

## **UTILIZATION OF A SEMI-EMPIRICAL AND A TABULATED CHEMISTRY APPROACH FOR THE TWO-PHASE FLOW NUMERICAL SIMULATION OF A “STABILIZED COOL FLAME” REACTOR: A COMPARATIVE STUDY**

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### **ABSTRACT**

Droplet evaporation in a “stabilized cool flame” environment leads to a heated, highly homogenous gaseous mixture that can be subsequently either burnt or utilized in liquid fuel reforming applications for fuel cell systems. “Stabilized cool flames” manifest themselves in the low-temperature hydrocarbon oxidation region representing essentially a process during which the fuel is partially oxidized, but not burnt. With the aim of numerically investigating the physico-chemical phenomena occurring in a diesel oil fed, atmospheric pressure, tubular, “stabilized cool flame” reactor, an in-house developed, two-phase, Eulerian-Lagrangian RANS computational fluid dynamics (CFD) code has been used. In order to simulate the cool flame reactivity, a twofold model development procedure has been followed by utilizing the fitting parameter technique. In the first case, a “semi-empirical” model has been developed, based on physico-chemical reasoning coupled with information from available experimental data. In the second case, a tabulated chemistry approach was utilized in order to estimate both the heat release and fuel consumption rates due to cool flame reactions. Numerical predictions of the CFD code utilizing both cool flame modelling approaches have been compared with available reactor temperature measurements, achieving satisfactory levels of agreement, while requiring limited computational resources.

### **1. INTRODUCTION**

Liquid fuels are extensively used in a large variety of technical combustion applications such as furnaces, boilers, internal combustion engines, gas turbines and rockets. The fuel is usually introduced in the combustion chamber by means of a spray injection system with the aim of increasing the fuel surface area thus accelerating the rate of evaporation and subsequent combustion. In conventional systems, the droplets, exposed to the surrounding turbulent, high-temperature gaseous environment, are evaporated and burnt in a temporally and spatially semi-sequential process. The involved autoignition phenomena depend on a multitude of processes, both physical and chemical in nature, such as atomisation, evaporation, turbulent mixing, free radical generation and exothermic reactivity. Mixture preparation is one of the most important autoignition rate-controlling parameters. Poor mixing of the fuel and oxidant streams leads to mixture inhomogeneities that affect combustion efficiency and result in enhanced pollutant formation. Temporal and spatial separation of the two main phenomena involved, namely evaporation and combustion, can lead to better mixing conditions, by essentially producing a gaseous “premixed” mixture. Such a technique is practically utilized in novel low-NO<sub>x</sub> Lean Premixed Prevaporized (LPP) burners of liquid fuelled gas turbines. An innovative way to accomplish the separation of the two processes is to evaporate the liquid fuel in a “stabilized cool flame” environment, prior to combustion. The additional heat produced by the exothermic cool flame reactions enhances droplet evaporation, resulting in the production of a well mixed, heated (yet below autoignition temperature), homogeneous mixture of air and fuel vapour, allowing the use of premixed combustion techniques. In addition, the products of the low-temperature oxidation cool flame reactions are known to play an important role in the reforming of fuels into hydrogen-rich gas. Ongoing research on “stabilized cool flame” mixture preparation suggests that this process may be used as part of a diesel oil reforming technology for utilization in fuel cell systems [1, 2].

The scope of the present work was to numerically investigate the physico-chemical behaviour of a diesel oil spray evaporating in a “stabilized cool flame” environment with the aim of providing better understanding of the involved phenomena. Toward this end, an in-house developed, two-phase Computational Fluid Dynamics (CFD) code was used to predict the spatial evolution of the evaporating spray. In order to model the effects of cool flame reactions on the heat and mass transfer phenomena, a twofold approach has been followed. On one hand, a dedicated semi-empirical approach was developed to computationally simulate the cool flame heat release rate. The model was based on physico-chemical reasoning coupled with experimental data. On the other hand, a tabulated chemistry model was formulated, utilizing a semi-detailed chemical kinetics oxidation scheme to produce a multitude of data, resulting from numerous simulations in an ideal Perfectly Stirred Reactor (PSR). The obtained data matrix, stored as a “look-up table”, links heat release and fuel conversion rates to the selected characteristic controlling variables, namely temperature, fuel concentration and residence time. After being implemented in the CFD code, the proposed models were validated and evaluated by comparing numerical predictions to experimental data obtained in a tubular, atmospheric pressure, diesel spray, “stabilized cool flame” reactor.

## 2. COOL FLAMES

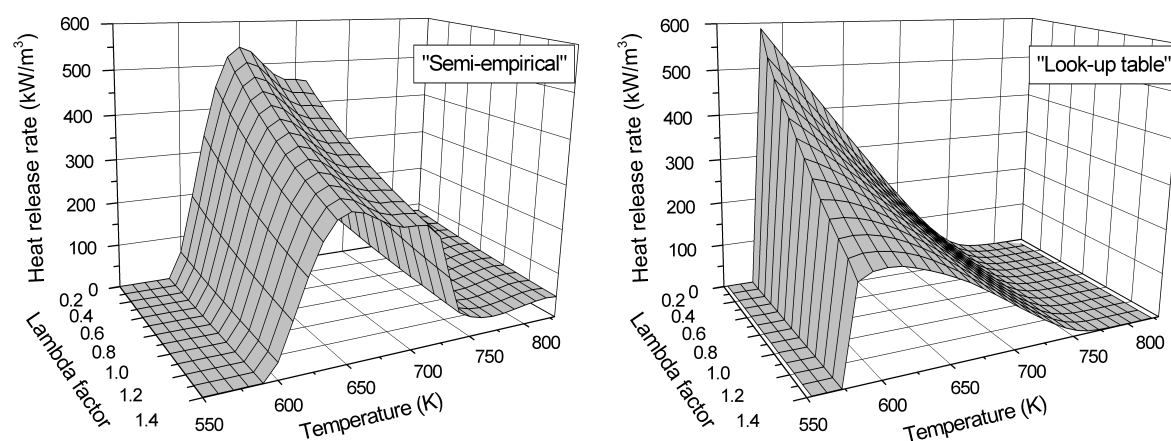
When alkane fuels reside either partially or fully mixed in an oxidizing atmosphere, in the temperature range of 500K-800K, the complex chemical reactions involved result in a “two-stage ignition” process in which the conventional “hot” ignition is preceded by a self-quenching temperature pulse known as “cool flame”. Generally, cool flames can be perceived as a low-temperature oxidation process during which the fuel is partially oxidized but not burnt; they are characterized by a faint pale bluish light that is attributed to the chemiluminescence of excited formaldehyde [3]. During the hydrocarbon 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 and are dominated by an exothermic degenerately branched chain reaction involving one or more important long-lived intermediates. In the temperature region of cool flame emergence, both thermal and kinetic feedback phenomena are important; a competition between termination and branching reactions arises, since the former occasionally exhibit higher activation energies than the latter [3, 4]. As a result, for a characteristic temperature range, a Negative Temperature Coefficient (NTC) of the reaction rate emerges, i.e. the overall reaction rate decreases with increasing temperature. The NTC is a rather unique phenomenon of hydrocarbon oxidation and is considered to be the main distinguishing property of cool flames, representing a barrier for autoignition to occur. In an open flowing system, it is possible to “stabilize” the cool flame reactions by exploiting the NTC phenomenon; in this case, heat losses at the system’s boundaries are compensated by the heat generation attributed to exothermal chemical activity and a “stable” thermo-chemical state is achieved, without a “hot flame” ignition being observed. Experiments have shown that when “stabilized cool flames” are realized in open flowing systems, the air/fuel mixture temperature increases up to 200K in the flow direction and stabilizes at the raised level [1, 2, 5]. During this process, no “conventional” ignition occurs and only 2-10% of the fuel mass, and therefore of the respective available thermal energy attributed to the fuel’s heating value, is being “consumed” [5]. The realization of liquid fuel evaporation in a “stabilized cool flame” environment generates a well mixed, heated and residue-free air/fuel vapour mixture, which can be subsequently utilized either in premixed combustion applications or in fuel reforming devices that produce hydrogen-rich gas for use in fuel cells [1, 2].

## 3. COOL FLAME MODEL DEVELOPMENT

There is scarce information in the open literature regarding the numerical modelling of non-igniting “stabilized cool flames”, especially in the frame of a CFD code. In order to effectively simulate the autoignition behaviour of conventional fuels, several characteristics such as two-stage ignition and NTC phenomena need to be modelled. However, cool flames are usually seen as a merely “transitional stage” that leads to ignition and are not confronted “per se” during hydrocarbon autoignition behaviour predictions. This kind of simulations is normally performed using either detailed or reduced chemical kinetics models [3, 4, 6] and they frequently regard the vigorous, high-temperature, high-pressure in-cylinder internal combustion engine environment, being consequently “fine-tuned” for such conditions. As a result, there is a serious lack of chemical kinetic models capable of reproducing cool flame behaviour in low-temperature, low-pressure conditions, such as those encountered in a “stabilized cool flame” reactor. Incorporating detailed or even reduced chemistry kinetic models into multidimensional, two-phase CFD computational approaches to account for non-igniting “stabilized cool flames” is currently not a straightforward procedure due to their excessive computational requirements and due to lack of relevant experimental data for the intermediate species concentrations, necessary to serve as validating means [4, 6]. The scope of the current study was the formulation of a simple, dedicated, low computational cost model, capable of incorporating the effects of “stabilized cool flame” reactions in a two-phase droplet evaporation CFD code, with the aim of acquiring a more in-depth comprehension of the respective thermo-kinetic phenomena. Towards this direction, two alternative approaches have been developed, namely the “semi-empirical” and the “look-up table” models. The former consists of a semi-empirical correlation derived on the basis of both experimental data fitting and chemical reasoning, whereas the latter regards the development of a tabulated chemistry approach, utilizing a semi-detailed chemical kinetics oxidation scheme.

### 3.1 “Semi-empirical” Model

Utilizing a wealth of temperature profile measurements from an atmospheric pressure, “stabilized cool flame” reactor, a 5<sup>th</sup> order polynomial equation has been generated by applying a curve-fitting procedure, correlating the cool flame heat release rate per unit volume with the mean local mixture temperature [7, 8]. To calculate the amount of heat released due to the cool flame exothermic reactions, a plug-flow reactor analysis has been employed, taking into account the mixture’s thermal losses through the reactor’s wall [5]. Since the correlation emanated from experiments conducted in an actual “stabilized cool flame” reactor, it is inherently capable of capturing and reproducing the very important NTC region. It is well documented [3, 4, 9] that the main operational parameters affecting the cool flame characteristics are pressure, temperature and fuel concentration. Since the current study focused on atmospheric pressure reactors and no data were available for different pressure levels, it was decided to examine the effects of the two latter parameters, namely temperature and fuel-air mixture fraction (expressed via the lambda factor), on the thermal behaviour of the system. Thus, a correction factor was introduced to the original correlation (which had been deduced based on the experimental case of constant lambda factor equal to 1.27) of the “semi-empirical” model to account for the effect of the fuel concentration variation. Various reports in the literature [6, 9] suggest that the overall cool flame reaction rates, and subsequently the amount of heat released, intensify when the fuel’s total concentration is increased.



**Figure 1:** Comparison of predicted heat release rate, as a function of temperature and total lambda factor, utilizing the “semi-empirical” and the “look-up table” model.

However, there are no consistent correlations available attempting to quantify this tendency. As a result, the correction factor applied to the original correlation was based on the widely applied “inverse proportional” principle, allowing also for under-relaxation. The suggested correction factor has exhibited encouraging quantitative prediction results, in the case of CFD simulations of “stabilized cool flame” reactors [7, 8].

### 3.2 “Look-up table” Model

An alternative approach, utilizing a chemical kinetics mechanism, has been developed in order to depart from the strictly experimental foundation of the “semi-empirical” model. In this case, in order to avoid the inflicted excessive computational burden, the chemical kinetics scheme is not introduced directly to the CFD code, but it is used to construct a “look-up table” which is in turn implemented in the code [10]. Almost all available chemical kinetic models in the autoignition region deal with high-temperature, high-pressure in-cylinder internal combustion engine environment and are “fine-tuned” for such conditions. As a result, there is a serious lack in the literature of kinetic schemes capable of reproducing the NTC behaviour in low-temperature, atmospheric pressure conditions, such as those encountered in the reactor under consideration. In addition, there are no chemical kinetic schemes currently available for the “actual” diesel fuel, which is essentially a mixture composed of a plethora of complex hydrocarbon components including alkanes, naphthenes and aromatics. The extensive work on fuel oxidation kinetics is confined primarily to single-component reference fuels such as n-heptane and iso-octane. Therefore, for modelling purposes, it is usually assumed that the diesel oil’s chemical and physical properties can be sufficiently described by n-heptane, commonly used as a “simulant” for diesel oil [11] since n-heptane’s cetane number is very similar to that of diesel.

A comparative study assessing the performance of seven n-heptane oxidation, chemical kinetic mechanisms in a low pressure Jet-Stirred Flow Reactor [12], revealed that the mechanism of the Chalmers University [11], involving 57 species and 290 reactions, exhibits a satisfactory thermo-chemical performance, while at the same time does not impose a high computational cost. Thus, this mechanism was selected to create a “look-up table” by performing a multitude of Perfectly Stirred Reactor (PSR) simulations. A PSR is practically a constant volume flow reactor in which the feed is instantaneously, continuously and rigorously mixed with the reacting fluid, thus achieving spatially uniform conditions of temperature, pressure and composition throughout the entire reactor volume. The mathematical model of a PSR consists of differential equations, the number of which depends on the number of chemical species involved in the kinetic mechanism implemented, for the mass, energy and species conservation. By arithmetically solving the numerical system of the differential equations, the thermo-chemical conditions at the reactor’s outlet can be estimated. In order to construct the “look-up table” database, three operational parameters were varied, namely reactor inlet temperature, lambda factor and residence time, within a prescribed range covering the experimentally determined typical values occurring in “stabilized cool flame” reactors (inlet temperature extents from 550K to 820K, lambda factor ranges from 0.2 to 1.4 and residence time values span 0.001-0.2s). For each triplet combination (eventually the resulting matrix consisted of 11648 elements), values for both volumetric heat release rate, as well as fuel consumption rate were computed and stored.

Predicted cool flame heat release rates as a function of temperature and fuel concentration are depicted in Figure 1, utilizing both developed models. In the case of the “look-up table” model, predictions refer to an atmospheric pressure PSR that exhibits a residence time equal to 0.1sec. This parametric study revealed a number of noteworthy features in relation to the thermal behaviour of the system in the examined range of operational parameters. The most prominent observation was that for both models, the predicted heat release values are increasing with decreasing lambda factor values (i.e. with increasing fuel concentration), signifying an enhancement of cool flame reactivity at fuel-rich conditions. This remark is consistent with literature reports [6, 9], suggesting that a particularly strong effect of initial fuel concentration on the rate of reaction is observed in the NTC region of n-heptane oxidation. However, the predicted

absolute values of heat release rates in the sub-stoichiometric region ( $\lambda < 1$ ) using the “semi-empirical” model are higher than the respective ones utilizing the “look-up table” model. The opposite remark is valid in the over-stoichiometric region ( $\lambda > 1$ ). For the “semi-empirical” model case, the overall distribution of the original ( $\lambda_c = 1.27$ ) heat release curve is maintained throughout the entire lambda variation region. Furthermore, the figure indicates that the temperature at which the exothermic heat production rate acquires its maximum value is independent of the lambda factor value. The introduction of an under-relaxation term in the correction factor results in a smoother distribution of the surface gradients. In the case of the “look-up table” model predictions, the “peak” of the curve, corresponding to the low-temperature limit of the NTC region, becomes more pronounced in the low lambda factor region, resulting to steeper curve slopes at the NTC region. However, in this case the temperature corresponding for which the exothermic heat production rate acquires its maximum value is decreasing with decreasing lambda factor. This corresponds to a “shift” of the entire low temperature chemistry towards lower temperatures when the system’s initial fuel concentration is increased, an observation consistent with similar remarks found in the literature [13].

#### 4. STABILIZED COOL FLAME REACTOR

Air/fuel vapour mixture temperature measurements conducted in an atmospheric pressure, “stabilized cool flame” reactor at the EST, RWTH-Aachen were used for model validation [5]. The reactor is an 1.0m long metal pipe of 0.1m internal diameter. The insulated pipe wall embodies heating elements that enable accurate control of the device’s thermal boundary conditions. Temperature profiles in both axial and radial directions are recorded using a number of retractable thermocouples. Following an initial pre-heating stage, air is supplied to the reactor through a perforated disk, utilized to maintain homogeneous flow turbulence levels. A water-cooled, 60 deg. hollow cone, Simplex pressure atomizer is fixed at the centre of the perforated disk, injecting diesel oil into the reactor. The droplets, subjected to the surrounding environment of preheated air, promptly evaporate; the emerging fuel vapours sustain the “stabilized cool flame” reactions. A steady-state mode of operation is achieved, featuring the following characteristics: immediately downstream the fuel injection plane a sudden temperature drop is observed, owed to the fuel’s latent heat of evaporation. However, further downstream, an increase in the mean temperature of the order of 100K-150K is observed reaching a nearly constant value at an axial distance of approximately 0.3m without, however, the mixture being actually ignited and burnt. The outlet temperature at the downstream end of the reactor is eventually, due to cool flame exothermal reactions, higher than the respective inlet temperature but still lower than the autoignition point. The additional amount of heat released in the process represents roughly 7.5% of the available thermal energy due to the fuel’s heating value [5].

#### 5. COMPUTATIONAL MODELLING

The in-house developed 2PHASE CFD code was used for the numerical simulations [14, 15]. The continuous phase is treated as a steady, incompressible, turbulent flow that is computed by solving the Reynolds-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 the RNG k- $\epsilon$  turbulence model in conjunction with standard wall functions for the near-wall boundary conditions; convective wall heat transfer is also taken into account. The Lagrangian treatment is adopted for the dispersed phase, where a large number of droplet “parcels”, each one representing a number of real droplets with the same properties, are traced through the flow-field. Each parcel’s trajectory is calculated by solving the instantaneous droplet motion equations in a three-dimensional Cartesian frame of coordinates (in order to avoid the singularity that droplet radial position may assume by applying cylindrical coordinates), with the use of a 4<sup>th</sup> order Runge-Kutta method. The droplet motion equations take account only of the drag and the gravitational force, since the density ratio of the fuel over the carrier gas is, in the test case examined, well higher than unity, thus rendering virtual mass, pressure forces and history effects on the droplet motion negligible. Droplet turbulent dispersion is modelled using a Lagrangian stochastic separated flow model, sampling random Gaussian gas velocity fluctuations, while accounting for the crossing trajectories and eddy lifetime effects [16]. The gas and liquid phases are coupled by calculating source-sink terms for the interfacial momentum, turbulent energy, thermal energy and species concentration exchange (two-way coupling), following a modified version of the PSI-cell approach [17]. Cool flame heat release rates are introduced as local heat source terms to each computational cell. In order to improve the accuracy of the droplet mass-flow rate predictions near the symmetry axis and to avoid strong artificial accumulation near the centreline far downstream the inlet plane, a “drift correction” term is applied to the turbulent dispersion model, in the transverse direction [18]. The evaporation model of Bellan and Harstad [19], which takes into consideration the non-equilibrium phenomena that may appear in the gas-droplet interface, is implemented in the code, according to results of a comparative study [15].

The computational domain, measuring 0.9m axially by 0.05m radially, was discretized using 94\*35 non-uniform, cylindrically axisymmetric, rectangular grid nodes. The grid was refined close to the nozzle tip to improve local flow resolution. This grid arrangement yielded similar results to those obtained by using a 143\*52 nodes grid, thus demonstrating grid independence. The continuous phase (air) was considered to enter the test region, having a top-hat velocity profile, corresponding to the experimentally determined mass flow rate value of 3.58 g/s, with an average temperature of 623K, which was also the assumed constant temperature of the reactor’s insulated wall. The spherical diesel oil droplets were assumed to be injected in the flow-field from 10 discrete starting locations, equally distributed across the atomizer inlet plane. According to fuel consumption measurements, the total liquid phase mass flux was considered to be 0.2211 g/s, yielding a mean mass loading of 6.2%, corresponding to a total power of 8.7kW and a global lambda factor value of 1.27. The initial droplet velocity and size distributions at the nozzle injection plane were

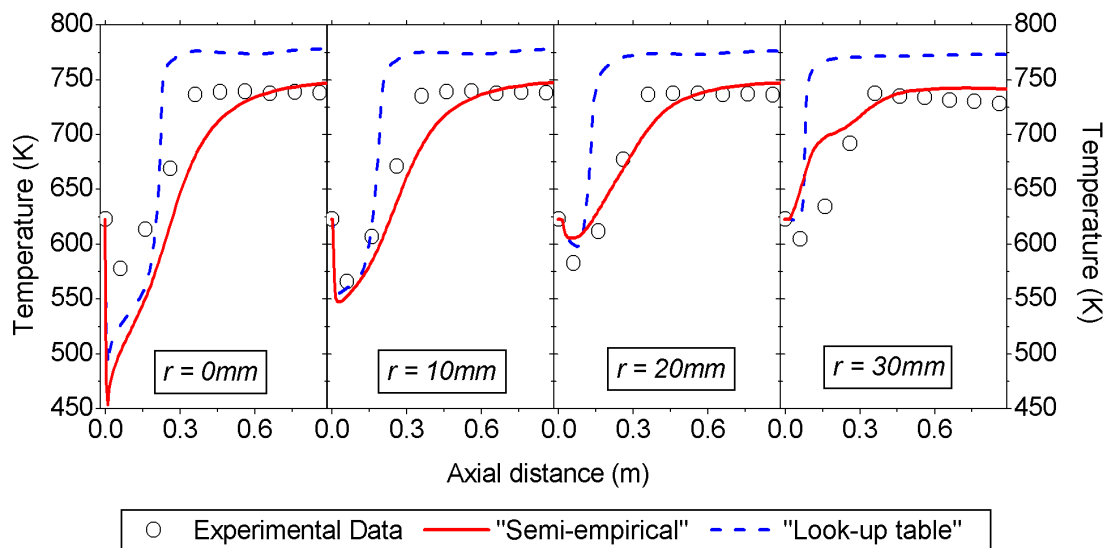
obtained by interpolating PDPA experimental measurements for a Simplex pressure atomizer, similar to the one used in the considered reactor [20]. The droplet injection temperature was assumed to be 393K, according to measurements of the water-cooled nozzle temperature. A total number of 300 000 computational droplet “parcels” were injected and tracked throughout the flow-field for 30 two-way coupling iteration cycles, in order to keep statistical fluctuations associated with stochastic particle tracking at an acceptable level. A “hybrid” representation for diesel oil was used, i.e. the chemistry corresponded to n-heptane whereas the liquid fuel properties, needed for the Lagrangian calculations, were of the actual diesel oil.

## 6. RESULTS

Computational simulations of the fluid flow inside an atmospheric pressure, tubular, “stabilized cool flame” reactor have been performed and the results are presented in Figure 2, where CFD code predictions are compared to experimental measurements of axial mixture temperature profiles. In the case of the “semi-empirical” model predictions, temperature predictions agree reasonably well with the experimental data, enabling the code to accurately describe the establishment of a downstream steady-state temperature. Mixture heating-up rates are well reproduced and the axial position of the main exothermal activity ( $x=0.15\text{m}$  to  $0.45\text{m}$ ) is properly captured. In general, overall agreement is quite satisfactory, confirming that the model is able to effectively reproduce the general trends observed in the experiments. Computational results utilizing the developed look-up table model (dashed line) are generally in good qualitative agreement with the respective measurements, being capable of adequately describing the main features of the flow, i.e. the sudden increase in temperature downstream the local “minimum”, which emerges in the droplet evaporation region, as well as the consequent attainment of a constant temperature level, up to the reactor’s outlet. Although the axial position of the main exothermal activity is properly captured, discrepancies regarding the downstream steady-state temperature levels are observed, as predictions suggest higher values (of the order of 50K) than the respective measured ones. Additionally, the predicted temperature gradients in the main exothermal activity region are generally steeper than the respective measured values, suggesting that under the specific flow conditions of the considered test case, the cool flame induced heat release rates are over-estimated by the developed model. This behaviour may be attributed to a variety of reasons, such as inaccuracies in the assumed boundary and inlet conditions, the lacking ability of the currently available chemical kinetic schemes to sufficiently describe the low-temperature, low-pressure oxidation characteristics of hydrocarbons [12], or the use of n-heptane as a “simulant” of the much more complex diesel oil, which is actually a multi-component mixture. Moreover, the incompatibility between the zero-dimensional PSR model utilized for the reactivity data matrix generation and the spatially non-uniform actual experimental conditions may have lead to the observed temperature over-predictions; this remark is in agreement with similar observations found in the literature [21], suggesting that the utilization of purely kinetics-controlled reaction techniques yield consistently faster reaction rates than the respective experimentally determined values.

## 7. CONCLUSIONS

Two modelling approaches have been developed and assessed in order to numerically simulate the “stabilized cool flame” phenomenon in a non-igniting, atmospheric pressure reactor, utilizing a two-phase CFD code. A “semi-empirical” model was derived using an algebraic expression, deduced from experimental measurements correlating cool flame heat release rates with temperature. The addition of a fuel concentration correction term improved the model’s predictive capabilities.



**Figure 2:** Comparison of axial profiles of measured temperatures with numerical simulations across the reactor, utilizing the “semi-empirical” and the “look-up table” model.

The second approach, dubbed the “look-up table” model, was based on a semi-detailed chemical kinetics scheme for n-heptane oxidation, utilizing 290 reactions and 57 species. The kinetic scheme was used in order to construct a look-up table, for a variety of temperature, fuel concentration and residence time combinations. Numerical predictions agreed quite satisfactorily with available experimental data, being able to capture reasonably well the general trends observed in the experiments, as well as the major characteristic features of the flow inside a cool flame reactor. However, some discrepancies were observed in the case of the “look-up table” model predictions; these were attributed to a variety of reasons, both of physical and chemical nature. However, the tabulated chemistry approach is very promising in order to depart from the empirical foundation of the algebraic correlation model. Both models are particularly convenient for use in the context of a CFD code, because they do not impose heavy computational load in contrast to the much more cumbersome and numerically stiff direct solution of chemical kinetics differential equations. The developed computational tool may be reliably used to predict the operational behaviour of atmospheric “stabilized cool flame” reactors, thus assisting the designing optimisation procedure of such technological devices.

## 8. ACKNOWLEDGEMENTS

The present study has been financially supported by the E.U. in the frame of an EU-project (Contract No. ENK6-CT-2000-00317). The authors are grateful to Dr. Ing. K. Lucka and Dr. Ing. N. Steinbach (both at EST-RWTH Aachen, Germany) for providing the cool flame reactor experimental datasets.

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