

DROPLET EVAPORATION ASSISTED BY “STABILIZED COOL FLAMES”: SCRUTINIZING ALTERNATIVE CFD MODELLING APPROACHES

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ABSTRACT

Controlled liquid fuel droplet evaporation under “stabilized cool flame” (SCF) conditions can lead to a homogeneous, heated air-fuel vapour mixture that can be subsequently either burnt or utilized in fuel reforming of fuel cell applications. In this work, an “in-house” Computational Fluid Dynamics (CFD) code is used to simulate the turbulent, two-phase, multi-component and reacting flow-field, developed in a “SCF-assisted”, atmospheric pressure, evaporating Diesel spray, loop - type reactor. A parametric study of various alternative modelling approaches is performed. The two-phase flow (air-liquid droplets) is modelled using either the Euler-Euler or the Euler-Lagrange concept. Also, the cool flame chemical activity is simulated by utilizing, alternatively, an “on-line” direct chemical kinetics integration method or an “off-line” chemical simulation storage and retrieval technique. The performance of the various alternative approaches investigated in this work is assessed by comparing predictions with available experimental data, obtained in the examined reactor. The emerging computational results suggest that both approaches are capable of effectively simulating the complex interacting physical and chemical phenomena occurring in SCF devices.

LIST OF ACRONYMS / SYMBOLS

DI: Direct Integration
LUT: Look – Up Table
NTC: Negative Temperature Coefficient
ODE: Ordinary Differential Equation
Rec 1-3: Recirculation Zones 1-3
SCF: Stabilized Cool Flame
TC 1-3: Test Cases 1-3

x: Axial Distance [m]
r: Radial Distance [m]

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 and improve the evaporation and combustion rates. In conventional spray combustion systems, the incomplete mixing of the liquid fuel droplets and fuel vapours with the surrounding air leads to inhomogeneities in the mixture that lessen the overall efficiency of the process and enhance the

formation of pollutants. Towards achieving better mixing conditions in the air-fuel vapour mixture, a novel approach, taking advantage of the Stabilized Cool Flame (SCF) phenomenon, has been proposed by Lucka and Koehne (1999). In this case, the two main phenomena, namely droplet evaporation and fuel combustion, are essentially separated, resulting in a highly homogeneous, heated (though without being ignited) mixture, allowing the use of premixed combustion technologies.

Cool flames were initially observed in hydrocarbon fuel autoignition under elevated pressure conditions and represent essentially a low temperature oxidation process during which the fuel is only partially oxidized. They manifest themselves in the range of temperatures where transition between low temperature and high temperature mechanisms occurs (Lignola and Reverchon, 1987; Harrison and Cairnie, 1988) and according to Sheinson and Williams (1973) they are associated with the appearance of a faint pale bluish light, attributed to the chemiluminescence of excited formaldehyde, occurring preferentially under fuel-rich conditions. Cool flame reactions are generally exothermic in nature, producing modest amounts of heat. The low-temperature hydrocarbon oxidation region is usually characterized by a Negative Temperature Coefficient (NTC) behaviour, in which the overall reaction rate decreases with increasing temperature.

By exploiting the NTC phenomenon as a chemical “barrier” for auto-ignition to occur (Gray and Felton, 1974), it is possible to “stabilize” the cool flame reactions in an open flowing system under atmospheric conditions. In this case, heat losses at the system’s boundaries are balanced by heat generation owed to the exothermal chemical activity and steady-state thermo-chemical conditions are achieved, without being followed by a “hot” ignition (two-stage ignition). When a SCF is confined in open flowing systems, only 2-10% of the fuel mass is “consumed” in cool flame reactions (Lucka and Kohne, 1999). However, the mixture temperature increases up to 200K in the flow direction and stabilizes at the raised, yet below auto-ignition temperature, level. Experimental work conducted by Steinbach (2002) has shown that the occurrence of atmospheric pressure Diesel oil SCF is favoured under fuel-rich conditions in the temperature range of 550-800K. The utilization of the SCF phenomenon in a dedicated “liquid fuel evaporation” device, results in the enhancement of the liquid fuel spray evaporation rate, producing a well mixed, heated and

oxidant-fuel vapour mixture. This mixture can be either subsequently burnt, utilizing premixed combustion technologies, or reformed into hydrogen-rich gas for use in fuel cells (Naidja *et al.*, 2003). A significant number of publications can be found in the open literature, reporting CFD simulations performed for high temperature and pressure Diesel engine conditions, utilizing either reduced (Belardini *et al.*, 1996), or detailed (Tao *et al.*, 2000) kinetic schemes. However, the numerical modelling of non-igniting SCFs, especially in the frame of a CFD code, is scarce.

The scope of this work is to scrutinize two alternative CFD approaches for the modelling of an atmospheric pressure, loop - type SCF reactor, where diesel spray is evaporated due to its interaction with a pre-heated air stream. Experiments presented in this work provide information on the examined reactor's thermal field and are also used for the validation and assessment of the implemented computational approaches. Computations are performed with the implementation of an "in-house" developed CFD code, which incorporates either the Euler - Euler (two - fluid) or the Euler - Lagrange methodology for the description of the flow field developing inside the reactor. In order to account for the thermal yield observed in the examined loop - type SCF reactor and evoked by the exothermal, oxidative reactions associated with the cool flame phenomenon, two different approaches have been followed: (a) a global chemical kinetic oxidation mechanism proposed by Zheng *et al.* (2004), consisting of 7 species and 7 global reactions (S7), which is directly linked to the CFD code and computations are performed via the "on-line" Direct Integration (DI) approach, (b) a Look - Up Table (LUT) approach has been developed by incorporating data from a large number of chemical kinetic simulations performed with the use of a semi-detailed mechanism, consisting of 290 reactions and 57 species (S57) (Tao *et al.*, 2004).

COMPUTATIONAL APPROACHES

The 2PHASE CFD Code Fluid Flow Solver

Simulations have been performed with the use of the "in-house" developed CFD code 2PHASE, which has been previously validated over a wide range of applications involving two-phase, multi-component and reactive flows (Founti and Klipfel, 1998; Katsourinis and Founti, 2004; Kolaitis and Founti, 2003) and utilizing either the Euler-Euler or the Euler-Lagrange methodology. In this work, both methodologies are incorporated in order to assist the understanding of the physical and chemical phenomena emerging inside the examined atmospheric pressure loop - type SCF reactor. An overview of the 2PHASE fluid flow solver is presented by Founti *et al.* (2007).

Computational Modeling Of Low Temperature Diesel Oxidation Phenomena (Cool Flames NTC Region)

Comprehensive kinetic mechanisms, describing hydrocarbon fuel auto ignition phenomena, usually consist of hundreds of species and thousands of chemical reactions. As a result their direct implementation in CFD codes is practically impossible due to the obvious computational cost limitations. To overcome this problem efforts are focused on systematically "reducing" available detailed kinetic schemes, in order to propose simpler and more flexible mechanisms with the ability to: (a) retain

and reproduce the essential chemical information for specified temperature, pressure and residence time conditions and (b) be incorporated and directly integrated in a CFD code, ensuring low computational cost. Thorough reviews of the available kinetic models reduction methodologies, as well as the existing reduced and detailed mechanisms can be found in the literature (Griffiths, 1995; Simmie, 2003).

It should be noted though, that the detailed description of diesel fuel oxidation chemical kinetics is still an open question. It is common practice to use n-heptane as a "simulant" fuel for Diesel oil in cases of auto ignition modelling, since the cetane numbers of both fuels are very close (Montgomery *et al.*, 2002). N-heptane is also favoured because it is among the largest chain hydrocarbon fuels for which detailed and accurate chemical mechanisms have been developed. The latter can be used as a template for the development of reduced chemical kinetic schemes.

The "Direct Integration" (DI) Approach

Global mechanisms (which utilize global reactions to minimize the reaction set) consist of less than ten (fictitious/real) species and global reactions (Halstead *et al.*, 1977; Schreiber *et al.*, 1994). Following a comparative assessment in a case of an atmospheric pressure, plug-flow SCF reactor (Chatzopoulou *et al.*, 2007), the 7 - step model (S7) of Zheng *et al.* (2004) has been selected to provide information on the fuel's oxidation characteristics in the examined case, via the direct integration approach (Katsourinis and Founti, 2008). The S7 model comprises of seven global reactions and seven active species. In order to take into account the effect of the low temperature chemical oxidation phenomena associated with the SCF phenomenon in the flow and thermal field developing inside the examined reactor, the system of energy and concentration conservation ordinary differential equations, resulting from the S7 scheme, is solved using an adaptation of the DVODE (Variable Coefficient Ordinary Differential Equations solver) integration package (Brown *et al.*, 1989), which is linked to the 2PHASE CFD code. Therefore a coupled solver has been developed, which implements the following procedure. The fluid flow solver calculates values of the characteristic controlling variables (temperature, species concentrations, residence time) at each computational cell. The ODE solver uses these values as inlet conditions for the integration of reaction rates, heat release rates, fuel consumption and intermediate species formation concentration rates, whose differential equations are provided by the implemented mechanisms. The resulting calculations form the necessary source / sink terms which are added in the energy and species conservation equations of the fluid flow solver to account for the effect of the occurring chemical reactions in the SCF reactor. This procedure is repeated at each iteration step of the fluid flow solver and for each computational cell and hence the influence of the chemical reactions as described by the implemented mechanisms is "directly integrated" in the computational tool. It should be noted that in this work, computations performed via the DI approach, implement the Euler-Euler concept for the description of the two-phase flow field developing inside the examined SCF reactor.

The “Look-Up Table” (LUT) Approach

In principle, global schemes demonstrating a small number of species and reactions and emerging from the implementation of systematic reduction methods, are reliable and can be utilized as substitutes of detailed mechanisms in reactive cases where the incorporation of CFD computations is necessary. However, due to their simplicity and lack of detailed description of the occurring chemical phenomena, their accuracy is questionable and must be assessed. Hence it is important to establish alternative approaches with the scope of “indirectly” linking detailed or semi-detailed chemical kinetic schemes in a CFD code. In this work, a tabulation method linking a semi-detailed chemical kinetic to the 2PHASE code, has been adopted as an alternative approach to the DI and thus avoiding this high computational burden. Following a comparative assessment of a variety of n-heptane oxidation kinetic mechanisms in low pressure Jet-Stirred Flow and Plug-Flow reactors (Kolaitis and Founti, 2009), a semi-detailed model developed at the Chalmers University of Technology, involving 57 species and 290 reactions (Tao et al, 2004) was selected for the look-up table (LUT) generation, an approach initially described by Kolaitis and Founti (2006). This mechanism is practically a reduced version of the detailed kinetic scheme of Lawrence Livermore National Laboratories (Curran *et al.*, 1998), consisting of 544 species and 2446 reactions and is accurate exhibiting, at the same time, low computational cost. More specifically, the kinetic mechanism was used to generate a “look-up table” (LUT) by performing a multitude of PSR simulations, in which the three major operational parameters, namely the reactor inlet temperature, the inlet fuel concentration (expressed via the lambda factor value) and the residence time, are varied. The range of variation for each parameter corresponded to experimentally determined typical values, occurring in SCF reactors. More specifically, inlet temperature values extended from 550K to 820K, lambda factor values ranged from 0.2 to 1.4 and residence time values spanned 0.001 - 0.2s, thus leading to a final database matrix consisting of 11648 elements. For each triplet combination, values for both volumetric heat release rate, as well as fuel consumption rate were computed and stored. Cool flame heat release rates calculated by the developed cool flame models are introduced to the CFD code as local heat “source” terms; the respective values for the fuel consumption rates, obtained by the LUT model, are introduced as fuel species “sink” terms.

In this work, computations performed via the LUT approach, implement the Euler-Lagrange methodology for the description of the two-phase flow field developing inside the examined SCF reactor.

LOOP TYPE SCF REACTOR SET UP

The experiments have been conducted in the Laboratory of Heterogeneous Mixtures and Combustion Systems of the National Technical University of Athens. An experimental, atmospheric pressure SCF loop-type reactor (Figure 1) with in-built recirculation zones, which has been designed, constructed and operated at the EST laboratory of RWTH-Aachen, has been used. Its concept is based on an axisymmetric cylindrical metal configuration with insulated walls. Two concentric cylinders form the main body of the reactor. A commercial pressure atomizer is fixed at the centre of the

cylindrical cross-section disc, located at the upstream plane of the reactor, and injects the liquid fuel into it. A centrally located bluff body (recirculation disc) is used downstream the atomizer forcing the mainstream gas mixture to recirculate between the inner (recirculation tube) and outer cylinders, ensuring complete oxidation of the liquid fuel and aiming to stabilize the phenomenon. The external cylinder’s diameter gradually decreases downstream the bluff body in order to create recirculation zones, increase velocities and thus produce a more homogeneous gas mixture at the outlet of the reactor. The preheated air supply to the reactor causes the evaporation of the liquid fuel spray and also plays the role of the oxidative means for the chemical reactions associated with the cool flame phenomenon to occur. It is supplied radially, from a rectangular cross-sectioned side port placed at the inlet of the reactor, but enters the main body of the reactor (liquid evaporation – cool flame region) axially, through eight peripheral holes of the same diameter. These holes are located symmetrically around the liquid fuel’s inlet, to ensure that the spray injected from the nozzle is uniformly mixed and thus evaporated. Detailed measurements of the gas mixture temperature inside the SCF reactor are obtained with the use of one retractable thermocouple (Therm1).

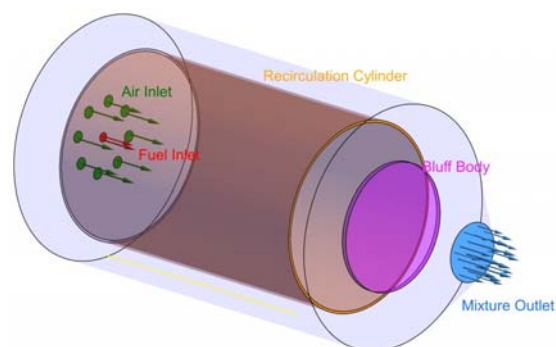


Figure 1: General layout of the SCF loop type reactor and the measuring range of the utilized thermocouple.

The thermocouple is capable of moving at distances between $x=0\text{m}$ and $x=0.11\text{m}$ downstream the reactor’s inlet, along the extended recirculation zone developed between the internal and external cylinder walls. Experiments presented in this work are conducted for three different test cases (TC 1-3) corresponding to diesel sprays evaporating in air streams preheated at $T_{in,1}=633\text{K}$, $T_{in,2}=683\text{K}$ and $T_{in,3}=733\text{K}$ respectively. However, due to heat losses at the reactor walls, the air inlet temperature at the main body of the reactor (liquid evaporation – cool flame region) was also experimentally determined. Measurements showed that the preheated air stream enters the main body of the reactor with $T_{in,1}=620.47\text{K}$, $T_{in,2}=664.12\text{K}$ and $T_{in,3}=708.3\text{K}$, for Test Cases 1-3, respectively. These values have been used as air inlet temperatures for the presented computations. In the examined cases the air to fuel ratio as expressed by the lambda factor is kept constant at $\lambda = 1.2$, while the total power was 9.2kW.

RESULTS

For both kinetic simulation approaches (DI/LUT) the computational domain constitutes the main body of the

reactor, where the examined mass transfer (droplet evaporation) and reactive (cool flame reactions) phenomena occur. It measures 0.21m axially by 0.05m radially and is discretized using 421x103 non-uniform, cylindrically axisymmetric, rectangular grid nodes. The grid is refined close to the nozzle tip to improve local flow resolution. The mean mass loading of the flow is calculated to be 14.1%. Initial droplet velocities and volume fractions at the nozzle injection plane are obtained by extrapolating experimental measurements available by Sommerfeld and Qiu (1998), for a Simplex pressure atomizer, similar to the one used in the experiments. Inlet velocities of the carrier fluid are calculated by splitting the total air-volumetric flow rate over the total surface of the eight peripheral holes. It should be noted though, that in the particular case of the DI approach where the Euler-Euler concept is implemented, liquid droplets are considered to be mono dispersed with a mean droplet size diameter of 25 μ m. In all examined cases, the reactor wall temperatures were set constant and equal to the respective preheated air stream inlet temperatures.

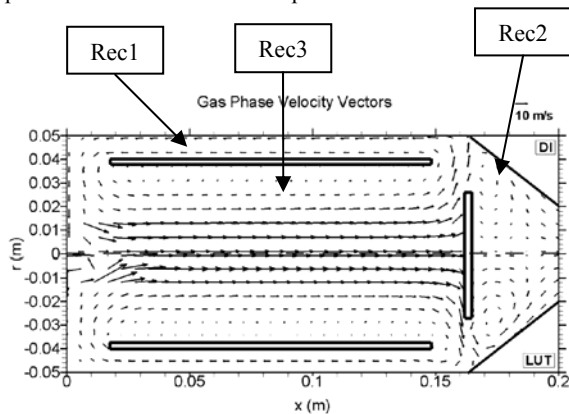


Figure 2: Predicted gas phase velocity vector plot throughout the simulated geometry (DI / LUT approach).

Figure 2 gives an overview of the simulated flow field by presenting predicted air velocity vectors for TC 3, when implementing both DI and LUT approaches. It is evident that the presence of the recirculation tube and the bluff body, force a certain portion of the flowing gas mixture to recirculate. The extended recirculation zone (Rec1) as well as the ones observed downstream and upstream the re-circulation disc (Rec2 / Rec3) play an important role in achieving better mixing between the air and fuel (liquid-vapour) streams. The extended recirculation zones evidently increase mixture residence times inside the reactor and thus control reaction and heat release rates associated with the SCF phenomenon. This results in the production of a more homogeneous gas mixture at the outlet of the reactor. Higher values of air velocity are computed downstream the nozzle and along the symmetry axis and this can be attributed to the characteristics of the inlet-air geometry, comprising a row of eight peripheral holes with very small diameter (5mm each) as well as to the interaction with the high velocity droplet spray injected from the central nozzle. It is evident that both implemented approaches (DI / LUT) succeed in capturing the basic characteristics of the flow field developing inside the loop-type reactor.

In Figure 3, predicted fuel vapour mass fraction contours are presented throughout the simulated geometry for TC 3. Fuel vapour concentration values demonstrate a gradual

increase in regions close the nozzle, owing to the mass transfer phenomena (evaporation), occurring between the preheated air stream and the injected liquid fuel. This increase is restricted downstream the reactor, due to the initiation of the exothermal low temperature oxidative reactions (owing to the cool flame phenomenon), occurring between fuel vapour and the preheated air stream and resulting in the fuel's partial consumption. It is shown that the stochastic nature of the Euler-Lagrange concept leads to higher gradients of fuel vapour mass fraction values in Rec1 and Rec3 when the LUT approach is implemented. Respective predictions obtained by the DI approach (incorporating the Euler-Euler concept) do not exhibit a similar trend in these regions. It should be noted though, that in the reactor's outlet both approaches predict a uniform distribution of fuel vapour mass fraction values, indicating that a homogeneous gas mixture is formed.

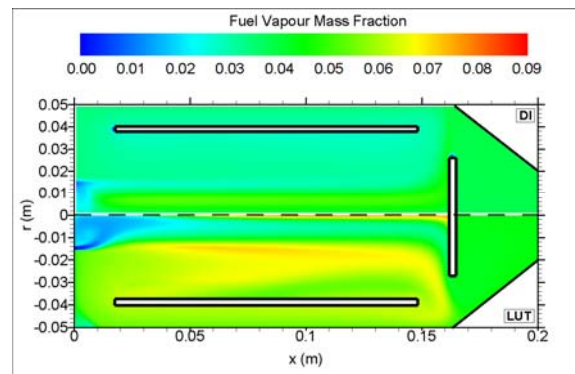


Figure 3: Predicted fuel vapour mass fraction values throughout the simulated geometry for TC 3 (DI / LUT approach).

Computations implementing both approaches (DI / LUT) result to the predicted gas mixture temperatures shown in Figure 4, for TC3. In principle, the spatial evolution of the gas phase temperatures depends mainly on the two main phenomena occurring inside the examined reactor, namely droplet evaporation and low temperature oxidation (cool flame reactions and NTC region). In the upstream region and close to the symmetry axis, droplet evaporation is the dominant phenomenon and predictions yield temperature values lower than 708.3K, which corresponds to the air inlet temperature value.

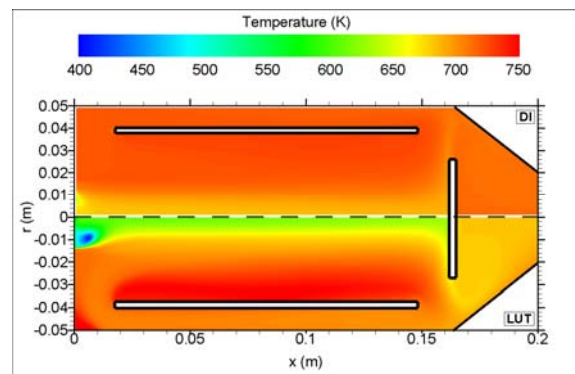


Figure 4: Predicted gas mixture temperatures (K) throughout the simulated geometry for TC 3 (DI / LUT approach).

It should be noted though, that in regions close to the nozzle and along the reactor's symmetry axis, predictions emerging from the implementation of the DI approach, demonstrate an over-prediction of the gas mixture temperatures, compared to the respective LUT predictions. Simulations using the DI approach show that in this region, predicted gas mixture temperatures reach values close to 650K, while the respective computations in this region using the LUT do not surpass 620 K. This discrepancy can be attributed to the behaviour of the fluid flow solver that has been utilized for each implemented approach and not on the chemical kinetic approach. It has been shown (Founti *et al*, 2007) that the Euler - Lagrange methodology tends to significantly under-predict measured gas mixture temperature values in regions close to the nozzle. Hence the DI approach implementing the Euler-Euler concept over-estimates temperature values when compared to the respective Euler-Lagrange computations. It should be noted that due to the low temperatures computed in this region by the Euler-Lagrange methodology (between 580K and 620K) the LUT approach is not activated (predicted heat release rates are significantly small). An increase in air temperatures, associated with the exothermal "cool flame" reactions, is achieved throughout the rest of the reactor's geometry. However, it should be noted that in TC3, predicted temperatures are not significantly higher than the air preheated temperature ($T_{in,3}=708.3$ K) due to the emergence of the NTC region. When the DI approach is incorporated, the highest air temperature values (approximately 725K) are predicted in regions close to the internal cylinder and the bluff body, where recirculation zones occur (Rec1, Rec2) and higher residence times for the gas mixture inside the reactor are computed. When the LUT approach is incorporated, peak air temperature values are predicted (approximately 750K) in the recirculation zone (Rec2) which is located upstream the recirculation disc, as well as in the upper part of the reactor, in the section between the outer cylinder and the reactor's inlet walls. In the reactor's outlet, computations utilizing the DI approach lead to higher temperature values than the respective predictions emerging from the LUT suggest. Overall, it is demonstrated that the LUT approach results to higher local temperatures. In order to assess the observed discrepancies between predictions of both implemented approaches and make a thorough analysis of their predictive capabilities, it is necessary to compare computational results, with the available experimental data.

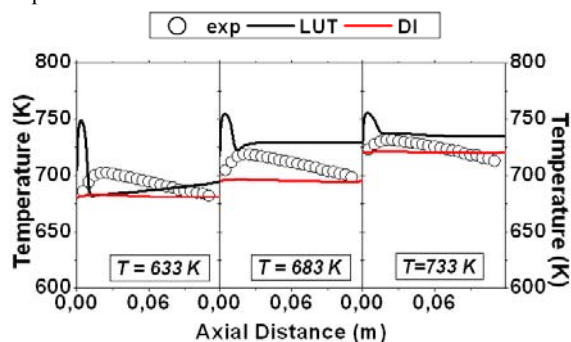


Figure 5: Gas mixture temperature axial profiles along the main re-circulation zone (Rec1) for TC 1–3. (DI / LUT approach).

Figure 5 presents measured and predicted gas mixture temperature distributions along the main recirculation region (Rec1) of the examined reactor, for all examined test cases (TC 1-3). The measurements suggest that temperature tends to increase up to $x=0.02$ m downstream the entrance of the flow and then decreases, however these variations are not significant (approximately 25K). Gas mixture temperatures in this region are mainly influenced by temperatures of both outer and inner cylinder walls, as well as the amount of heat released due to the reactivity of the air / fuel vapour gas mixture. It is demonstrated that the gradual increase of the air preheated temperature from 633K to 733K (TC1 to TC3), results in a respective increase of temperature values along Rec1. However, in TC3 the relative temperature increase is hindered due to the emergence of the NTC region.

Predictions obtained by the DI approach show that calculated temperatures tend to be lower than the respective measurements along Rec1, except from TC 3 where a good agreement between experimental data and computational results is found. On the contrary, predictions obtained by the LUT approach show that calculated temperatures along Rec1, tend to be higher than the respective measurements, for all examined Test Cases. The computed gas mixture temperature values do not significantly vary, with the exception of a noticeable temperature peak value (of approximately 750 K) predicted by the LUT approach for $x < 0.2$ m, for all examined Test Cases.

The overall agreement between measurements and computational results obtained by both approaches can be considered to be satisfactory, for all examined Test Cases, however some discrepancies are observed. These discrepancies can be associated with: (a) the assumption of constant wall temperatures that has been applied in the present computations, (b) the substitution of the complex Diesel oil multi-component mixture flowing inside the reactor by *n*-heptane and (c) inaccuracies in the assumed boundary conditions, mainly for the gas and droplet inlet velocities. Further work is needed towards that direction.

Discrepancies are also observed in Rec1 between predictions obtained by the DI approach and the respective ones emerging with the implementation of the LUT approach. These discrepancies can be attributed to the ability of the incorporated chemical kinetic schemes (S7, S57) to accurately describe the low-temperature, atmospheric-pressure oxidation characteristics of *n*-heptane. In regions near the reactor's outlet and Rec1, where the low temperature oxidative reactions play a dominant role in the development of the reactor's thermal field (the gas mixture's residence time values are increased) the performance of each implemented CFD approach is highly depended on the behaviour of the incorporated scheme. Given the fact that the majority of the available reduced or detailed mechanisms have been developed for internal combustion engine conditions, it is very difficult to find mechanisms with the ability of accurately capturing heat release rates in the low pressure, low temperature conditions of the examined system.

CONCLUSION

In this work, two alternative methodologies based on the implementation of an "in-house" developed CFD code are assessed, with respect to capturing the basic flow and

thermal characteristics of diesel spray applications evaporating in “Stabilized Cool Flame” (SCF) environments. The Direct Integration (DI) approach utilizes the Euler-Euler concept to account for the description of the flow field developing inside the examined reactor. A global *n*-heptane oxidation mechanism comprising 7 species has been directly linked to the CFD code, in order to compute the effect of the occurring low temperature oxidation phenomena in the reactor’s thermal field. The Look-Up Table (LUT) approach utilizes the Euler-Lagrange concept to account for the description of the flow field developing inside the examined reactor. A semi-detailed mechanism, consisting of 57 species (S57) has been indirectly linked to the CFD code, via an “off-line” chemical simulation storage and retrieval technique. Both implemented approaches succeed in capturing the basic physical and chemical phenomena occurring in an atmospheric pressure loop type (SCF) reactor. Computational results obtained by both approaches are compared with available temperature measurements along the reactor’s main recirculation region and the overall agreement is satisfactory. Discussion is focused on the specific conceptual characteristics of each implemented approach, with respect to improving their predictive capabilities.

REFERENCES

- BELARDINI, P., BERTOLI, C., BEATRICE, C., D’ANNA, A. and DELGIACOMO N., (1996), “Application of a reduced kinetic model for soot formation and burnout in three – dimensional Diesel Combustion Computations”, *Proceedings of the Combustion Institute*, **26**, 2517-2524.
- BROWN, P. N., BYRNE, G. D. and HINDMARSH, A. C., (1989), “VODE: A variable coefficient ODE solver”, *SIAM J. Sci. Stat. Comput.*, **10**, 1038 – 1051.
- CHATZOPOULOU, M., KATSOURINIS, D., SKEVIS, G. and FOUNTI, M., 2007, “Numerical simulation of a cool flame vaporizer: Comparison of lumped and detailed kinetic approaches”, *Proceedings of the European Combustion Meeting 2007*, Chania, Greece, April 11 – 13, Paper 21-10.
- CURRAN, H.J., GAFFURI, P., PITZ, W.J. and Westbrook, C.K., 1998, “A Comprehensive Modeling Study of *n* – Heptane Oxidation” *Combustion and Flame*, **114** (1-2), 149-177.
- FOUNTI, M., KATSOURINIS, D.I. and KOLAITIS, D., (2007), “Turbulent sprays evaporating under “stabilized cool flame” conditions: Assessment of two CFD approaches”, *Numerical Heat Transfer, Part B: Fundamentals Journal*, **52**(1), 51-68.
- FOUNTI, M. and KLIPFEL A., (1998), “Experimental and computational investigations of nearly dense two – phase sudden expansion flows”, *Experimental Thermal and Fluid Science*, **17**, 27-36.
- GRAY, B.G. and FELTON, P.G., (1974), “Low-Temperature Oxidation in a Stirred-Flow Reactor-I. Propane”, *Combustion and Flame*, **23**, 295-304.
- GRIFFITHS, J.F., (1995), “Reduced kinetic models and their application to practical combustion systems”, *Progress in Energy and Combustion Science*, **21** (1), 25-107.
- HALSTEAD, M., KIRSCH, L. and QUINN, CP., (1977), “The auto ignition of hydrocarbon fuels at high temperatures and pressures – Fitting of a mathematical model”, *Combustion and Flame*, **60**, 30-45.
- HARRISON, A.J. and CAIRNIE, L.R., (1988), “The Development and Experimental Validation of a Mathematical Model for Predicting Hot-Surface Autoignition Hazards Using Complex Chemistry”, *Combustion and Flame*, **71**, 1-21.
- KATSOURINIS, D.I. and FOUNTI M.A., (2004), “Introducing a two – fluid approach for the modelling of “Stabilized Cool - Flame” Phenomena”, *Proceedings of the 19th Annual Conference on Liquid Atomization and Spray Systems*, 148-153, Nottingham, UK.
- KATSOURINIS, D.I. and FOUNTI M.A., (2008), “CFD modeling of a ‘stabilized cool – flame’ reactor with reduced mechanisms and a direct integration approach”, *Chemical Engineering Science*, **63** (2), 424-433.
- KOLAITIS, D.I. and FOUNTI M.A., (2003), “Scrutinizing Evaporation Models for Computational Modelling of Turbulent Sprays”, *Proceedings of the 9th International Conference on Liquid Atomization and Spray Systems*, Paper 2-18, Sorrento, Italy.
- KOLAITIS, D.I. and FOUNTI M.A., (2006), “A Tabulated Chemistry Approach for Numerical Modeling Of Diesel Spray Evaporation in a “Stabilized Cool Flame” Environment”, *Combustion and Flame*, **145**(1-2), 259-271.
- KOLAITIS, D.I. and FOUNTI M.A., (2009), “On the Assumption of Using *n* – Heptane as a “Surrogate Fuel” for the Description of the Cool Flame Oxidation of Diesel Oil”, *Proceedings of the Combustion Institute*, **32**, 3197-3205.
- LIGNOLA P.G. and REVERCHON, E., (1987), “Cool Flames”, *Prog. Energy Combust. Science*, **13**, 75-96.
- LUCKA K. and KOEHNE, H., (1999), “Usage of cold flames for the evaporation of liquid fuels”, *Proc. 5th Int. Conf. On Technologies and Combustion For A Clean Environment*, Lisbon, Portugal, **1**, 207-213.
- MONTGOMERY, C.J., CREMER, M.A., CHEN, J.Y., WESTBROOK, C.K. and MAURICE, L.Q., (2002), “Reduced chemical kinetic mechanisms for hydrocarbon fuels”, *Journal of Propulsion and Power*, **18** (1), 192-198.
- NAIDJA, A., KRISHNA, C.R., BUTCHER, T. and MAHAJAN, D., (2003), “Cool flame partial oxidation and its role in combustion and reforming of fuels for fuel cell systems”, *Prog. Energy Combust. Science*, **29**, 155-191.
- SCHREIBER, M., SADAT SAKAK, A., LINGENS, A. and GRIFFITHS, J. F., (1994), “A reduced thermokinetic model for the auto ignition of fuels with variable octane ratings”, *Proceedings of the Combustion Institute*, **25**, 933 – 940.
- SHEINSON, R.S. and WILLIAMS, F.W., (1973), “Chemiluminescence Spectra from Cool and Blue Flames: Electronically Excited Formaldehyde”, *Combustion and Flame*, **21**, 221-230.
- SIMMIE, J.M., (2003), “Detailed chemical kinetic models for the combustion of hydrocarbon fuels”, *Prog. Energy Combust. Science*, **29** (6), 599-634.
- SOMMERFELD, M., QIU, H., (1988), “Experimental studies of spray evaporation in turbulent flow”, *Int. J. Heat Fluid Flow*, **19** (1), 10-22.
- STEINBACH, N., (2002), “Untersuchungen zum Zuendverhalten von Heizöl EL-Luft-Gemischen unter atmosphärischem Druck”, *Ph.D. Thesis*, RWTH-Aachen, Aachen, Germany.

TAO, F., GOLOVITCHEV, V.I. and CHOMIAK, J., (2000), "Self - ignition and early combustion process of n – heptane sprays under diluted air conditions: numerical studies based on detailed chemistry", *SAE Transactions, Society of Automotive Engineers*, Paper 2000-01-2931.

TAO, F., GOLOVITCHEV, V.I. and CHOMIAK, J., (2004), "A Phenomenological Model for the Prediction of Soot Formation in Diesel Spray Combustion", *Combustion and Flame*, **136(3)**, 270-282