Combustion and Flame 161 (2014) 222–239

Contents lists available at ScienceDirect

Combustion and Flame

journal homepage: www.elsevier.com/locate/combustflame

Large-eddy simulation of spray combustion in a gas turbine combustor

W.P. Jones *, A.J. Marquis, K. Vogiatzaki

Department of Mechanical Engineering, Imperial College London, Exhibition Road, London SW7 2AZ, UK

ARTICLE INFO

Article history:
Received 26 October 2012
Received in revised form 16 July 2013
Accepted 17 July 2013
Available online 19 August 2013

Keywords:
Large eddy simulation
Pdf-methods
Stochastic field method
Spray

ABSTRACT

The paper describes the results of a comprehensive study of turbulent mixing, fuel spray dispersion and evaporation and combustion in a gas-turbine combustor geometry (the DLR Generic Single Sector Combustor) with the aid of Large Eddy Simulation (LES). An Eulerian description of the continuous phase is adopted and is coupled with a Lagrangian formulation of the dispersed phase. The sub-grid scale (*sgs*) probability density function approach in conjunction with the stochastic fields solution method is used to account for *sgs* turbulence-chemistry interactions. Stochastic models are used to represent the influence of *sgs* fluctuations on droplet dispersion and evaporation. Two different test cases are simulated involving reacting and non-reacting conditions. The simulations of the underlying flow field are satisfying in terms of mean statistics and the structure of the flame is captured accurately. Detailed spray simulations are also presented and compared with measurements where the fuel spray model is shown to reproduce the measured Sauter Mean Diameter (SMD) and the velocity of the droplets accurately.

1. Introduction

Numerical simulations complement traditional experimental approaches and can provide a valuable aid to the design of combustion devices with low emissions and more efficient operation. These simulations require accurate models to represent the interaction of turbulence with chemical reactions, and, depending on the complexity of the combustion process additional models for two-phase flows interactions, radiative heat transfer and soot formation may be required. To date practical combustion devices such as gas turbines are mostly designed based on the experimental findings of expensive high quality tests. Simulations of similar geometries could constitute a more economic alternative to experiments but these are rather limited at the present time. The main reason for this is that the computational constraints often lead to simplifications such that the simulations are unable to describe all of the complex and interacting physical phenomena taking place over a wide range of length and time scales.

One of the most prominent areas of modern research evolves around liquid fuel combustion. Liquid fuels have a high volumetric and mass energy density and are easy to store and transport. In a practical combustor liquid fuel is atomised into small droplets in order to increase the surface area of fuel exposed to the hot gases and to facilitate rapid vaporisation and mixing with the surrounding air. In addition to this process, in many devices, the spray is injected into a swirling air flow that enhances the mixing between the fuel and the air and thus the evaporation rate. The combustion performance and emissions are mainly influenced by the atomisation of the liquid fuel, the dispersion and evaporation of the fuel droplets and the mixing of fuel and air. Thus the accurate prediction of the spray dynamics and combustion process is extremely important to determine flame stability over a wide range of operating conditions, to ensure safe and efficient utilisation of energy, and to better understand the mechanisms of pollutant formation.

Reynolds Averaged Simulations (RANS) are currently a major tool for gas turbine combustion chamber designers, but over the last few years Large Eddy Simulation (LES) has undergone considerable development and is starting to make a significant contribution to the design process. In LES a spatial *filter* is applied to the equations of motion. The large energy-containing motions are then computed directly while the effects of the small sub-filter scale motions are modelled. This makes LES an appropriate tool to capture the complicated phenomena including unsteady effects present in a practical combustor.

LES has been applied to the simulation of a wide range of premixed and non-premixed combustion processes demonstrating the ability of the method to migrate from an academic to an industrial tool [1–3]. Crucial steps in this migration have been the development of numerical algorithms that are flexible enough to handle complex configurations, yet accurate enough to simulate turbulence and its interaction with the physical and chemical processes taking place in a plurality of phases.

In the present work a coupled Eulerian (for the gas-phase flow) and Lagrangian (for the liquid-phase flow) formulation is used to

* Corresponding author.
E-mail address: w.jones@imperial.ac.uk (W.P. Jones).

0010-2180/$ - see front matter © 2013 The Combustion Institute. Published by Elsevier Inc. All rights reserved.
http://dx.doi.org/10.1016/j.combustflame.2013.07.016

Nomenclature

$\mathbf{a}$	particle acceleration
B	Spalding mass transfer number
C_D	drag coefficient
C_o	model constant ($C_o = 1$)
Cp_ℓ	liquid specific heat capacity
C_s	Smagorinsky parameter
C_V	model constant ($C_V = 1$)
dt	time interval
$d\mathbf{W}_t$	increment of the Wiener process
F_D	drag force
F_g	gravitational force
f_i	momentum exchange between the carrier gas and the dispersed flow
$\mathbf{g}$	gravitational acceleration
h	specific enthalpy
h_{fg}	latent heat of evaporation
k_{sgs}	*sgs* kinetic energy
$\dot{m}$	rate of mass addition to the continuous phase per unit volume through droplet evaporation
m_p	particle mass
$\dot{\mathcal{N}}$	rate of change of droplet number through droplet break-up and coalescence
N	number of species
N_s	number of scalars ($N_s = N + 1$)
p	pressure of the gaseous phase
$\widetilde{P}_{sgs}(\underline{\psi})$	ensemble of N stochastic fields for each of the N_s scalars
$\widetilde{\mathrm{P}}_{spr}$	*sgs* spray *pdf*
$\dot{\mathcal{R}}$	rate of change of the droplet radius through evaporation
r	droplet radius
Re	Reynolds number based on the droplet diameter
Sc_g	gas phase Schmidt number at the particle position
Sh	Sherwood number
$Sh^{(d)}$	deterministic part of the Sherwood number
$Sh^{(st)}$	stochastic part of the Sherwood number
$\widetilde{S}_{ij}$	filtered rate of strain tensor
$\dot{\mathcal{T}}$	rate of change of droplet temperature caused by heat transfer from the surrounding gas phase
u_j	velocity of the gaseous phase
$\widetilde{\mathbf{u}}_p$	filtered gas velocity at the particle position
v	droplet velocity
$\mathbf{v}_p$	velocity of the pth particle

Greek Symbols

Γ'	total – molecular plus *sgs* – diffusion coefficient
Δ	filter width
η_i	$[-1,1]$ dichotomic random vector
θ	droplet temperature
μ_{sgs}	*sgs* viscosity
ξ_α^n	stochastic fields for $1 \leqslant n \leqslant N$, $1 \leqslant \alpha \leqslant N_s$
ρ	density of the gaseous phase
ρ_ℓ	density of the liquid phase
ρ_p	filtered gas density at the particle position
σ	Schmidt number
σ_{ij}	viscous stress of the gaseous phase
τ_{ij}^{sgs}	*sgs* stress
τ_p	particle relaxation time
τ_{sgs}	*sgs* mixing time scale
τ_t	sub-grid time scale which determines the rate of interaction between the particle and turbulence dynamics
ϕ_α	species α
$\dot{\omega}_\alpha$	species α reaction rate

represent the spray dynamics and the interaction between the gas and liquid phases flow [4–9]. The Eulerian–Lagrangian framework represents a natural approach for flows where a dispersed phase is present. It allows direct modelling of the actual processes that individual droplets undergo (such as break-up, droplet dispersion, and wall interactions) in contrast to the more indirect modelling dependence of these processes on the volume fraction of the droplets or their number density distribution required by alternative Euler–Euler approaches. The restriction however of the adopted approach is the need for computationally efficient algorithms especially when the number of droplets is large.

In this paper LES calculations are presented for two operating conditions of a single sector combustor operating at a pressure of 4 bar pressure for which DLR has performed detailed measurements [10,11]; in particular an isothermal simulation (namely test case E), and a reacting simulation (namely test case A). The focus of the work here is the assessment of the predictive capability of LES with sub-grid scale models for spray dispersion and evaporation and subsequent combustion. The emphasis of the work is placed on the effect of the unresolved velocity and temperature fields on the droplet statistics especially in the region close to the injection point.

2. Burner geometry

The configuration under investigation is the DLR Generic Single Sector Combustor (GENRIG): a detailed description can be found in [10,11]. Velocities and droplet sizes of the evaporating sprays were measured with Phase Doppler Anemometry (PDA) and temperature was measured with Laser-Induced Fluorescence (OH-LIF). A photograph of the set-up used in the experiments can be seen in Fig. 1. The computational domain used for the CFD calculations consists of two parts: a cylindrical component (80 mm long) that surrounds the two radial air swirlers which are fed by pre-heated air from a plenum, and a rectangular combustor (300 mm long) with a converging duct at the exit as it is shown in Fig. 2. The fuel (commercial aviation kerosene) used for the combusting test is supplied by two opposing fuel lines to an annular fuel gallery, and from there to a vertical slot through a circular array of 36 orifices that surround the base of a prefilmer (see Fig. 3a). The actual pipes, through which the fuel enters, are not included in the computations. Instead the liquid fuel is injected in the form of droplets via an annular ring (represented by 1000 discrete locations[1] from which droplets are injected at random) at an axial location just downstream of the fuel injector prefilmer lip. In addition, the combustor walls have a series of effusion air cooling holes, however as this occurs downstream of the region of interest the effusion cooling air was omitted from the present analysis. A structured, multi-block mesh of the DLR generic combustor was created using ICEM CFD v.11, and consisted in total of 2.2 million cells and 137 blocks [12]. The mesh is refined at the exit of the swirler and the size of the smallest cells is 0.5 mm (see Figs. 2 and 3). The size of the largest cells is 5 mm and are located in the middle section of the combustor. The simulations were carried out using 16 cores of a Linux cluster comprising Intel Xeon E5404 2.0 GHz CPUs.

[1] It would also have been possible to inject droplets at random locations around the annular ring. However given the uncertainty in spray boundary conditions it is doubtful that this would bring any significant changes.