

Analysis of Premix Flame and Lift-Off in Diesel Spray Combustion using Multi-Dimensional CFD

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ABSTRACT

A detailed analysis is performed upon the results of CFD combustion simulations of several diesel fuel spray flame experiments. Simulations are validated against measurements from a constant volume combustion chamber testcase [9]. Particular emphasis is made in the analyses to identify mechanisms associated with the 'lift-off' phenomena characteristic of contemporary high injection pressure diesel engine combustion. A recently developed industry state of the art RANS hybrid combustion model (Extended Coherent Flame Model - 3 Zones) [41] is used which takes account of both a propagating (premixed) flame combustion mode as well as the conventionally assumed diffusion flame mode used in most diesel combustion models. The location of and development of a propagating reaction front, obtained from analysis of the progress variable within the model, is studied in relation to the lift-off behaviour. The entrainment of air upstream of the lift-off is quantified from the CFD simulated field results and compared with values estimated from an empirical model [38] considered in recent experimental studies [34]. The fuel vapour field is also examined and compared with recent field data experiments of fuel concentration [22].

INTRODUCTION

Understanding of the diesel spray flame has advanced significantly during the last decade, notably with the now familiar conceptual view of Dec [26, 12] and subsequent studies of Siebers *et al.* [19] and co-workers at Sandia National Laboratories in highlighting the role of lift-off. From a simulation perspective

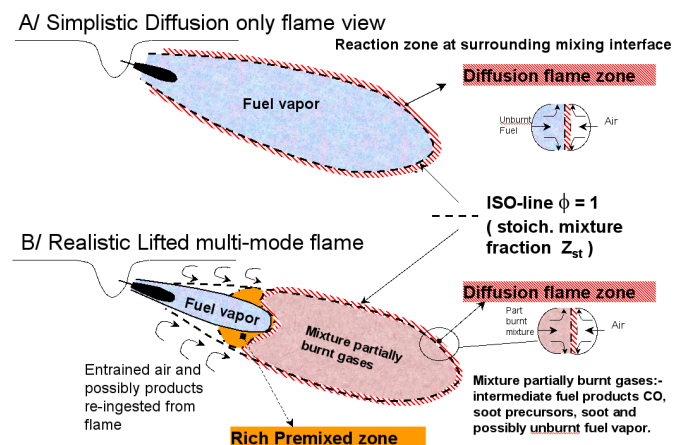


Figure 1: Conceptual views of spray flame

the contribution of Chomiak and Karlsson [4] stands out as bringing fresh focus to the requirements imposed on a combustion model for diesel spray flame simulation.

Surprisingly, given the evidence of a lifted flame structure and the emphasis upon a partially premixed mode of combustion within the diesel flame, simulation models used in industry have remained strongly entrenched in the non-premixed view of diesel flame and the dominance of a diffusion flame structure.

In Fig. (1) upper (A) a cartoon is drawn which represents a diesel flame if it were entirely existing as a diffusion flame, where the reaction zone is located solely at the surrounding mixing interface between the fuel vapour and air (oxidiser).

The simplistic view of Fig. (1)(A) is not realistic, more especially with increasing injection pressures and reducing nozzle hole size, the flame structure is now predominantly of a multi-mode nature where strong entrainment and inherent premixed burning occurs, this shown in the lower Fig. (1)(B/).

Further, the 'premixed' burning mode is not simply a short transient as indicated from the familiar characteristic 'premixed spike' which occurs at the early stage of combustion. Rather there is a continual resident 'premixed' combustion whose location immediately upstream of where soot is observed, suggests that accurate simulation of this flame structure is of major importance and probably of greater priority in terms of model development than employing expensive detailed kinetics in the soot modelling.

A further complication to the behaviour of the lifted flame structure is in regard to relative penetration of the liquid spray compared to the lift-off location as described by Siebers et al. [9].

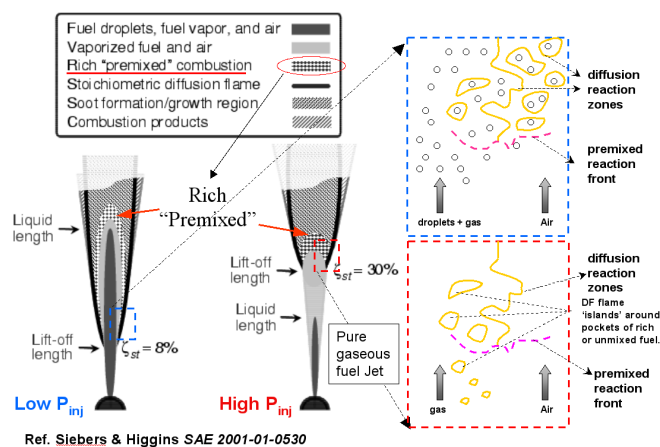


Figure 2: Conceptual view of flame structure local to the lift-off and the relative penetration of liquid into the flame.

In Fig. (2) the top righthand sub-figure is an adaptation of the conceptual picture of spray combustion by Demoulin and Borghi [14], and is shown as an embedded small scale feature within a figure taken from [9]. The second left main figure in 2 indicates how the influence of increased injection pressure and reduced hole size leads to the situation where liquid penetration is much shorter than the flame lift-off such a pure gaseous jet fuel-air mixture is entering the flame zone. Hence in the lower right-hand sub-figure 2 the situation reduces to a gaseous only jet meeting something similar to a triple flame structure observed in laminar flow. Under turbulent flow conditions the structure is more complex but does retain a familiar three branched structure.

The consequence of this gas-jet only characteristic is to place less regard on the difficult physics attached to sub-modeling the liquid spray, since the droplets are no longer interacting directly within the flame zone. Modeling effort may then be focused on the partially premixed regime comprising some sort of ensemble of triple flamelets.

FLAME STABILISATION There have been two main categories of theory for explaining the stabilisation mechanism of a turbulent jet lifted flame:- the propagating premixed flame theory [29] and a quenching theory [45].

Variations around each of these two main theories have been proposed and examined in the research literature. The theory relying upon a premixed propagating flame appears to have been discounted on the basis that the flame propagation speed, even given the enhancement by high turbulence intensity providing increased local flame surface wrinkling effects, cannot be sufficiently high to compete with the high velocities of the oncoming premixed fuel stream. In any respect, the assumption of a fully premixed condition, especially in the context of a liquid spray, seems unrealistic in this theory. The 'quenching theory', also referred as a 'critical scalar dissipation rate' theory [8] or diffusion flamelet extinction theory has gained considerable support in the numerical research but has also been acknowledged (by one of its originators [46]) to be not wholly responsible as the stabilising mechanism and in fact stabilisation by a premixed flame propagation could be the more valid[46]. It should be noted however that the vast majority of the stabilisation studies are made in regard to gas jets.

The latest understanding in regard to diesel spray (i.e. liquid jet) flame stabilisation seems to point at some type of auto-ignition induced propagating reaction front. A concept of this type is described by Vogel et al. [43] suggesting that a simultaneous partnership of auto-ignition(AI) and premix flame(PF) is responsible, this concept will be discussed in light of the present studies in the conclusions section. A recent review of the studies made on diesel flame lift-off has been made in [58] which emphasises the curious dilemma that numerous model studies based on alternate mechanisms appear to yield (at least qualitatively) correct lifted flame simulations.

In summary to this introduction, the author's present objective has been to employ a contemporary industrial CFD simulation and examine it's capability to capture the underlying flame structure as evident from the experimental laser imaging studies of a quasi-steady lifted diesel spray flame.

The credibility of combustion simulation with CFD for even qualitative prediction of pollutant, must be founded on the basis that the simulation agrees with the *basic physics of where and in which mode of combustion reaction occurs*. To otherwise arrive at the quantitatively correct pollutant prediction without observing a correct flame structure cannot be a correct approach.

SIMULATION METHOD

DIESEL LIQUID JET FUEL SPRAY An essential pre-requisite for spray combustion simulation is to establish the correct distribution and state of mixedness of the fuel vapour produced as result of the liquid jet atomisation and evaporation processes. The sub-modelling of these spray processes is a difficult task and is itself the subject of a large body of literature and on-going research searching to improve the accuracy of predictions. In the present work the industry standard Discrete Droplet Lagrangian (DDL) method [11] as implemented in the STAR-CD [1] code is used. The deficiencies of this method (DDL) for achieving accurate a priori prediction are appreciated since quite a long time [15] with the most common criticism being a strong mesh dependency especially in the near nozzle region where the liquid drop density is high. Alternatives to the DDL approach based on Eulerian two-phase approach have been developed in recent years e.g. [28, 60, 25] but as yet few appear to have reached application in the industry [51] or are not seeing widespread use. The computational economy and robustness of the DDL approach remains highly attractive to industry as does its capacity for tuning. While the merit of tuning constants may be questionable, nonetheless using a DDL approach it is possible to calibrate the coefficients of the atomisation and breakup sub-models to obtain a match against experimental data - typically the global liquid and vapour penetration histories as interpreted from mie-scattering and schlieren methods. It is however difficult to achieve a match with both of liquid and vapour penetration. In some studies e.g. [44], the calibration of the model constants with spray experiment has been automated by using genetic algorithm driven optimisation methods.

In the present studies an exhaustive calibration/sensitivity assessment of the spray model has not been conducted. Instead, and fortuitously, a reasonable match has been found using default parameter settings as judged by comparison with the global penetration and fuel vapour *field* concentration measurements [21].

A summary of the spray sub-model parameters is shown in Table 1, please refer to [1] for more details. Of particular note is the specification of a nozzle hole

exit area contraction coefficient C_a , which takes into account the reduced cross section of the emerging liquid jet at hole exit and its corresponding increase in momentum. This C_a value is obtained from spray momentum measurements which provide a next level of information beyond the common discharge coefficient C_d measurement and is particularly important in the case of a sharp edge hole such as the one used in the Sandia test case.

Spray Process	submodel / parameter
Nozzle flow	1-D orifice $C_d = 0.80$ and $C_a = 0.86$
Atomisation	Huh
Secondary Break-up	Reitz-Diwaker
Droplet Momentum	Standard(STAR) correlation

Table 1: Submodels used in spray model

COMBUSTION MODEL - ECFM3Z The combustion model used is the Extended Coherent Flame Model in 3 Zones (ECFM3Z) which was developed by the Groupement Scientifique Moteur (GSM) consortium by partners IFP, Renault and PSA Peugeot-Citroen. It has been implemented in the STAR-CD code by CD-Adapco [36] in partnership with Renault but is also available in other commercial CFD software codes IFP-C3D [35, 23, 50] and recently AVL-FIRE [52].

The ECFM3Z methodology is described in detail by Colin *et al.* [41]. A brief summary description is provided here to highlight some of the key features.

The general principle of the model is to combine combustion sub-models for each of auto-ignition (AI), premixed propagating flame (PF) and diffusion flame (DF) simultaneously inside a concept which takes account of the local sub-grid state of the gases i.e. their composition and temperature, by applying a simple form of double conditioning. This is achieved by considering the mixing state to occur in three zones and for the reaction state of the gases to correspond to either unburnt or burnt gases mixture. In mathematical terms the mixing space is defined by a three point dirac delta probability distribution function (PDF) Fig. (3). For the reaction state a reaction progress variable ($c = 1 - Y_{Fu}/Y_{TF}$) is defined to track the increase of burnt gases relative to unburnt gases. Hence the progress variable 'c' assumes a double-dirac (unburnt or burnt) PDF description. This double conditioning (for each of mixing and reaction states) is applied to the cell mean values solved by the transport equations in CFD simulation. It is important that the conditioned (sub-grid) values of composition and temperature are used in each of the component combustion reaction rate models. This approach serves to

account for the turbulence-chemistry interaction due to micro-scale fuel and temperature stratification.

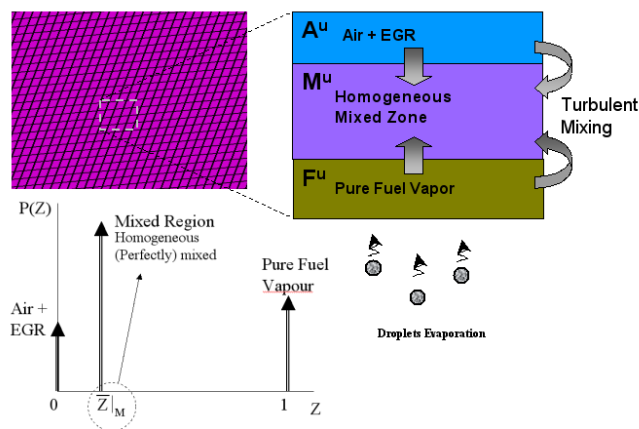


Figure 3: Sub-grid mixing model

FUEL REACTION RATE AND CHEMICAL KINETICS

Auto-ignition The auto-ignition (AI) model used in the present work is based on the double delay with tabulated reaction rate auto-ignition model described by Colin *et al.* [40]. The chemical mechanism of Curran *et al.* [5] for *n*-heptane was used in creating the auto-ignition delay (for cool-flame) and reaction rate (for high temperature) loop-up database. Two additional transport equations are solved to track the cell-wise ignition progress for each of cool-flame and the high temperature ignition chemistry. Actually, in the present test case (1000K, 40bar) there is likely no benefit from accounting for cool-flame chemistry.

Premix propagating flame The expression for fuel consumption rate due to the premixed propagating

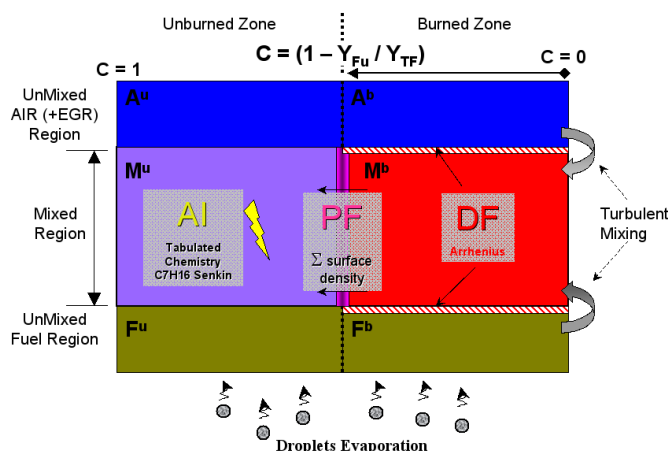


Figure 4: Conceptual sub-grid view of the ECFM3Z combustion model

flame (PF) combustion in the ECFM3Z model is provided by the method of a coherent flame model (CFM) based on the composition in Mixed and Unburnt gases region:

$$\bar{\omega}_{fu}^u = \bar{\rho}^{u,M} |M Y_{fu}^M|_M U_L \Sigma \quad (1)$$

where the unstrained laminar flame speed U_L is obtained from a correlation after [37] with corrections for a wider range of equivalence ratio and for high pressures. A transport equation is solved for the turbulent flame surface area density Σ . In essence, the combustion chemistry of the PF is obtained from the U_L and the influence of the turbulent flow-field interacting with the combustion is brought by the model transport equation for Σ . Further details can be found in [2, 41] and their supporting references.

Diffusion flame For the diffusion flame burning mode an eddy-breakup concept is considered whereby the fuel consumption rate is taken as proportional to the mixing rate of fuel and air into the hot 'burnt' gases region. This means that fuel which is transferred into the burnt gases region (e.g. pockets of fuel vapor too rich to burn by PF or vapor produced by droplets which have penetrated into regions of burnt gases) is effectively consumed almost instantaneously, delayed only by the fast but finite rate of a reduced step 'post-flame' oxidation kinetic.

EMISSIONS SUB-MODEL In the present simulations an industry standard empirically based soot model (ERC soot model [42]) is used, the model describes each of the two competing sub-processes for soot formation and soot oxidation following Hiroyasu [18, 20]. The soot oxidation rate follows Nagel and Strickland-Constable [39]. This model responds to the local concentration of a soot inception species (in this case simply fuel concentration), the local temperature and pressure. In the ECFM3Z case, the local conditions are those conditioned in the mixed and burnt gases region. This two-step empirical soot model is maybe not today considered state-of-the art, (a more sophisticated soot modelling approach based on the method-of-moments for particle size soot distribution in combination with a flamelet library is available within the STAR-CD code), however for purposes of the present studies focusing on the reaction zone structure, it was considered sufficient to employ the standard empirical soot model for qualitative comparison.

EXPERIMENTAL AND COMPUTATIONAL SET-UP

The experimental database available from the 'Engine Combustion Network' ECN website [61] established by Sandia Laboratories using measurements in a

constant volume combustion chamber has been used to provide validation against the simulations. This constant volume experimental facility is described in detail in numerous studies published by researchers at Sandia laboratories since year 2000 [19, 9].

The present simulations are for the 'baseline' case *n*-heptane fuel injected at 150MPa through a 100 μ m diameter hole into an ambient gas condition of 1000K and 14.8kg.m⁻³. This case is considered to provide a well characterised experiment which is relevant to the case of a heavy-duty diesel engine where a single main injection event is dominant and a quasi-steady so called 'mixing-controlled' flame structure is pre-dominant. Perhaps a more accurate description is to say '*injection rate controlled*' as evident from the heat release rate profile.

The use of 100 μ m hole diameter in production DI diesel engine injectors is already in practice. One possible inconsistency when compared with present state of the art injector nozzle hole design is that the Sandia nozzle 100 μ m hole is a sharp edge entry cylindrical hole, whereas current practice now employs rounded(hydro ground) hole entry and convergent cone shaped holes. Nevertheless, the key benefit from the experiment is that the nozzle hole has been well characterised from previous measurements. Specifically, a hole area exit contraction coefficient (*C_a*) is supplied from spray momentum measurements which provides a specification for the injection velocity of the liquid spray.

Injection	
Nozzle hole dia.	100 μ m
Fuel@Temp	N-Heptane@373K
Inj.Pressure Delta	150 MPa
Inj. Mass / duration	17.8mg / 6.8msec
Noz.hole contraction	<i>C_a</i> = 0.86
Mean Injection velocity	$\bar{U}_{inj}$ = 633m/sec
Ambient gas	
Oxygen	21%
density ρ	14.8 kg/m ³
temperature	1000 K
pressure	$\cong$ 41 Bar
Global measurements	
Liquid penetration	9.2mm
Ignition Delay	0.53 msec
Lift-Off-Length(LOL)	17mm

Table 2: Sandia baseline N-heptane experiment

SIMULATION SETUP A two-dimensional axisymmetric mesh has been used in the STAR-CD CFD simulations. The initial 'M1' mesh Fig. (5) used was constructed with a resolution typical of industry engine in-cylinder calculations, having approximately

1mm cell size near the nozzle. The rather peculiar graded mesh structure is inherited from some previous investigations (not shown here) made by one of the co-author's, using a three-dimensional grid constructed and solved using the engine specific software IFP-C3D code (also employing the ECFM-3Z combustion model). The three dimensional model containing 90,000 cells was produced as a pseudo engine cylinder 90 degree sector model having the same volume as the Sandia combustion chamber. The equivalent resolution 2-D axisymmetric domain contains 2760 cells. The equivalent 90,000 cell 3-D model was also tested in the STAR-CD code and yielded the same results as the 2-D axisymmetric, but with a very substantial(x10) increase in computation time. All subsequent detailed post-processing and field analyses have been made using the 2-D STAR-CD axisymmetric model which allows for much faster run-time and economic handling of the large transient results datasets and post-processing.

The 2-D axisymmetric grid is based on a 30 degree sector one cell thick in the theta direction. The size of the domain is created having the same 108mm dimension from the nozzle hole to the incident chamber wall and a radial dimension 56mm to provide an equivalent volume (for 1/12th hole) compared to the actual experiment.

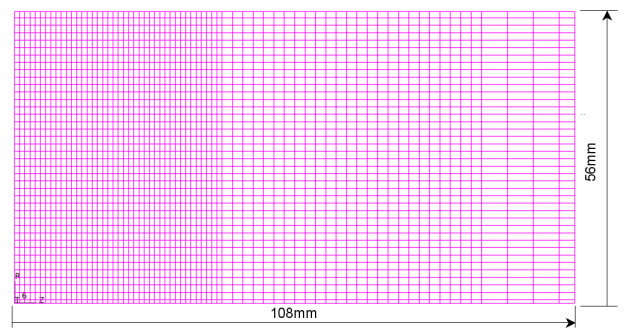


Figure 5: Standard (M1) 2D axisymmetric computational mesh. 2760cells. near nozzle 1mm.

Subsequent to the analysis of the field results from the M1 grid case a refined grid was produced by adaptively refining the original grid using the combination of fuel vapour scalar gradient and velocity gradient taken from the original solution at 3.0msec. The refined grid is denoted as 'M2ARb' and contains 5382cells, see Fig. (6).

In the numerical solution, a second-order accurate discretisation scheme (MARS [1]) is employed for the momentum and the turbulence transport equations, with first-order UD for the scalars. Timestep size is user specified according to the demands of different phases of the injection and combustion. A

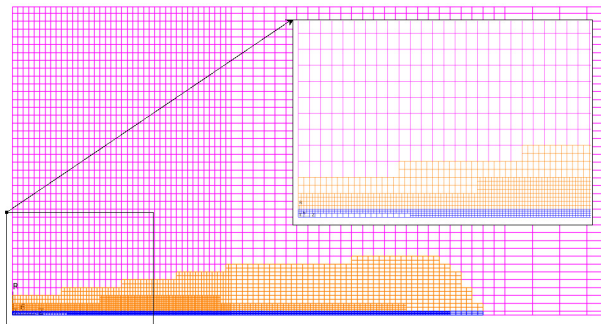


Figure 6: Adaptively refined 'M2ARb' grid - 5382cells, near nozzle=0.25mm

nominal overall timestep 0.5×10^{-6} sec is used, this is a conservative value well within the courant number limitations for the refined case grid, a minimum timestep 1×10^{-7} sec is applied during the auto-ignition and premixed burn period. Corresponding to the minimum timestep a sufficiently high (2×10^7 /sec) injection parcel rate is specified for the stochastic DDL model. Calculation time for a 10msec period (where EOI is at 6.8msec), is approximately 7 hrs (M1) or 15 hrs (M2) running on a single dual-core 2.5GHz AMD PC. For solution on a comparable resolution three-dimensional grid (90,000 cells) the calculation time is approximately > 48hrs dependent on less conservative (larger) timestep size.

DETERMINATION OF THE FLAME LIFT-OFF LENGTH The phrase '*flame lift-off length*' (hereafter denoted LOL) has become a common place term describing the distance between the nozzle and a location downstream where there is first appearance of high temperature reactions. In the majority of previous CFD simulation comparing with liftoff experiment, some examples being [54, 13], the criteria selected from the CFD simulation to indicate a flame lift-off length has been a rather arbitrarily chosen iso value of temperature in the range from 1600K thru 2200K. The experimental method of quantifying lift-off by employing OH chemiluminescence is described by Higgins and Siebers [10]. Images of light emission filtered at 310nm, characteristic of excited state OH species, are interpreted as indicating the location and approximate concentration of high temperature reaction of diesel fuel. The location denoted as flame lift-off length is determined by constructing an axial profile of the peak relative intensity of the 310nm images averaged over many images. The constructed axial profile Fig. (7) has been found to exhibit a characteristic point of rapid rise before levelling off, thereby allowing application of a threshold value to quantify a location where the high temperature flame is deemed to start. Further details of the precise

experimental method can be found in [31].

In the CFD simulations the field of *mean* OH species has been examined in a similar way as for the experiment to yield an axial profile of the peak value (obtained across the radial section at each axial station) and a threshold is chosen as a diagnostic for the location of the flame lift-off. In the charts Fig. (17) and Fig. (18) two alternate threshold values are shown, an axial profile of the peak Temperature is also shown for reference. It should be apparent that precise determination of LO distance is sensitive to choice of criteria.

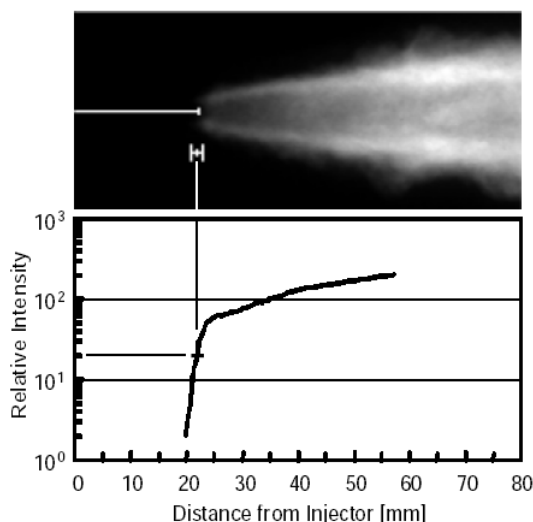


Figure 7: Sample picture from the experiment [10] showing how the axial distribution of peak OH-LIF image is analysed to obtain a liftoff distance. (extracted from for a 180um DF2 case)

RESULTS AND DISCUSSION

INERT CASE - FUEL SPRAY VAPOUR FIELD Fig. (8) shows the fuel vapour concentration field from CFD simulation compared with the experimental images obtained from the Rayleigh scattering technique [21, 22].

Fig. (10) shows the global penetration history where the liquid matches closely the experiment penetration (9.2mm) but the vapour penetration is slightly under-predicted.

In the experiment the global vapour penetration history is quantified by interpreting schlieren images which represent density gradients [55]. In the CFD field the furthest extent of fuel concentration greater than mass fraction 0.5% ($FVMF > 0.005$) is used for the vapor penetration and the the liquid penetration is an axially integrated 99% of total liquid mass.

Fig. (11) shows the global penetration history for the refined grid M2ARb which shows a slightly improved