. In single-phase flow, it is argued that the algebraic equations approach the partial differential equations in the limit of zero cell size (so-called consistency in Lax' equivalence theorem). In LPT of dispersed two-phase flow, the droplets are assumed to be points which move in the continuous gas phase. If the grid is refined in this case, the point approximation weakens as the grid spacing approaches the droplet size. No continuous phase is left in the cell, and the computation of local gas properties at that point cannot be justified. It can therefore not be proven that the differential equations are recovered in the limit of zero cell size.

A region which clearly violates the model assumptions is the near-field of the liquid jet. The atomization of a liquid jet to fine droplets is a research objective as it is still debated if an intact liquid core exists. The dense spray in the jet region is difficult to penetrate with current optical diagnostics. Likewise, the dense spray region leads to modeling difficulties with current modeling techniques. Therefore understanding of the two-phase