INTRODUCING A TWO – FLUID APPROACH FOR THE MODELING OF "STABILIZED COOL – FLAME" PHENOMENA

D. Katsourinis, M. Founti*

Heterogeneous Mixtures and Combustion Systems, Thermal Engineering Section,
School of Mechanical Engineering, National Technical University of Athens,
Heroon Polytechniou 9, Polytechnioupoli Zografou, 15780 Athens, Greece
Tel. +30-210-7723605, Fax. +30-210-7723527, *email: mfou@central.ntua.gr

ABSTRACT

An in-house developed computational fluid dynamics code implementing a Eulerian-Lagrangian approach is extended in this work by introducing a model based on the two – fluid approach (Euler / Euler). This model's performance is tested by comparing predictions with available experimental data obtained for an air – water spray. The calculated air and water velocity profiles show that the overall agreement using the two-fluid approach can be considered satisfactory, establishing the applicability of the model. Particle tracking (Euler / Lagrange) simulations have also taken place for the same experimental test case. A comparison between both approaches calculations indicates that no significant differences can be observed with respect to their predictive capability. However, the Lagrangian approach yields slightly better results than the Euler-Euler approach downstream the water-nozzle.

1. INTRODUCTION

Liquid fuel atomization, in the form of a spray, is commonly used in oil-fired furnaces and boilers, diesel engines and gas turbines in order to increase the fuel surface area and thus accelerate the vaporization and combustion rates. In conventional liquid spray flame combustion, incomplete mixing of the fuel vapors and of the liquid fuel droplets with the surrounding combustion air, leads to in-homogeneities in the fuel vapor-air mixture and deteriorates the overall efficiency of the process.

In this work, a new computational tool is introduced based on, the so – called, two – fluid approach. The work is motivated by the need of obtaining detailed description of the flow and thermal field inside a "stabilized cool – flame vaporizer", where a liquid-duel spray is first evaporated and then the fuel steam is partially oxidized but not burnt [1,2]. This low temperature oxidation process is termed as stabilized cool flame evaporation and couples mass and heat transfer phenomena with "low-temperature" chemical kinetic mechanisms. It is apparent that, the numerical modeling of the complex phenomena occurring during cool flame vaporization necessitate the use of dedicated two-phase flow modeling approaches capable of capturing in detail the mass and heat transfer phenomena both in the dense and the dispersed spray region. This study is classified under the general frame of work of acquiring more in depth information about the physical and chemical phenomena occurring in the "cool – flame" region.

Cool flames are characterized by a faint pale bluish light that is attributed to the chemiluminescence of excited formaldehyde [2]. They manifest themselves in the range of temperatures where transition between low temperature and high temperature mechanisms occurs. Experimental work is currently in progress in various laboratories throughout the world, studying the physical and chemical phenomena involved in the "cool – flame" phenomenon [3,4,5]. These experiments conducted in various cool – flame vaporizers, have shown that when "stabilized cool flames" are realized in open flowing systems, the air/fuel mixture temperature increases up to 200K in the flow direction and stabilizes at the raised level. During this process, no "conventional" ignition occurs and only 2-10% of the fuel mass, and therefore of the respective available thermal energy attributed to the fuel's heating value, is being "consumed" [5].

Until now there is scarce information in the open literature regarding the numerical modelling of non-igniting "stabilized cool flames", especially in the frame of a CFD code. Towards this end, an in-house developed, two-phase Computational Fluid Dynamics (CFD) code, based on the Eulerian / Lagrangian approach has been employed in the past to predict the spatial evolution of the evaporating spray. In order to model the effects of cool flame reactions on the heat and mass transfer phenomena, a twofold approach has been followed. On one hand, a dedicated semi-empirical approach has been developed to computationally simulate the cool flame heat release rate [6], while on the other hand, a look –up table has been formulated by incorporating data from a large number of chemical kinetics simulations [7]. However, the complexity of heat and mass transfer phenomena occurring inside a "cool - flame" vaporizer, combined with the numerous exothermic chemical reactions involved, gives rise to the need of obtaining precise information of the flow and thermal field in regions close to the nozzle, where the flow is dense. Furthermore, it must be taken into account that there is considerable lack of experimental data in dense spray regions, where also numerical predictions with the use of the Lagrangian particle tracking approach method are problematic.

Consequently, the implementation of a two – fluid model (Euler – Euler) is presented here for the simple case of a non – evaporating water spray in air. Future work will focus on the simulation of the flow characteristics using the Euler / Euler approach inside a "cool – flame" vaporizer, especially close to the fuel spray injection nozzle. Such calculations can provide appropriate inlet conditions, (inlet velocities and droplet size) for the Lagrangian simulations to yield accurate results at the rest of vaporizer's geometry where a dilute spray flow field exists. However, at this stage the performance of the implemented two - fluid model is validated against experimental data available in the literature.

2. COMPUTATIONAL APPROACH

Generally, two approaches are commonly employed for predicting the behavior of the liquid phase in spray applications. The Lagrangian approach considers a large number of droplet "parcels", representing a number of real droplets with the same properties. Each parcel's trajectory is calculated by solving the instantaneous droplet motion equations. In the Eulerian approach, both phases are treated as interpenetrating continuums and are governed by a set of differential equations representing conservation laws (two –fluid model). However, various modifications of the two – fluid approach can be found in the literature.

As a consequence of the two concepts, the Eulerian approach can be more appropriate for dense spray regions, while the Lagrangian tracking method is usually more successful in dilute spray flow fields. Both methods have been successfully employed in the past for predicting flow and temperature fields in various cases of non – evaporating and evaporating sprays [8,9].

The work focuses on the development of a new CFD computational tool based on the two - fluid approach (Euler – Euler) to assist the understanding of the physical and chemical phenomena involved in the "cool flame" phenomenon, especially in regions close to the spray injection nozzle. The new computational tool's performance is tested by comparing predictions against available experimental data. Additionally, simulations with the use of both Euler and Lagrange approaches take place and resulting predictions are assessed.

Simulations have been performed with the use of the computational fluid dynamics code, 2 – Phase, developed in the Laboratory of Heterogeneous Mixtures and Combustion Systems of NTUA. This code has been previously, successfully applied [10,11,12] in a wide range of two-phase flows using the Lagrangian approach.

The code is extended here by implementing a two – fluid model. As a result, both phases are treated as steady, incompressible, turbulent flows, which are computed by solving the time-averaged continuity (to calculate each phase's volume fraction) and momentum transfer, conservation equations. The resulting system of equations is solved via a finite volume method based on a staggered grid arrangement. Turbulence quantities for both phases are modeled using a modified version of the k-ε turbulence model by Sung et Al. [13]. Inter-phase momentum transfer between the continuous gas phase and the dispersed liquid phase has been introduced in the code, via the drag term calculated by the empirical correlation of Schiller and Naumann [14]. The drag coefficient is written as:

$$C_D=\max((24/Re_p)\,(1+0.15Re_p^{0.687}),0.44), \quad (1)$$

where Re_p : the Particle-Droplet Reynolds Number

In the case of the Eulerian / Lagrangian simulations, the continuous phase is treated as a steady, incompressible, turbulent flow, which is computed by solving the time-averaged continuity and momentum transfer, conservation equations. The resulting system of equations is solved via a finite volume method based on a staggered grid arrangement, using the SIMPLE algorithm. Turbulence quantities are modelled using a modified version of the k-ε turbulence model [13]. This model modifies the constants C_μ and C_2 of the standard k-ε model to account for the radius of curvature of the flow. The model has proved to yield better prediction accuracy than the standard k-ε model in re-circulating flows with abrupt area changes [15]. The Lagrangian treatment is adopted for the dispersed phase, where a large number of droplet "parcels", representing a number of real droplets with the same properties, are traced through the flow-field. Each parcel's trajectory is calculated by solving the instantaneous droplet motion equations in a three-dimensional Cartesian frame of coordinates (in order to avoid the singularity that droplet radial position may assume by applying cylindrical coordinates), with the use of a 4^{th} order Runge-Kutta method. The droplet motion equations take account of the drag and the gravitational force. Droplet turbulent dispersion is modeled according to a Lagrangian stochastic separated flow model, by sampling random Gaussian gas velocity fluctuations, while accounting for the crossing trajectories and eddy lifetime effects [16]. The gas and the liquid phase are coupled by calculating source-sink terms for the interfacial momentum, turbulent energy, thermal energy and species concentration exchange (two-way coupling), following a modified version of the PSI-cell approach [17].

3. EXPERIMENTAL DATA

The experimental data of Bulzan et Al. [18] are used for the validation of the implemented two – fluid computational model, as well as for the comparison between Euler – Euler and Euler – Lagrange predictions. These experiments use an axisymetric air-assist blast atomizer injecting water. As it can be seen in Fig. 1 the diameter of the nozzle's orifice is 3.18mm, while the inner diameter of the liquid tube is 0.39mm. The spray's direction is vertical downward within a large enclosure (1.8 by 1.8 by 2.4m high). The resulting two - phase flow field consists of air (as the carrier / atomizing phase) and water droplets (as the discrete / atomized phase). The air and water flow rates applied for this particular data set are 0.49g/s and 2.25g/s, respectively. The range of the measured droplet diameters is from 1 to 50μm and velocity

measurements are reported for droplet diameters of 4, 11, 18, 25, 32, 39 and 46μm. A complete set of measurements is obtained at axial locations from 5 to 50μm downstream of the nozzle.

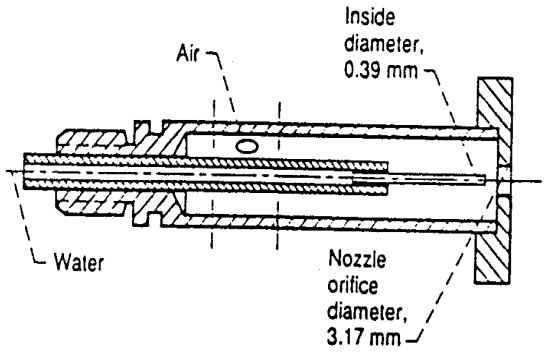

Figure 1: Air – assist nozzle used by Bulzan et Al. [18]

4. RESULTS

Simulations using both approaches have been carried out, by taking into consideration a computational domain, measuring 0.5m axially by 0.12m radially. This domain has been discretized using 282*73 non-uniform, cylindrically axisymmetric, rectangular grid nodes. The grid was refined close to the nozzle tip to improve local flow resolution. The continuous phase (air) was considered to enter the test region with a top-hat velocity profile, corresponding to the experimentally determined mass flow rate value of 2.25 g/s. Simultaneously, the liquid phase (water) was considered to enter the simulated domain having a top-hat velocity profile, applied to the inside diameter of the liquid tube (Fig 1). This profile also corresponds to the experimentally determined mass flow rate value of 0.49 g/s for water. For both the experimental and computational purposes, the liquid phase (water) droplets were considered as monodispersed, with a mean droplet size diameter equal to 18μm. In the case of the Lagrangian simulations, spherical water droplets were assumed to be injected in the flow-field from 5 discrete starting locations, equally distributed across the atomizer inlet plane. A total number of 10 000 computational droplet "parcels" were injected and tracked throughout the flow-field for 10 two-way coupling iteration cycles, in order to keep statistical fluctuations associated with stochastic particle tracking at an acceptable level.

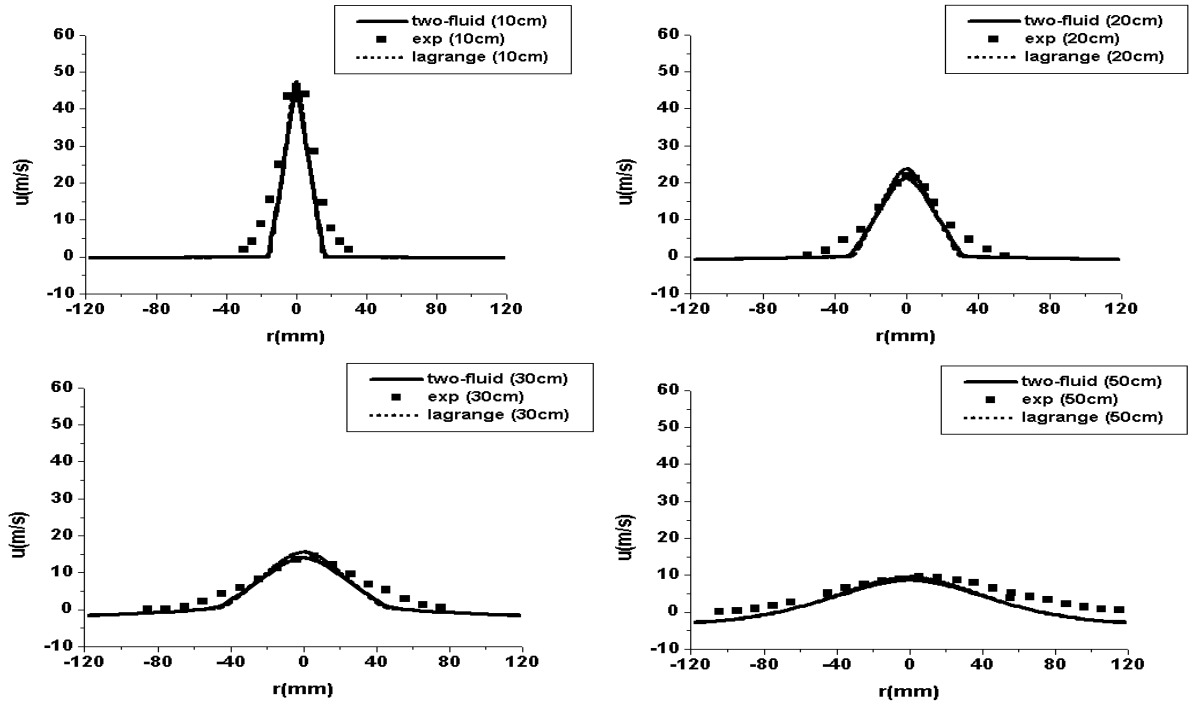

Figure 2: Axial air (gas phase) velocity radial profiles at various downstream distances from the nozzle: (i) square symbols: experimental data, (ii) continuous line: two – fluid approach calculations, (iii) dotted line: Eulerian – Lagrangian approach calculations

Measured and predicted axial mean air-velocity radial profiles (continuous phase) at various distances from the nozzle (10mm, 20mm, 30mm and 50mm) are depicted in Figure 2. It is apparent that, utilizing either of the implemented approaches properly captures the main features of the air velocity's flow field. Some very small differences can be observed in the radial profiles located 20cm and 30cm downstream the nozzle.

The overall performance of the implemented two – fluid model is quite successful and this argument can also be asserted by results exhibited in Figure 3, where the liquid phase (water) predicted axial velocity profiles are compared to measurements, at various downstream distances from the nozzle (10mm, 20mm, 30mm and 50mm), utilizing both the Eulerian and the Lagrangian approach. A detailed observation of Figure 3 indicates a slightly better predictive capability of the Lagrangian approach, for the dispersed phase (water droplets) especially for locations far downstream the nozzle.

The lack of detailed experimental data near the nozzle, in the dense phase region, is the major reason for the observed discrepancies between experimental data and computational results. Such data would provide more realistic inlet conditions (air - water velocities and volume fractions) for the computational simulations. Consequently, the anticipated advantages of the two-fluid approach in the near-nozzle region cannot be demonstrated.

Future work will include the introduction of an evaporation model, followed by the implementation of a model capable of predicting the droplet size distribution, after the liquid fuel is injected from the nozzle and before evaporating. Moreover a chemical kinetics model capable of predicting the additional thermal amount owing to the exothermal reactions occurring during the "cool flame" phenomenon will be developed. The resulting computational tool will be used to provide detailed predictions of the most essential flow and thermal parameters behavior inside a "cool flame" vaporizer, especially in regions near the nozzle characterized by dense flow. Euler – Euler and Euler – Lagrange predictions will be tested against experimental data, with the aim of developing an efficient, coupled two – phase flow solver. This solver will employ a more sophisticated method, which will at the same time use the Euler – Euler approach for dense spray regions, while the Euler – Lagrange approach will be applicable for the respective dilute spray regions.

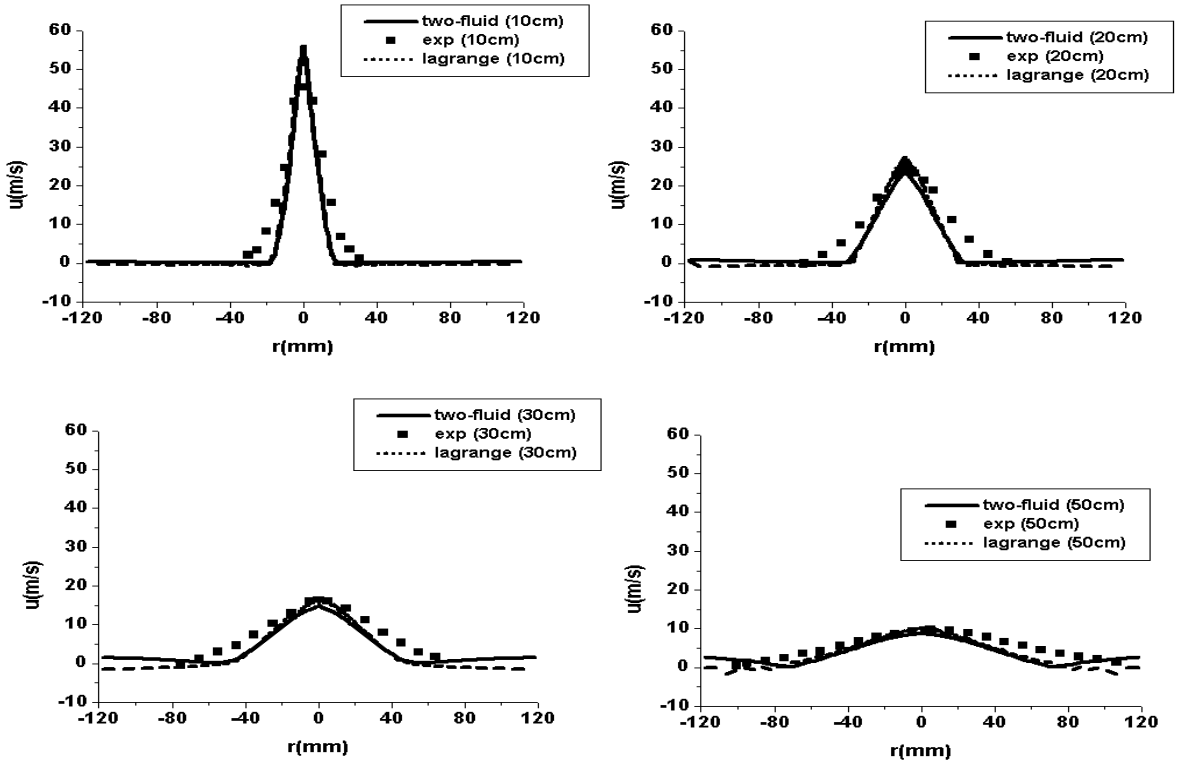

Figure 3: Axial water (liquid phase) velocity radial profiles at various positions – distances from the nozzle: (i) square symbols: experimental data, (ii) continuous line: two – fluid approach calculations, (iii) dotted line: Eulerian – Lagrangian approach calculations

5. CONCLUSIONS

The work of this paper focuses on the implementation of a new computational tool based on the two – fluid approach. At this stage of the study, this computational tool is validated against experimental data available in the literature for a test case of a non- evaporating spray. The predicted velocity profiles indicated that the performance of the two – fluid model could be considered as satisfactory as that of the Lagrangian spproach, leading to the conclusion that the developed computational tool succeeds in yielding reliable predictions of turbulent spray flow characteristics. No significant differences are observed between the overall predictive capacity of the two-approaches. Far from the nozzle, the droplet velocity profiles obtained with the particle tracking modeling approach, agree slightly better with the experimental data.

6. REFERENCES

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