A 3D CFD MODELLING STUDY OF A DIESEL OIL EVAPORATION DEVICE OPERATING IN THE "STABILIZED COOL FLAME" REGIME

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ABSTRACT

In a Diesel oil evaporation device operating in the "Stabilized Cool Flame" (SCF) regime, a thermo-chemically stable low-temperature oxidative environment is developed, thus preventing the mixture from being ignited. In this case, a well-mixed, heated air-fuel vapour gaseous mixture is produced, which can be subsequently fed either to premixed combustion systems or fuel reformer devices for fuel cells applications. In this work, the ANSYS CFX 11.0 CFD code is used to simulate the 3-dimensional, turbulent, two-phase, multi-component and reacting flow-field, developed in a Diesel oil "SCF" evaporation device. An innovative modelling approach, based on the fitting parameter concept, has been developed in order to simulate cool flame reactions. The model, based on physico-chemical reasoning coupled with information from available experimental data, is implemented in the CFD code and is validated by comparing numerical predictions to experimental data obtained from an atmospheric pressure, recirculating flow SCF device. Numerical predictions are compared with temperature measurements, achieving satisfactory levels of agreement. The developed numerical tool can effectively support the theoretical study of the physical and chemical phenomena emerging in practical devices of liquid fuel spray evaporation in an SCF environment, as well as the design optimisation process of such innovative devices (Figure 1).

NOMENCLATURE

Ai Model constants
Bi Model constants
Q Cool flame-induced heat release rate (W/m^3)
T Temperature (K)
λ Lambda factor (ratio of the actual air-to-fuel mass ratio over its stoichiometric value)

INTRODUCTION

Liquid fuel atomization, in the form of a spray, is commonly used in a large variety of technical combustion applications such as furnaces and boilers, Internal Combustion Engines (ICE) and gas turbines in order to increase the fuel surface area and thus accelerate 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 may reduce the overall energy utilization 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 recently proposed (Lucka and Koehne, 1999). In this case, the two main phenomena, namely droplet evaporation and fuel combustion, are essentially separated; the liquid fuel is allowed to evaporate (but not to burn) in an open-flowing chamber where low temperature oxidative cool flame reactions occur. The additional heat due to the exothermic reactions enhances droplet evaporation, resulting in the production of a highly homogeneous, heated (though not ignited) mixture of air and fuel vapour. The produced mixture can be either fed into premixed combustion devices, which allow better control over the combustion process, or utilized for reforming the fuel to a hydrogen-rich gas. Ongoing research on SCF mixture preparation suggests that this process may be used as part of a Diesel oil reforming technology for utilization in fuel cell systems (Hartmann et al., 2003).

The present work aims to numerically investigate the interacting physico-chemical phenomena occurring inside a SCF reactor. Toward this end, a commercial Computational Fluid Dynamics (CFD) code is used to simulate the SCF device. In order to model the effects of cool flame reactions on heat and mass transfer, a dedicated semi-empirical correlation is developed to numerically estimate the cool flame heat release rate. The model is based on physico-chemical reasoning coupled with experimental data and chemical kinetics simulations. After being implemented in the CFD code, the proposed model is validated and evaluated by comparing numerical predictions with experimental data obtained in an atmospheric pressure, Diesel spray, SCF reactor.

COOL FLAMES

Overview

Cool flames are essentially a low temperature oxidation process (500-800K) during which the fuel is only partially oxidized. Cool flames are characterized by the appearance of a faint pale bluish light, attributed to the chemiluminescence of excited formaldehyde. Cool flames appear, in the form of a self-quenching temperature and pressure pulse, during the two-stage ignition of hydrocarbon fuels and are associated with the "knocking" phenomenon in ICE. Cool flame reactions occur preferentially under fuel-rich conditions and are generally exothermic in nature, producing modest amounts of heat.

During hydrocarbon fuel autoignition, the operating kinetic mechanisms governing the chemical reactions are

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continuously changing according to the temperature of the air-fuel mixture. As a result, it is possible to define low- and high-temperature mechanisms, in which different oxidising schemes are effective. Cool flames manifest themselves in the range of temperatures where transition between low-temperature and high-temperature mechanisms occurs and are dominated by exothermic degenerately branched chain reactions involving important long-lived intermediate species (Lignola and Reverchon, 1987). Both thermal and kinetic feedback phenomena are important in the temperature region of cool flame emergence. As a result, a competition between termination and branching reactions arises, whenever the former exhibit higher activation energies than the latter (Griffiths, 1995). In this case, a Negative Temperature Coefficient (NTC) region emerges, corresponding to a decrease in the overall reaction rate with increasing temperature.

Stabilized Cool Flames

By exploiting the NTC phenomenon as a chemical "barrier" for autoignition (Gray and Felton, 1974), it is possible to "stabilize" the cool flame reactions in an open flowing system. 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 "conventional" ignition. Experimental evidence suggests that when SCF are realized in an open flowing system, the air-fuel mixture temperature may increase up to 200K in the flow direction and subsequently stabilize at the raised level (Lucka and Koehne, 1999). Only 2-10% of the fuel's available thermal energy is being "consumed" when non-igniting SCF operation is achieved. The occurrence of atmospheric pressure Diesel oil SCF is favoured under fuel-rich conditions in the temperature range of 550-800K (Steinbach, 2002). 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 residue-free 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).

Attention to cool flames has been mainly driven by the fact that they are associated with "knocking" phenomena in spark ignition ICE, therefore most of the respective studies deal with the high-temperature, high-pressure conditions prevailing inside the engine cylinder (Aggarwal, 1998). However, there is a scarcity of information regarding non-igniting SCF, both in terms of experimental investigation and of numerical modelling of the respective phenomena, especially in the frame of a CFD code. The numerical modelling of the complex interacting chemical and momentum-, heat- and mass-transfer phenomena occurring inside a SCF reactor necessitates the use of a dedicated modelling approach.

Stabilized Cool Flame Reactor

An atmospheric pressure, recirculating flow SCF reactor, developed by OWI gGmbH (Aachen, Germany), has been used to validate the developed cool flame model. The reactor consists of a 162.5mm long cylinder with an inner diameter of 102mm, which is attached to a 40 deg. converging nozzle with a 25mm circular outlet (Figure 1). A 54mm diameter metal disk (bluff body) is fixed at the downstream end of the cylindrical part of the reactor, in order to generate the main recirculation zone. To assist the establishment of a steady recirculation region, a "recirculation cylinder" of 80mm diameter is installed upstream the recirculation disk. The recirculation zone assists the reactor's stability, thus allowing extending its operational point to fuel-rich conditions. A water-cooled, 60 deg. hollow cone, Simplex pressure atomizer is used for Diesel oil injection through a central 2mm circular opening, whereas the preheated air-stream enters the reactor through 8 circular holes, with a diameter of 5mm, that are circumferentially positioned at a distance of 15mm from the central axis.

The thermally insulated reactor is equipped with 3 retractable thermocouples that allow recording temperature profiles in various positions inside the reactor. The two thermocouples measuring axial profiles are positioned along the symmetry axis and the main recirculation zone, whereas an additional thermocouple measuring the radial temperature profile is placed 1mm upstream the bluff body (yellow lines in Figure 1).
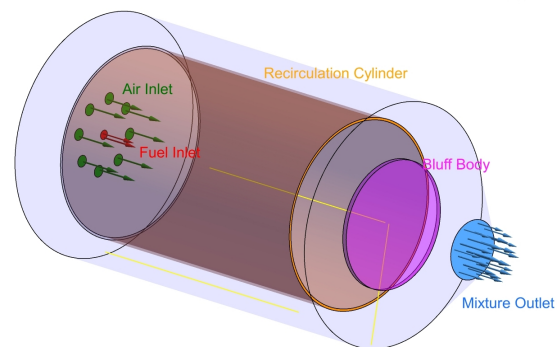
Figure 1: Sketch of SCF reactor and measuring ranges of the thermocouples.

NUMERICAL SIMULATION

The ANSYS CFX Computational Fluid Dynamics Code

The numerical simulations are performed using the ANSYS CFX 11.0 code, which is a general purpose and widely validated CFD software suite. In this study, the code is set to solve the three-dimensional partial differential equations that describe fluid flow, heat transfer and species transport. The flow is assumed to be steady, incompressible, turbulent and multi-component. Thus, the Favre-averaged equations for the conservation of mass, momentum, turbulent energy, species concentration and thermal energy are solved, using a finite control volume method based on a collocated unstructured grid arrangement. The RNG k-ε model is utilized to simulate the turbulent flow (Yakhot et al., 1992). A conjugate heat transfer model is also used to determine heat transfer phenomena in flow regions occupied by heat conducting solids (bluff body, recirculation cylinder).

Modelling of Cool Flame Reactions

In general, cool flames are not taken into account in CFD simulations of turbulent combustion phenomena, with the sole exception of ICE in-cylinder studies, where they are implicitly dealt under the frame of the "ignition delay time" collective modelling (Collin et al., 2005). As a result, in order to simulate a non-igniting SCF reactor utilizing a CFD code, there arises a need to develop an

appropriate model. Cool flames, especially the low-temperature NTC region that is of major importance for the SCF behaviour, are considered to be a kinetically controlled phenomenon characterized by "slow" chemistry (Pilling, 1997). Therefore, multi-step finite-rate chemical reactions have to be taken into account (Kolaitis and Founti, 2009a). Incorporating a detailed chemical kinetics mechanism into a multi-dimensional CFD code is still not a straightforward procedure due to both the excessive computational requirements and the shortage of relevant intermediate species measurements, necessary to serve as validating means (Montgomery et al., 2002). Consequently, an alternative modelling approach is developed, aiming to formulate a simple, dedicated, low computational cost model, capable of describing with sufficient accuracy the main thermo-chemical characteristics of the SCF reactions, being at the same time suitable for incorporation in a CFD code.

The developed model is based on the "parameter fitting" technique (Pilling, 1997), where each individual computational cell is assumed to be an "infinitely fast mixing" Perfectly Stirred Reactor (PSR) with spatially uniform temperature and mixture composition (Kong et al., 2001). A large number of temperature measurements (Steinbach, 2002), obtained in an atmospheric pressure linear SCF reactor under fuel-lean conditions (λ_e=1.27), is utilized in order to determine local heat release rate values, by employing a thermodynamic analysis for the quantification of heat losses. As a result, a 4th order polynomial, Equation (1), is generated by applying a curve-fitting procedure (Founti and Kolaitis, 2005), correlating the experimentally determined cool flame induced volumetric heat release rate Q_e (W/m^3) to the mean temperature (T). The respective polynomial constants (A_i) are given in Table 1.

$$Q_e(T) = \sum_{i=0}^{4} A_i T^i \qquad (1)$$

$$\frac{Q_{CF}(T,\lambda)}{Q_e(T)} = B_0 + B_1 e^{B_2 \lambda} \qquad (2)$$

Literature evidence suggests that an increase in the fuel concentration leads to the intensification of the overall cool flame reaction rate (Dagaut et al., 1995). In order to quantify the effect of fuel concentration, a chemical kinetics mechanism is utilized to formulate a correction factor, correlating the temperature-dependent experimentally obtained values, $Q_e(T)$, with the local fuel concentration (expressed via the lambda factor). Since there are no chemical kinetic schemes available for the "real" Diesel oil fuel, which is essentially a mixture consisting of a plethora of components, it is assumed that its chemical and physical properties can be sufficiently well described by n-heptane (Montgomery et al., 2002). The semi-detailed kinetic mechanism of the Chalmers University (Tao et al., 2004), involving 290 reactions and 57 species, is used to perform a large number of numerical simulations, utilizing the PSR assumption. An exponential decay function is capable of reproducing very well the values obtained by the numerical experiments (Kolaitis and Founti, 2006). The developed correlation, Equation (2), enables the calculation of the local cool flame heat

release rate $Q_{CF}(T,\lambda)$ as a function of both temperature and fuel concentration; the values of the corresponding constants (B_i) are given in Table 1.

Temperature range	598 K – 750 K	750 K – 925 K
A_0	− 7.426822x10^2	+ 9.311440x10^6
A_1	− 1.217922x10^5	− 6.522844x10^3
A_2	+ 4.952730x10^2	− 6.206470x10^1
A_3	− 6.597038x10^{-1}	+ 1.126900x10^{-1}
A_4	+ 2.879051x10^{-4}	− 5.377180x10^{-5}
B_0	0.47154	
B_1	1.37276	
B_2	− 0.76665	

Table 1: Model constants for Equations (1)-(2).

Inlet and Boundary Conditions

The unstructured grid used for the numerical simulations comprises of 2,012,274 tetrahedral elements (Figure 2). This resolution is adequate to ensure grid independence since the flow-field obtained with this grid arrangement does not deviate more than 2% when compared to the one obtained using 2,352,827 elements. The grid is refined close to the solid boundaries in order to improve the local resolution of the developing boundary layers.
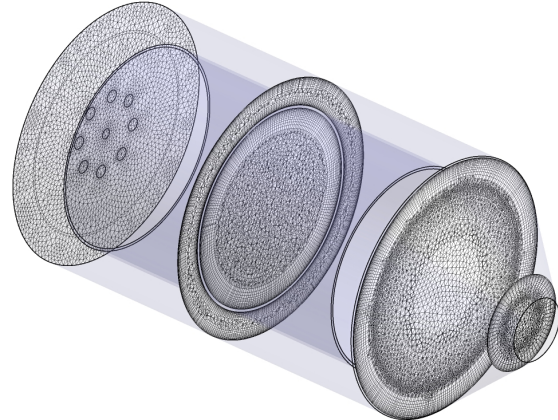
Figure 2: Computational grid distribution.

In order to validate the developed model in a large range of operational conditions, 3 different test cases have been considered (Table 2). All cases correspond, generally, to the same power. Test Case 1 serves as a "basis" for comparison; in Test Case 2 the inlet temperature is raised by almost 100K, whereas in Test Case 3, the air flow rate is decreased by approximately 40%.

Test Case	Volumetric Air Flow	Air Inlet Temperature	Lambda factor	Power
1	10.95 m^3/s	621 K	1.2	9.2 kW
2	11.14 m^3/s	710 K	1.2	9.0 kW
3	6.56 m^3/s	574 K	0.7	9.3 kW

Table 2: Main characteristics of the considered cases.

The preheated air stream is considered to enter the reactor through the 8 circumferentially distributed holes,

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exhibiting a top-hat velocity profile, corresponding to the experimentally determined volumetric flow rate. The reactor's well-insulated outer walls are considered adiabatic; however, for the temperature estimation of both the bluff body and of the recirculation cylinder, conjugate heat transfer is taken into account.

A detailed Euler-Lagrange two-phase simulation is performed using 100,000 computational droplet "parcels" that are injected through the central circular opening. The initial droplet velocity and size distributions are obtained from available PDA measurements in a Simplex pressure atomizer (Sommerfeld and Qiu, 1998), similar to the one used in the considered reactor. The droplets are injected from 10 discrete radial positions that span from 0mm to 9mm from the symmetry axis; a stochastic process is used to determine the actual droplet initial position, velocity and diameter. The mean and rms values for both droplet axial velocity and droplet diameter utilized at the 10 injection points are shown in Figure 3. The droplet injection temperature is assumed to be 393K, according to surface temperature measurements of the water-cooled nozzle.
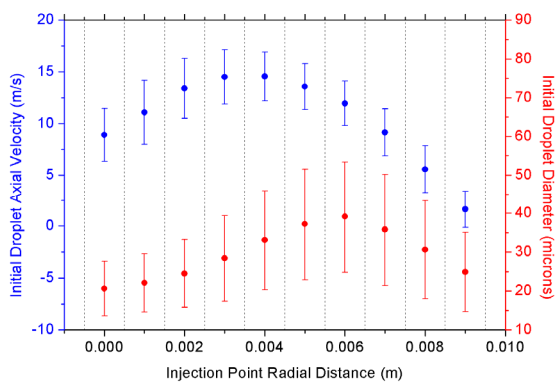
Figure 3: Inlet conditions at the droplet injection points.

RESULTS AND DISCUSSION

The complex two-phase flow-field that develops inside the SCF reactor is evident in Figure 4, which depicts predictions of the gas mixture velocity vectors for Test Case 1.
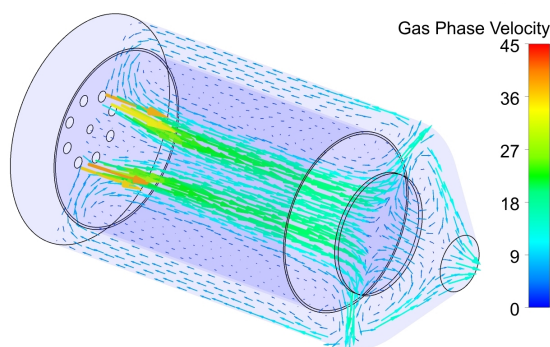
**Figure 4**: Predictions of gas phase velocity vectors.

In the outer zone of the reactor, the main direction of the flow is reversed, due to the existence of the bluff body disk and the recirculation cylinder, thus increasing the mean residence time of the mixture. Also, a strong

recirculation zone appears downstream the bluff body but, due to the converging nozzle, the flow is again fully developed at the reactor's outlet.
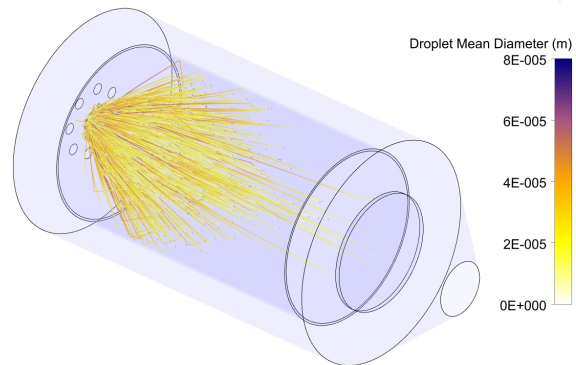
Figure 5: Predictions of droplet trajectories and droplet diameter evolution.

Figure 5 depicts the trajectories of a representative number of "computational" parcels, obtained by the Euler-Lagrange simulation. The trajectories are coloured according to the local mean droplet diameter. A typical hollow cone spray pattern is observed. The large majority of the droplets are completely evaporated close to the injection region. However, despite the high temperature environment, some droplets do not evaporate completely before reaching the inner side of the recirculation cylinder, thus they impinge on it. Almost no droplets manage to reach the bluff body; the developing recirculating fluid-flow structure (c.f. Figure 4) prevents any partially evaporated droplet from reaching the reactor's outlet.
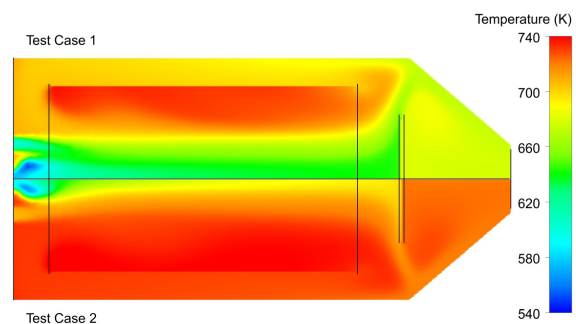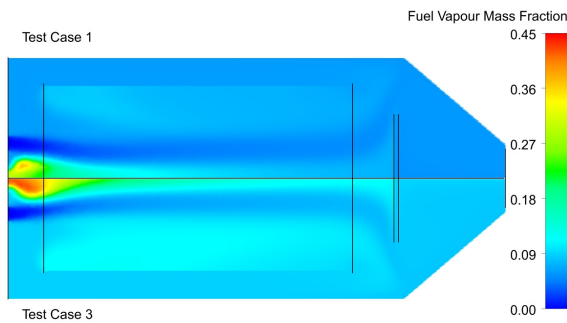

Figure 6: Comparison of predictions of gas temperature.

Temperature predictions for Test Cases 1 and 2 are presented in Figure 6. Higher temperatures are observed in the outer region of the main core of the flow, due to the combined influence of the adjacent recirculation cylinder, which is maintained in high temperature and the low velocity field that contributes in locally "freezing" the flow. In both cases, a homogeneous, heated (yet below ignition temperature) air-fuel vapour mixture is produced at the outlet of the device, which can be subsequently used either in premixed combustion devices or for fuel reforming applications.

Predictions of the Diesel oil's vapour mass fraction, for Test Cases 1 and 3, are shown in Figure 7. It is evident that, due to turbulent mixing and diffusive and convective mass transfer phenomena, the air-vapour mixture becomes

diluted, achieving homogeneous conditions at the reactor's outlet. The higher mean values observed in Test Case 3, correspond to the higher global fuel concentration (c.f. Table 2).

Test Case 1

Test Case 3

Figure 7: Comparison of predictions of Diesel oil vapour mass fraction.

Predictions of the cool flame-induced heat release rate, corresponding to Test Cases 1 and 3, are depicted in Figure 8. In Test Case 1, substantial chemical activity is observed in the main recirculation region, developing in the outer part of the reactor, thus confirming its vital role in the thermo-chemical stability of the developing flow-field. Another region that exhibits high heat release rate values is the recirculation zone that emerges downstream the bluff body. In this region, the multi-component mixture is subjected to intense mixing (c.f. Figure 4), which results in the enhancement of the chemical activity.

Test Case 1
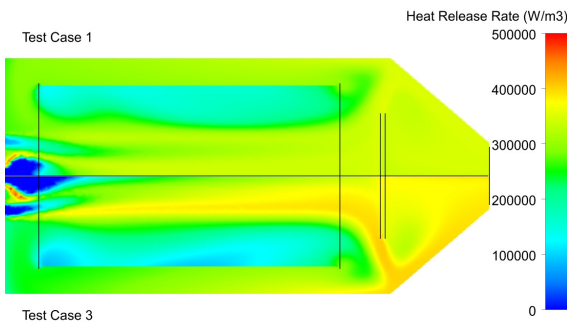
Test Case 3

Figure 8: Comparison of predictions of cool flame heat release rate.

In Test Case 3, higher heat release rate values are observed, since cool flame chemical activity is favoured in fuel-rich conditions (Dagaut et al., 1995). It is evident that, contrary to "conventional" combustion devices where chemical reactions occur mainly in a very "thin" flame zone, cool flame reactivity zones are highly extended and cover a significant part of the device's volume.

Validation of the Results

In Figure 9, temperature predictions along the reactor's symmetry axis ($r = 0mm$) are compared to available experimental data (Kolaitis and Founti, 2009b), for all the considered Test Cases. The thermal field inside the SCF reactor features the following characteristics: downstream the fuel injection plane, the droplets, subjected to the surrounding preheated air environment, promptly evaporate; the emerging fuel vapours sustain the cool flame exothermal reactions, which lead to an increase in the mean temperature. Steady-state operation is achieved since a nearly constant temperature is observed throughout the reactor's core without, however, the mixture being "conventionally" ignited and burnt.

For Test Cases 1 and 2, numerical results are found to under-predict the observed temperature values by 20-30K; a slightly better agreement is achieved in Test Case 3. However, the general trend is, in all cases, qualitatively similar to the experimentally observed trends. The observed discrepancies are associated with the measurement accuracy as well as with simplifications and inaccuracies in the modelling assumptions (e.g. initial conditions).
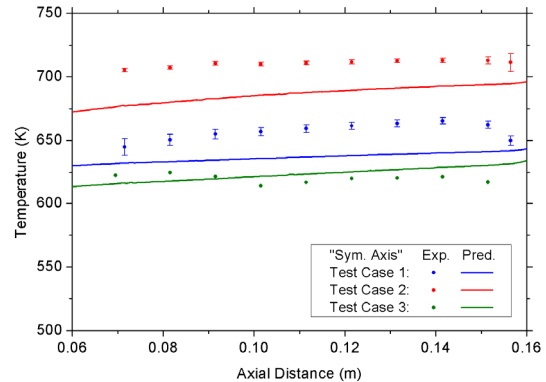

Figure 9: Comparison of predictions with temperature measurements along the symmetry axis.

A similar behaviour is observed in Figure 10, which depicts temperature predictions in the main recirculation region ($r = 46mm$). Predictions qualitatively agree with the measured values; however, only in Test Case 2 there is a very good quantitative agreement. In the other cases, temperatures are generally over-predicted, a fact attributed to the adiabatic boundary conditions utilized for the outer reactor's walls.
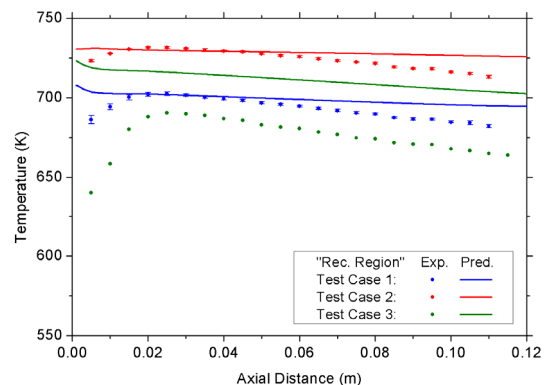
Figure 10: Comparison of predictions with temperature measurements along the main recirculation region.

In Figure 11, predictions are compared to the measured radial temperature profile, 1.0 mm upstream the bluff body disk. Once more, reasonable qualitative and quantitative agreement is observed, given that the mean error does not exceed 25K. In this case, conjugate heat transfer phenomena play an important role since the surface temperature of the bluff body is strongly dependent on the developing thermal field.
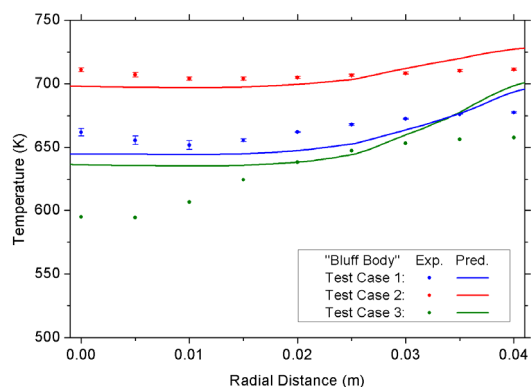
Figure 11: Comparison of numerical results with temperature measurements across the bluff body.

In general, in all cases and all measuring positions, the obtained numerical results lie quite close to the available experimental data, despite the complexity of the occurring physico-chemical phenomena and the simplifying assumptions that were made to formulate the simulation. This observation suggests that the developed tool may be reliably used to support the design process of SCF-assisted Diesel oil evaporation devices.

CONCLUSION

A dedicated modelling approach, based on the "parameter fitting" technique, has been developed and assessed in order to numerically simulate the SCF phenomenon, utilizing a commercial CFD code, in a non-igniting, atmospheric pressure, Diesel oil reactor. The cool flame model has been derived using an algebraic expression deduced from experimental data correlating cool flame heat release rates with temperature. The model has been further improved by utilizing a chemical kinetics mechanism, in order to take into account the effects of fuel concentration variations. The developed model has proved to be particularly convenient for use in the context of a CFD code. Validation tests in a recirculating flow SCF reactor showed that the developed computational model exhibits an encouraging performance, yielding results within a satisfactory level of accuracy. Major flow features and the cool flame-induced heat release characteristics have been well reproduced, thus enabling the utilization of the developed numerical tool for the investigation of the thermal behaviour of SCF reactors, as well as for the support of the design optimization process.

REFERENCES

AGGARWAL S.K., (1998), "A Review of Spray Ignition Phenomena: Present Status and Future Research", *Prog. Energy Combust. Sci.*, **24**, 565-600.

COLIN O., DA CRUZ A. P. and JAY S., (2005), "Detailed chemistry-based auto-ignition model including low temperature phenomena applied to 3-D engine calculations", *Proc. Combustion Institute*, **30**, 2649–2656.

DAGAUT P., REUILLON M. and CATHONNET M., (1995), "Experimental Study of the Oxidation of n-Heptane in a Jet Stirred Reactor from Low to High Temperature and Pressures up to 40 Atm", *Combust. Flame* **101**, 132-140.

FOUNTI M.A. and KOLAITIS D.I., (2005), "Numerical simulation of diesel spray evaporation exploiting the "stabilized cool flame" phenomenon", *Atomization Spray*, **15**, 1-18.

GRAY B.G. and FELTON P.G., (1974), "Low-Temperature Oxidation in a Stirred-Flow Reactor-I. Propane", *Combust. Flame*, **23**, 295-304.

GRIFFITHS J.F., (1995), "Reduced Kinetic Models and their Application to Practical Combustion Systems", *Prog. Energy Combust. Sci.*, **21**, 25-107.

HARTMANN L., LUCKA K. and KOEHNE H., (2003), "Mixture preparation by cool flames for diesel-reforming technologies", *J. Power Sources*, **118**, 286-297.

LIGNOLA P.G. and REVERCHON E., (1987), "Cool Flames", *Prog. Energy Combust. Sci.*, **13**, 75-96.

KOLAITIS D.I. and FOUNTI M.A., (2006), "Numerical modelling of transport phenomena in a diesel spray "stabilized cool flame" vaporizer", *Combust. Sci. Technol.*, **178**, 1087-1115.

KOLAITIS D.I. and FOUNTI M.A., (2009a), "On the assumption of using n-heptane as a ''surrogate fuel" for the description of the cool flame oxidation of diesel oil", *Proc. Combustion Institute*, **32**, 3197-3205.

KOLAITIS D.I. and FOUNTI M.A., (2009b), "Numerical Simulation of Diesel Spray Evaporation in a "Stabilized Cool Flame" Reactor: A Comparative Study", *Flow, Turbulence and Combustion*, **82**, 599-619.

KONG S.C., MARRIOTT C.D., REITZ R.D. and CHRISTENSEN M., (2001), "Modeling and Experiments of HCCI Engine Combustion Using Detailed Chemical Kinetics with Multidimensional CFD", *SAE Proceedings*, Paper No. 2001-01-1026.

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, 207-213, July 12-15.

MONTGOMERY C.J., CREMER M.A., CHEN J.Y., WESTBROOK C.K. and MAURICE L.Q., (2002), "Reduced Chemical Kinetic Mechanisms for Hydrocarbon Fuels", *J. Propul. Power*, **18**, 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. Sci.*, **29**, 155-191.

PILLING M.J. (Ed.), (1997), "Low-Temperature Combustion and Autoignition", Comprehensive Chemical Kinetics, **35**, Elsevier, Amsterdam.

SOMMERFELD M. and QIU H.H., (1998), "Experimental studies of spray evaporation in turbulent flow", *Int. J. Heat Fluid Flow* **19**, 10-22.

STEINBACH N., (2002), "Untersuchungen zum Zuendverhalten von Heizoel EL-Luft-Gemischen unter atmosphaerischem Druck", *Ph.D. Thesis*, RWTH-Aachen, Germany.

TAO F., GOLOVITCHEV V.I. and CHOMIAK J., (2004), "A phenomenological model for the prediction of soot formation in diesel spray combustion", *Combust. Flame*, **136**, 270-282.

YAKHOT V., ORSZAG S.A., THANGAM S., GATSKI T.B. and SPEZIALE C.G., (1992), "Development of turbulence models for shear flows by a double expansion technique", *Phys. Fluids A*, **4**, 1510-1520.