DIESEL SPRAY EVAPORATION MODELLING IN A "COOL FLAME" ENVIRONMENT: A NOVEL APPROACH

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Abstract

An innovative approach for the separation of evaporation from the combustion process can take advantage of the damped "cool flame" phenomenon. To investigate this phenomenon a "cool flame" vaporizer reactor has been numerically simulated using a computational fluid dynamics code. A novel semi-empirical approach is developed, based on experimental data to calculate the heat release due to cool flame phenomena. The model overcomes problems of high computational demand, normally required in the implementation of chemical kinetics models describing low-temperature alkane oxidation. Two test cases are computationally simulated: a "single" spray evaporation case, serving to validate the CFD code, and a "cool flame evaporation" case, used for the development of the "cool flame" model. The good agreement between experiments and predictions confirm the ability of the model to capture reasonably well the general trends observed in the experiments.

Introduction

Oil fired furnaces and boilers, diesel engines and gas turbines utilize liquid fuel sprays in order to increase the fuel surface area and thus accelerate the vaporization and combustion rates. Conventional liquid fuel burning technologies inject the fuel into the combustion chamber through a nozzle that atomises it, producing a spray comprising many droplets, typically the order of a few tens of microns in diameter. The droplets, subjected to the high temperatures of the combustion chamber, are evaporated and burnt in a sequential process. During this procedure, there may arise problems owing to the incomplete mixing of the fuel vapours with the combustion air. The separation of the two phenomena, namely evaporation and combustion, could lead to the alleviation of inhomogenities in the fuel vapour-air mixture. A satisfactory mixing of the gaseous mixture can be thus achieved before initialisation of the combustion process.

A novel way to accomplish such "separation" is to evaporate the fuel with the use of a process based on the "cool flame" phenomenon. The cool flame evaporation is a very promising process that could prove to be more efficient compared to the conventional liquid fuel evaporation methodologies, since it allows the use of premixed combustion technologies, which are known to exhibit a wide range of advantages, like reduction in emissions of soot, NOx, CO and unburned HCs. The scope of the present work is to numerically simulate a "cool flame" vaporizer reactor, using a computational fluid dynamics (CFD) code, in order to acquire more in-depth information about the occurring physical and chemical phenomena that are involved in the process. For this purpose a novel semi-empirical approach is developed to computationally simulate the cool flame characteristics.

The "Cool Flame" Phenomenon

The phenomenon described as "cool flame" is essentially a low temperature oxidation process during which the fuel is partially oxidized but not burnt [1] and it is mainly observed during the autoignition process of hydrocarbon fuels. Whenever alkane fuels have to reside partially or fully mixed in an oxidizing atmosphere at high temperatures, ignition can occur in a *multistage* mode, subsequently following completely different schemes of oxidation. At temperatures below 500°C, the complex chemical reactions involved result in a *twostage ignition* process in which "hot" ignition is preceded by a self-quenching temperature pulse referred to as a "cool flame" [2]. During the autoignition process, the operating kinetic mechanisms change continuously according to the temperature of the air-fuel mixture. 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 [1] and are dominated by an exothermic degenerately branched chain reaction involving one or more important long-lived intermediates. In the temperature range of cool flame occurrence, the combustion process develops with a *negative temperature coefficient* of the reaction rate, i.e. the cool flame process is able to self-accelerate and to self-decelerate. This ability is considered to be the main distinguishing property of cool flames, since the homogenous self-quenching ability of an autocatalytic process is a rather unique feature. When an air/n-heptane mixture flows through a heated tube, autoignition occurs at around 500°C. At lower temperatures, in a darkened room, it is possible to discern a pale blue light, which is attributed to the cool-flame reactions. Under specific fluid-flow and temperature conditions, the cool flame phenomenon can be stabilized, converging to a stationery state, without a "hot" flame ignition being observed. In this state, any slight perturbation of the system can be damped by the cool flame reactions, leading to the restoration of the stable, steady state operational condition. Experiments have shown that in this case, the mixture's temperature increases by 10-150K in the flow direction and stabilizes at the raised level, virtually independently of the air/fuel ratio and the type of fuel used [3]. During this process, no ignition occurs in the form of a virtually 100% conversion of the fuel, since only 2-10% of the fuel is consumed. The limitation of the occurring chemical reactions is based on complex fuel-specific mechanisms. In conclusion, the use of the stabilized cool flame technology can lead to a process able to achieve complete and residue-free evaporation of liquid hydrocarbon mixtures.

Description of a Cool Flame Reactor

Two series of experimental datasets from an operational cool flame reactor have been used for the validation of the developed "cool-flame evaporation" computational model. The experiments have been conducted in an experimental cool flame reactor (vaporizer), which has been designed, constructed and operated at the RWTH University of Aachen - EST laboratory [3]. The available data regarded carrier fluid-fuel vapour mixture temperature profiles along the reactor [4].

The EST reactor consists of an insulated metal pipe, 1m long, with an internal diameter of 0.1m, in which a number of radially movable thermocouples are installed. The carrier fluid (air or N_2), after being preheated, is supplied to the reactor through a perforated disk, used to control the flow turbulence level and homogenize the general fluid-flow characteristics. A commercial, water-cooled pressure atomizer is fixed at the centre of the perforated disk, injecting into the reactor diesel EL fuel, preheated at 120°C. The insulated cylindrical wall of the reactor embodies heating elements used to achieve homogeneous thermal boundary conditions along the reactor. A movable, water-cooled quench is placed at the downstream end of the pipe, in order to reduce the mean mixture temperature, so as to avoid any autoignition phenomena that may arise. Two series of experimental datasets were available:

Test case 1: The first dataset pertains to a "simple" evaporation case, where a diesel spray evaporates in a preheated stream of inert medium (N_2). The initial temperature of the stream is 350°C and the walls of the reactor are kept at the same constant temperature. The mechanisms involved in the evaporation procedure are, in this case, purely "physical". The experiments indicate a drop in the carrier fluid temperature downstream the injection plane, which is attributed to the (latent) heat required by the fuel in order to evaporate.

Test case 2: In the second case, the diesel spray is injected in a preheated airstream of the same initial temperature (350°C). The walls of the reactor are again kept at a constant temperature of 350°C. The main feature of the flowfield, observed experimentally, is that at axial positions far downstream the fuel injection plane, an increase in the mean carrier fluid temperature of the order of 100K is observed, without, nevertheless, the mixture being actually burnt. This temperature rise is attributed to the exothermal reactions occurring due to the presence of the "cool flame" phenomena that emerge in this case ("physico-chemical" evaporation process). The "additional" amount of heat released during the process represents roughly 2-5% of the fuel's heating value and intensifies the evaporation process, permitting the shortening of the vaporizer's total length compared to the purely "physical" evaporation case.

Computational Modelling

In order to numerically simulate the spray-injection in a "cool flame" reactor, a modified version of the 2PHASE CFD code, developed in the Laboratory of Heterogeneous Mixtures and Combustion Systems of NTUA, has been used. The code is based on the Eulerian-Lagrangian computational formulation for the continuous and dispersed phases, respectively and has previously been validated in a variety of diverse two-phase flow cases [e.g. 5, 6]. The continuous phase is treated as a steady, incompressible, turbulent flow, which is computed by solving the time-averaged continuity, momentum transfer, energy and species 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 [7]. This model modifies the constants C_µ and C₂ 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 recirculating flows with abrupt area changes [6].

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 flowfield. 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 4th order Runge-Kutta method. The droplet motion equations take account of the drag and the gravitational force. Droplet turbulent dispersion is modelled 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 [8]. 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. In order to improve the accuracy of the droplet massflow rate predictions near the symmetry axis, a "drift correction" term is applied to the turbulent dispersion model, across the transverse direction [9]. The droplet evaporation process is simulated by solving the droplet mass and energy balance differential equations, using the Abramzon and Sirignano model [10], which is a revised form of the "classic" infinite conductivity model, incorporating the effects of Stefan flow on heat and mass transfer. The choice of the evaporation model was based on a comparative evaluation of three different models [11]. The fuel vapour and the gas phase species properties are determined using the well-known "1/3-rule", the standard additive rules for ideal gas and the Wilke mixing rule.

Development of a semi-empirical cool flame model

The developed model aims to predict the gas temperature and fuel vapour concentration fields inside a cool flame reactor. The evaporation rate of a spray in a "cool flame" environment is expected to increase due to the additional heat provided by the exothermic reactions of the cool flame process. Dedicated models are needed in order to estimate this additional amount of heat assisting the evaporation. An extensive literature survey has shown that the modelling of the cool flame phenomenon is usually done in the frame of alkane autoignition behaviour predictions, using detailed or reduced chemical kinetics models [1,12,13]. Such models are generally used to study autoignition of homogeneous and heterogeneous mixtures in situations where transport and geometrical aspects can be simplified to one-dimensional computations. However, incorporating detailed chemistry models into multidimensional, two-phase computations is currently not feasible due to their excessive computational requirements [13]. On the other hand, the incorporation of a reduced kinetics model in the case of a non-igniting cool flame phenomenon would not be a straightforward procedure, due to lack of experimental data for the intermediate species concentrations, necessary to serve as validating means. It should be also stressed here, that there seems to be a lack in the literature with respect to the modelling of the "damped" cool flame phenomenon, in cases that do not lead to autoignition using a chemical kinetics approach in the frame of a CFD code-which is in fact proposed in this work.

The current modelling approach aims to develop a simple, low-cost computational model with wellunderstood range of validity that could predict the additional amount of heat owing to the cool flame, within an acceptable level of accuracy. Bearing that in mind, it was decided to opt for an analytical semi-empirical model, which would assist the effort to acquire a more in-depth comprehension of the physico-chemical phenomena involved in the process, while at the same time it would serve as a "basis" for further development. Towards this end, an algebraic equation, correlating the amount of volumetric heat produced by the exothermal cool flame reactions to the local temperature of the mixture, has been used as a first-level approach. This equation has been produced by the EST laboratory, University of Aachen, utilizing a wealth of temperature profile measurements [3,4] conducted in the cool flame reactor described above. The experiments have been conducted for a variety of initial temperatures of the mixture for a constant value of the mixture's lambda factor - defined as the ratio of the actual air-to-fuel mass ratio over its stoichiometric value - equal to 1.27.

In order to calculate the amount of heat released by the cool flame exothermic reactions per unit volume, a plug-flow reactor analysis has been employed, taking into account the mixture's thermal losses to the reactor's wall [4]. A 5th order polynomial (Eq. 1) was fitted to the experimental data points as depicted in Figure 1.



Figure 1. Temperature dependence of the volumetric thermal power released by the cool flame induced exothermal reactions. *Symbols*: Measurements, *Continuous line*: Polynomial correlation (Eq. 1)

$$Q^* = \{-2.9 \cdot 10^{-4} T^5 + 0.96 \cdot T^4 - 1265 \cdot T^3 + 832228 \cdot T^2 - 2.7 * 10^8 \cdot T + 3.583 \cdot 10^{10}, 598K < T < 733K$$
(1)
$$-0.266 \cdot T^3 + 635.9 \cdot T^2 - 1265 \cdot T^3 - 505411 \cdot T + 1.338 \cdot 10^8, 733K < T < 830K$$

Q represents the volumetric heat released by the cool flame reactions [W/m³], while *T* corresponds to the mean mixture temperature [K]. From the form of the correlation curve, it is evident that there exists a regime of *negative temperature coefficient*, spanning from approximately 400°C to 460°C, which is an indispensable characteristic of the cool flame phenomenon [1,12].

It is known [13] that the main operational parameters affecting the cool flame phenomenon are pressure, temperature and the fuel-air mixture fraction. The experiments used here [3], were conducted under atmospheric pressure conditions and no data were available for different pressure levels. Therefore, for the modelling purposes, the amount of heat released by the exothermic cool flame reactions was assumed to depend mainly on the mixture's temperature and the local fuel concentration, expressed via the lambda factor.

In addition and in order to take into account the effect of the variation of the fuel concentration, a correction factor has been introduced to the original correlation which was deduced based on the case of a constant lambda factor, equal to 1.27. Various reports in the literature [13,14] suggest that the overall cool flame reaction rate, and subsequently the amount of heat released, seem to intensify when the fuel's total concentration is increased. Nevertheless, there are no consistent correlations available that quantify this phenomenon. As a result, the correction factor applied to the original correlation was based mainly on the widely applied "inverse proportional" principle. The adopted relation that links the experimentally determined value of $Q^*(T)$ with the "corrected" one, $Q(T,\lambda)$, is shown in Eq. 2. Starred quantities refer to the experimental values, λ is the mixture's lambda factor and α is an empirical correction factor, used to calibrate the correction term.

$$Q(T,\lambda) = \frac{\lambda^*}{\lambda} \left(1 + \frac{|\lambda - \lambda^*|}{\lambda - \lambda^*} \alpha^2 Q^*(T) \right)$$
⁽²⁾

The r.h.s. first term of Eq. 2 is the ratio of the experimental lambda factor ($\lambda^*=1.27$) over its actual value, enabling the model to describe the increase of the heat release rate with decreasing lambda values. The second term in the r.h.s. is an "under-relaxation" term, which smoothes out the rather "crude" inverse proportional approach of the first term and enables calibration of the model, by altering the value of the correction factor α .

In order to introduce the "cool flame" model to the CFD code, the computational domain was divided in radial "slices" (each "slice" corresponding to an axial computational node) and the mean temperature for each slice was calculated. A volumetric heat "source" term was then determined by implementing the mean "slice" temperature into Eq. 1. This additional "source" term was subsequently distributed in every computational cell of the considered "slice", using the volume of each cell as a weighting factor. The calculated additional heat "source" terms were then implemented in the fluid thermal energy transport equation together with the heat "sink" terms associated to the droplets' latent heat of evaporation. It was found that after some initial numerical fluctuations the two-phase coupling procedure converged to a rather steady state.

Results

Spray Evaporation in an Inert Atmosphere

The computational domain, measuring 1m axially by 0.05m radially, is discretized using 143*52 nonuniform, 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 6.1%. The initial droplet velocities and size distribution at the nozzle injection plane are obtained by interpolating experimental measurements available for a Simplex pressure atomizer [15], similar to the one used in the experiments. Inlet velocities of the carrier fluid are approximated assuming a top-hat profile. A total number of 30 000 droplet "parcels" is injected and tracked throughout the flowfield, for 15 two-way coupling iteration cycles.

In Figure 2 measured and predicted nitrogen-fuel vapour mixture temperatures along the reactor for 4 positions in the radial direction are depicted. All the main features of the reactor's temperature field, especially in the spray core region, where a steep temperature drop exists, are properly captured. However, the axial evolution of the mixture temperature is slightly overpredicted for the outermost radial positions (r=20mm-30mm). Sources of discrepancies between experiments and predictions may be (a) errors associated with the followed measurement technique [4] (since liquid droplets may still be present near the nozzle, affecting measurement accuracy), (b) inaccuracies in the assumed boundary conditions, mainly for the gas and droplet inlet velocities and (c) the considered "pure-liquid" approach for the calculation of the thermodynamic properties of the actually multicomponent mixture of Diesel oil - spray evaporation characteristics are strongly influenced by the liquid fuel properties [10,11,13]. Nevertheless, an overall satisfactory agreement between numerical

predictions and measurements is achieved, rendering the developed CFD code a valuable tool that can be reliably used for the modelling of dilute evaporating sprays.



Figure 2. Nitrogen-fuel vapour mixture temperature axial profiles along 4 radial positions. Symbols: Measurements, Continuous Line: Predictions.

Spray Evaporation in a "Cool Flame" Environment

The grid, boundary and initial conditions used for this case are the same with the respective ones used in the previous test case, except that here the carrier fluid is air instead of N_2 . In order to demonstrate the necessity of using a "cool flame" model, at first predictions have been performed using no such model, thus simulating "physically-controlled" evaporation conditions. By inspection of Figure 3 (dotted line), it is evident that "physical" evaporation is unable to adequately describe the temperature field inside the reactor, since it does not take into account the "source" heat terms attributed to the cool flame reactions. Consequently, while the experimental data suggest that downstream the reactor a rather uniform temperature of 460°C is achieved, the "physical" evaporation predictions yield downstream temperatures with values lower than 350°C, corresponding to the air temperature at the inlet plane, since in this case only the latent heat "sink" terms are considered.

In the second attempt, the polynomial correlation (Eq. 1) has been implemented and the computational predictions using the described procedure are depicted in Figure 3 (dashed line). It is obvious that the inclusion of the polynomial correlation that accounts for the heat release due to the "cool flame" exothermic reactions, yields much more reasonable results compared to the "physical" evaporation" predictions. The empirical model reproduces well one of the main features of the experimental data, which is the increase of the downstream temperature at levels well above the inlet value of 350° C. In fact, the model predictions of the temperature at the outlet of the reactor (x=0.9m) lie quite near the experimentally measured values, whereas the model seems to fail to follow the observed temperature increase rate.



Figure 3. Air-fuel vapour mixture temperature axial profiles along 4 radial positions. *Symbols*: Measurements, *Continuous line*: Predictions using Eq. (2), *Dashed line*: Predictions using Eq. (1), *Dotted line*: Predictions without "cool flame" model (physically-controlled evaporation).

Finally, predictions after the implementation of the proposed corrected correlation (Eq. 2), using a correction factor value of α =0.2, are depicted in Figure 3 (continuous line). It is evident that Eq. (2) represents a clear improvement over the original polynomial correlation, since in this case the predictions agree reasonably well with the experimental data, being able to describe accurately the establishment of a downstream steady-state temperature. Although there appear some discrepancies in the value of the mixture temperature at the exit of the reactor, overall agreement is quite satisfactory, confirming that the model is able to capture quite well the general trends observed in the experiments. The evident improvement of the model predictions with the inclusion of the correction factor, suggests that the cool flame exothermic reactions heat release does not depend only on the mixture's temperature. The local fuel concentration has also to be taken into account in order to properly estimate the heat release rate due to the cool flame reactions.

Conclusions

A novel attempt has been presented to numerically simulate a non-igniting, damped cool flame reactor, using a multidimensional, two-phase CFD code. Comparison of predicted temperatures with available experimental data indicated that the major characteristic features of the flow inside a "cool flame vaporizer" can be captured reasonably well, using a semi-empirical cool flame heat release correlation. The adopted approach is particularly convenient for use in the context of a CFD code, because it does not impose heavy computational load in contrast to the much more cumbersome and numerically stiff chemical kinetics differential equations. A temperature dependent polynomial correlation has been used for the calculation of the heat release rate of the cool flame reactions yielding reasonable results. Agreement with experimental data has been further improved by introducing to the polynomial correlation a correction to take into account the local fuel concentration. There is a great need for more detailed experimental data for validating purposes, since considerable effort is still required for the proper prediction of the reactor's flow field.

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