Proceedings of GT2006
ASME Turbo Expo 2006: Power for Land, Sea and Air
May 8-11, 2006, Barcelona, Spain

GT2006-90956

VALIDATION OF A PARTIALLY-PREMIXED COMBUSTION MODEL FOR GAS TURBINE APPLICATIONS

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ABSTRACT
The principal requirements of industry, with respect to the numerical simulation of gas turbine combustors, are computational efficiency and algorithm robustness, together with an accurate representation of the complex fundamental processes. This paper examines the performance of the premixed combustion models implemented in the commercial CFD package Fluent™, in order to validate the ability to model combustion in the context of a premixed gas turbine combustor. The predictions of the model are found to compare well with the experimental results available, demonstrating robustness and computational efficiency.

Keywords: turbulent premixed combustion, turbulent flame speed

NOMENCLATURE

Sc_t	Turbulent Schmidt number
c	Progress variable
μ_t	Turbulent viscosity
Sc	Reaction progress source term (s-1)
n	Number of products
$\vec{V}$	Velocity vector
Y_i	Mass fraction of species i
$Y_{i,ad}$	Mass fraction of species i after complete adiabatic combustion
ρ_u	Density of unburnt mixture
U_t	Turbulent flame speed
$A = 0.52$	Model constant
U_l	Laminar flame speed (m/s)
u'	RMS (root-mean-square) velocity (m/s)
$\alpha = k/\rho c_p$	Molecular heat transfer coefficient of unburnt mixture (thermal diffusivity) (m2/s)
$\tau_t = l_t/u'$	Turbulence time scale (s)
$l_t = C_D \dfrac{(u')^3}{\varepsilon}$	Turbulence length scale (m)
$C_D = 0.37$	Constant
$\tau_c = \alpha/U_l^2$	Chemical time scale (s)
$erfc$	Complementary error function
G	Stretch factor
ε_{cr}	Deviation of the distribution of ε
g_{cr}	Critical velocity gradient

INTRODUCTION
There has always been a considerable interest in premixed combustion because of its central importance in gas turbine technology. In recent years this has further increased due to the desire to reduce pollutants emissions. In this context the requirements of industry are quite practical. Here CFD is considered a useful development tool in the design process wherein a large number of alternative designs may be assessed before committing to expensive combustion rig or engine tests. The decreasing cost of computing power and the availability of accessible commercial Navier-Stokes solvers has led to the rapid growth in the application of CFD techniques throughout the combustion industry. Computational fluid dynamic simulations are now used to visualise the aerodynamics, the combustion environment and the emissions performance of combustors at the design stage. As a consequence of this there is a considerable demand for the further development

of physical combustion sub-models that can accurately describe premixed and partially premixed combustion in gas turbine combustors.

Unfortunately the prediction of premixed combustion is complex and involves many disciplines. Understanding the flame dynamics, in fact, implies the simultaneous solution of a turbulent problem (stirring and mixing), a chemical kinetics problem (oxidation of the fuel) and an acoustic problem (interaction of pressure and heat release fluctuations). Furthermore the underlying physics of combustion instabilities are not yet completely understood and the methods of numerical simulation are still being developed. On the numerical modelling side, the unstable combustion regime, typical of lean premixed flames, brings modelling complexities due to the requirement to represent the detailed chemical kinetics in addition to the influence of the underlying fluid dynamics.

As these problems are highly non-stationary, combustion simulations require the spatial and temporal resolution of the coupled physical and chemical problem. At the same time the development of new approaches to turbulence modeling including large eddy, detached eddy and direct numerical simulations, has led to modelling becoming the dominant approach for investigating combustion processes that are not readily, or economically, accessible through experimental programmes.. Indeed, other than by excessively expensive experimental programmes, design engineers have no other option.

Turbulent premixed combustion modelling still represents a major challenge in computational prediction methods. The combustion research community have over recent decades proposed a number of alternative premixed combustion models, differing from each other in the way that the underlying chemical kinetics are represented. Combustion modelling has progressed and refined from simple mixing models, for example eddy break-up, to models that attempt to represent the detailed chemistry of combustion including transported and presumed shape pdf models, for instance.

Complementary to developments in numerical simulation of combustion, modern laser measurement techniques, such as LDA and PIV, have considerably improved the investigative tools available to the researcher, making reliable benchmark data readily available.

The aim of this study is the validation of the partially premixed combustion model implemented in the commercial CFD package Fluent™, testing the ability of the model to describe fuel/air mixture non-homogeneities. Differences in local fuel distribution in fact are characteristics of practical devices and are of great significance in terms of pollution formation, thermo-acoustic and flame stability.

The analysis is carried out with the objective to determine if the model fulfils the industrial requirement of the adequate representation of advanced combustion phenomena, retaining at the same time computational efficiency and robustness.

The stretch effect correction of the model, which is needed at high turbulence intensities, is also introduced and discussed in some detail.

DESCRIPTION OF VALIDATION CASES

The computational results are validated against a series of experimental measurements supplied by Cranfield University and German Aerospace Centre (DLR) laboratories, representing two distinct combustor geometries. Full details are available in [1].

The first set of experimental data was obtained by Cranfield University in a series of measurements on a specially designed experimental burner. The resultant data were utilized to validate the development and application of a Turbulent Flame Closure (TFC) premixed combustion model in a series of CFD predictions using the in-house code, SOFIE. Full details are available in [2].

The experimental rig consisted of a laboratory scale burner where propane and air was mixed at lean equivalence ratios (typically Φ=0.8), resulting in a premixed stabilized flame. Fig. 1 and 2 illustrate the rig. The fuel enters through the base of the burner into a cavity separated from the mixing tube by an injection plate. A rod passes through the centre of the tube to support the centre body, a turbulence generating plate and the injection ports. The fuel flows from the cavity through 16 sections of hypodermic tube connected to the injection ports by rubber tubing, which ran directly from the injection plate to the injection plane. The air passes through the remaining holes in the plates and mixing takes place upstream of the second plate, which forms the injection plane. The air enters through four diametrically opposed pipes located upstream of the injection plane. The studies were conducted at atmospheric pressure.

The second set of experimental data is a result of a comprehensive investigation performed by DLR in the context of the European funded PRECCINSTA project (PREdiction and Control of Combustion INStabilities in Tubular and Annular gas turbine) on premixed swirling CH_4/air flames at atmospheric pressure in a gas turbine-like combustor with optical access. Further details may be found in [3,4,5].

The experimental conditions were ambient at atmospheric pressure and ambient temperature. The combustion chamber (Fig. 3 and 4) had a square section with transparent liner walls, in such a way to facilitate the observation and measurements by optical diagnostics including Laser Doppler Velocimetry, Raman spectroscopy and Laser Induced Fluorescence (LIF).

The combustor was fuelled by methane (CH_4). The injector was provided by Turbomeca and consisted of an experimental swirler with simple gimlets, provided with twelve valves. This component allowed the injection of the fuel by twelve orifices connected directly to the swirler arms, at the same time turning the flow to give it too a swirl component inside the chamber. The fuel was injected through twelve small holes in each of the swirler slots with a rather high momentum in order to achieve a high level of premixing (Fig. 5 and 6). The exhaust nozzle provides a transition from the rectangular cross-section combustion chamber to a cylindrical exhaust duct.

COMBUSTION MODELLING APPROACH

Variations of the model proposed by Zimont et al. [7] for premixed gaseous combustion at high Reynolds numbers are employed by both Fluent™ and SOFIE [2]. In its original form the model was only able to represent homogeneously premixed combustion, however recently the model has been extended to partially premixed problems.

In the Zimont model, the combustion process is represented in terms of a single scalar quantity, the progress variable, rather than solving individual species transport equations. The reaction progress variable is solved in order to predict the position of the flame front, which separates perfectly mixed reactants and burnt products. The evolution of the reaction is taken into account through the movement of the flame front progressing from unburnt reactants to burnt products. Therefore the premixed combustion model thus considers the reacting flow field to be divided into regions of burnt and unburnt species, separated by a flame sheet.

The flame front propagation is modelled by solving a transport equation for the Favre averaged progress variable c:

$$\frac{\partial}{\partial t}(\rho c) + \nabla \cdot (\rho \vec{V} c) = \nabla \cdot \left(\frac{\mu_t}{Sc_t} \nabla c \right) + \rho Sc \qquad (1)$$

The mean reaction rate is modelled as:

$$\rho Sc = \rho_u U_t \left| \nabla c \right| \qquad (2)$$

The influence of turbulence is accounted for by means of the turbulent flame speed U_t concept, based upon the assumption that the reaction rate is solely controlled by the turbulence, as shown in equation 2 (Turbulent Flame Speed Closure Model, TFC).

The advantage of using the turbulent burning velocity in the TFC model is that the influence of the underlying chemical kinetics can be included. The principal concern of modelling premixed combustion is in fact the definition of a model for the chemical source term that varies sensibly with both the chemical and turbulence time scales.

The speed U_t is normal to the surface of the flame and in turn is influenced by the laminar flame speed (function of the fuel concentration, temperature, molecular diffusion properties and generally by chemical kinetics) and by the alterations of the flame front. The flame in fact is continuously wrinkled and stretched by any turbulent eddies.

The wrinkling and thickening effect is modelled in terms of turbulence parameters and physico-chemical characteristics of the combustible mixture:

$$U_t = A(u^{'})^{3/4} U_l^{1/2} \alpha^{-1/4} l_t^{1/4} = A u^{i} \left(\frac{\tau_t}{\tau_c} \right)^{1/4} \qquad (3)$$

The present paper evaluates the performance of the partially premixed combustion model implemented in the commercial CFD package Fluent™ 6.1.22 validating it against detailed experiments. Furthermore the performance of Fluent™ was additionally compared to the CFD simulations carried out by Wood [2] who used an alternative implementation of the TFC model within the Cranfield University research CFD code SOFIE.

The difference in the TFC implementation between the commercial code Fluent™ and the academic code SOFIE lies in the manner in which the model has been extended to represent partially premixed combustion. This is fully described in [2].

Both SOFIE and Fluent™ solve additional transport equations for the mixture fraction and its variance, to determine the density and other properties of the reactants. A presumed shape probability distribution function is employed, which is assumed to be described by a beta function. Lookup tables are pre-computed for the specific fuel and operating conditions to improve upon computational efficiency.

The later experimental comparison (Fig. 22) showed a considerable effect of the flame stretch phenomena, which consists of an experimentally observed reduction in the turbulent combustion intensity at high turbulent velocities. This stretch effect is particularly important in low emissions gas turbines and it appears necessary to be taken in account in the combustion model.

In order to take this flame stretching into account, the source term for the progress variable ρS_C is multiplied by a stretch factor, G representing the probability that the stretching will not quench the flame; the 100% probability of an unquenched flame corresponds to the value $G = 1$.

The stretch factor, G, is obtained by integrating the log-normal distribution of the turbulence dissipation rate ε and introducing a complementary error function *erfc*:

$$G = \frac{1}{2} erfc \left\{ - \sqrt{\frac{1}{2\sigma}} \left[\ln \left(\frac{\varepsilon_{cr}}{\varepsilon} \right) + \frac{\sigma}{2} \right] \right\} \qquad (4)$$

Equation (4) contains the *critical turbulence dissipation rate* ε_{cr} ,expressed as function of a parameter named *critical velocity gradient* g_{cr}:

$$\varepsilon_{cr} = 15 \nu \, g_{cr}^2 \qquad (5)$$

The critical velocity gradient is the most significant parameter for tuning the TFC model flame stretch correction to the experimental data. A plausible value used in industrial combustor's simulations is $g_{cr} = 8000$ s^{-1}, as suggested in [7].

PROPANE FLAME VALIDATION CASE

The first case was modelled as two dimensional and axisymmetric. The computational domain describes just half of the facility, exploiting the rig's symmetries in terms of geometry and flow field features. The burner is also rotated through 90 degrees so the flow is from left to right rather than upwards as occurs in the actual device (Fig. 7).

In order to avoid the necessity of modelling the flow through the complex series of baffles that are within the burner, only the final part of the fuel injector was included. Turbulence properties were defined from the dimensions of the turbulence plate and experimental evidence (Table 1).

The second inlet boundary was defined at the same height as the first, and runs from the external wall of the burner to the wall of the flame tube. Again the flow was assumed to be uniform, with the estimated turbulence characteristics. The outlet of the burner was modelled with a zero gradient outflow boundary, placed sufficiently downstream of the burner that the reaction is expected to be complete.

The remaining boundaries were represented by non-conducting walls, giving an adiabatic solution. The geometry of the experimental rig is relatively simple suggesting the use of a quadrilateral structured grid for the whole domain. After grid dependency checks, the final grid contained approximately 44000 cells.

The full Reynolds Stress turbulence model (RSM) was chosen for the Fluent™ simulation. The SOFIE simulations reported in [2] were obtained using the standard k-ε turbulence model.

The Fluent™ premixed combustion model performance were qualitatively compared with the experimental measurements reported in [2]. Figures 8-11 compare the predictions produced by SOFIE and Fluent™ in terms of Favre averaged progress variable and reactant velocity.

Examination of the comparison of the axial velocity of the reactants shows appreciable agreement between the predictions and the experimental measurements. However an anomaly in the value assumed by the progress variable is observed.

The value of the progress variable can be generally considered a rough indication of the presence of the flame. A careful analysis of the progress variable contours reveals intermediate values which correspond to a region of recirculation (Fig. 12). Such a result means that the reaction takes place where it is not observed experimentally. The outcome is probably due to the interaction between the secondary air contribution and the main premixed fuel inlet.

Many authors (Biagioli et al., [8]; Polifke et al. [6]; Wood and Moss [9]) observed similar incongruities in premixed combustion models predictions.

A probable explanation of the latter anomaly involves the nature of the premixed combustion model. The fuel mass fraction is calculated from both the progress variable and the mixture fraction, and consequently variation in the progress variable, caused by the dilution of combustion products by the additional contribution of air from the secondary inlet, could introduce errors in the species concentration.

METHANE FLAME VALIDATION CASE

The PRECCINSTA burner rig was represented in detail, including all of the major components, the air plenum, the swirling burner and the square combustor (Fig. 13). In this combustor the air is fed into the burner from the plenum and mixes with fuel within the swirler slots and centre body channel, in such a way that none of the detail could be neglected.

The geometrical complexity of the configuration encouraged the use of a hybrid grid composed of grid blocks with unstructured tetrahedral elements and grid blocks with structured quadrilateral elements. The final grid contained approximately 16000000 cells. The size of the mesh was varied to resolve the major flow details, in the swirler it is highly refined because of the small scale details previously described, while in the combustion chamber the grid was chosen in order to match the best compromise between mesh density and solution quality (Fig. 13).

The zone along the chamber centreline was discretised with an increased resolution in order to account for the high gradients present in that region..

The boundary conditions were provided by DLR and related directly to the series of experimental tests which they had carried out (Fig. 14).

The fuel and air inlet mass flow corresponded to the case of stable combustion examined by DLR. The burner outlet was modelled with a zero gradient outflow boundary, placed sufficiently downstream of the burner that the reaction is expected to be completed (Table 2).

The results from unsteady reacting simulations were compared with the experimental data obtained by laser doppler anemometry measurements. The comparison was performed at a number of axial locations through the combustor.

The principal mechanisms of heat transfer on the combustor walls is both convection (the ambient air cools the walls) and radiation (the walls are transparent). However without quantitative data to define these boundary conditions, the combustor walls were considered to be adiabatic.

Considering the velocity field, the simulation results from Fluent™ show good agreement with the DLR experimental data (Fig. 15). The peak axial velocity is overestimated, but the lower value of the velocity field corresponding to the recirculation zone matches reasonably well with the measured one at each axial distance station.

The flame cone predicted by CFD is narrower than the real one. This conclusion is confirmed by the analysis of the tangential velocity field which illustrates a more intense recirculation zone (Fig. 16).

The temperature field follows the trends revealed by analysis of the velocity field. Looking at the temperature profiles (Fig. 17) it can be seen that the temperature at different axial stations proposed by Fluent™ is greater than that measured by spectroscopy. This discrepancy is easily explained bearing in mind that the calculations were performed under the assumption of adiabatic combustion chamber walls. Since radiation was not accounted for, the CFD simulations overpredict the temperature distribution.

At the same time, the computed temperature profiles are displaced with respect to the experimental data. This is due to the narrower jet flame prediction by Fluent™, which is inline with the corresponding velocity field.

THE FLAME STRETCH EFFECT

A detailed examination of the static temperature contours reveals an anomaly in the temperature field inside the swirler arms. The fuel mixture, in fact, is not supposed to burn inside the swirler or the injection cone. Though flame ignition inside the swirler is not observed experimentally, it does apparently occur in the simulation, as it is clearly shown in Fig. 19.

Fluent™ predicts ignition inside the swirler arms in the region of the fuel injection tube. Such high temperature pockets pass through the injector, albeit mixing and decreasing in temperature, although they still contribute to non-uniformity in the temperature distribution even in the combustion chamber (Fig. 20).

The result is justified looking at the laminar flame velocity contour, which is non-zero, and in accordance with equations 3 and 4, contribute to an increase in the progress variable transport equation source term (Fig. 21).

This non-physical behavior can be avoided by incorporating the effect of flame stretch. In such a situation the combustion is considered to be controlled by the flame stretch due to the high levels of turbulence.

Figure 22 shows the comparison between the experimental data and the results from Fluent™ with and without the flame stretching correction. The results have clearly improved when flame stretch is accounted for.

CONCLUSIONS

Comparison of the results with the measurements were pleasing, showing remarkable consistency between the computation and the experiments. The general level of agreement achieved indicates that the model is a valid approach for predicting premixed combustion even on large three-dimensional complex geometries. However a fundamental weakness was identified in applying the model in presence of inhomogeneities arising from the dilution of premixed reactants by secondary air. The situation just mentioned could be considered analogous to the addiction of dilution or cooling air in practical devices. In such circumstances an apparent region of intermediate progress variable arises from mixing of pure combustion products and oxidisers.

Although the partially premixed model demonstrates the ability to predict combustion in laboratories burners, the result should be still object of further investigations because the measurements experimental conditions did not match exactly the once occurring in practical devices. In particular the experimental facilities pressure was ambient, consequently far from the typical operating pressure found in industrial turbines.

Unfortunately the collection of experimental data on real gas turbine combustors is not trivial, due to the adverse conditions and limited optical access.

Furthermore it as been identified the necessity of implementing in the combustion model a correction factor for quenching due to flame stretching phenomenon, even more important in gas turbine combustors than in the experimental burners examined here. The latter consideration suggests a detailed analysis of the influence of the critical strain rate.

ACKNOWLEDGEMENTS

The authors gratefully acknowledge the valuable contribution from C. Masson at Cranfield University and the support from Dr. V. Sanderson, SIEMENS, Lincoln, UK throughout this project.

REFERENCES

1. Caracciolo L. 2005: 'CFD modelling of partially premixed combustion', MSc thesis, Cranfield University.

2. Wood J. P. 2004: 'Lean premixed combustion models at elevated pressure for the gas turbine.', Ph.D. thesis, Cranfield University, UK.

3. Weigand P., Duan X. R., Meier U. Et al. 2005: 'Experimental investigation of an oscillating lean premixed CH4 / air swirl flame in a gas turbine model combustor.' Proceedings of the European Combustion Meeting 2005.

4. Lartigue G. 2004: 'Simulation des grandes echelles et instabilites de combustion.', Mémoire de thèse, Institut National Polytechnique de Toulose.

5. Selle L., Lartigue G., Poinsot T. et al. 2004 : 'Compressible large eddy simulation of turbulent combustion in complex geometry on unstructured meshes.' Combustion and Flame, 137, pp 489-505.

6. Polifke W, Flohr P, and Brandt M. 2002: 'Modelling inhomogeneously premixed combustion with an extended TFC model.' Journal of Engineering for Gas Turbines and Power 124, pp 58-65.

7. Zimont V, Polifke W, Bettelini M, and Weisenstein W. 1998: 'An efficient computational model for premixed turbulent combustion at high Reynolds numbers based on a turbulent flame speed closure.' Journal of Engineering for Gas Turbines and Power 120, pp 526-532.

8. Biagioli F, Zimont V. L, and Syed K. J. 2001: '*Modelling and numerical simulation of gas combustion in DLE burners based on a turbulent flame speed closure approach*.' International Joint Power Generation Conference and Exposition, New Orleans, Lousiana, USA. June 4-7.

9. Wood J. P. and Moss J. B. 2003: 'Modelling partially premixed combustion using a turbulent burning velocity based closure.' European Combustion Meeting 2003, 25th-28th October, Orléans, France.

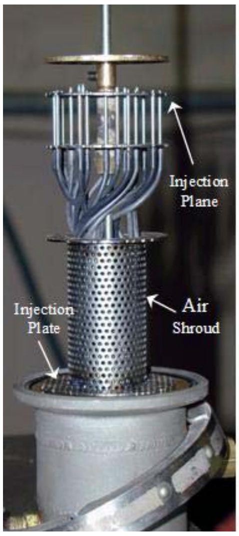


Figure 1. The internal baffles and injection system of the experimental burner.

Figure 2. The experimental burner.

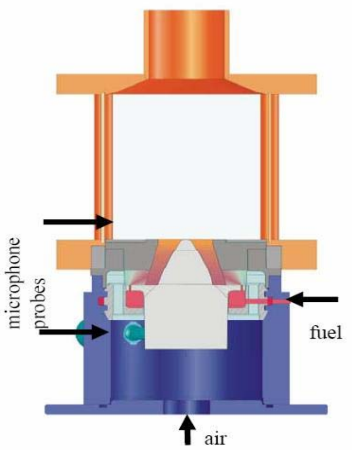


Figure 3. Complete experimental rig layout. Some basic geometrical properties are indicated.

Figure 4. Detail of DLR's combustion chamber.

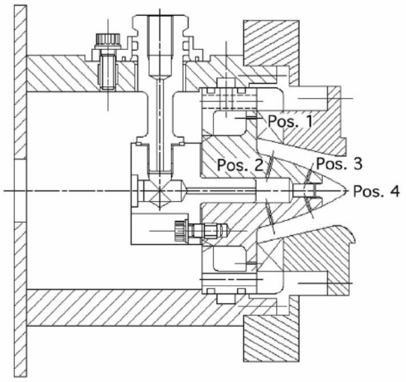


Figure 5. Technical drawing showing in section the injector, the fuel supplier and the swirler.

Figure 6. Swirler detail without the central cone.

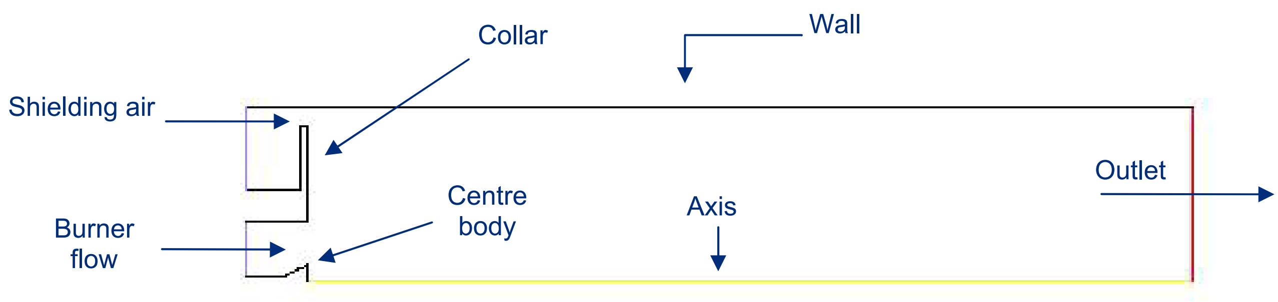
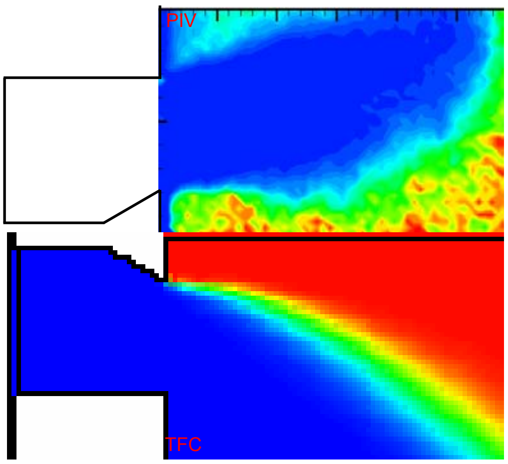


Figure 7. Computational domain and boundary conditions applied.



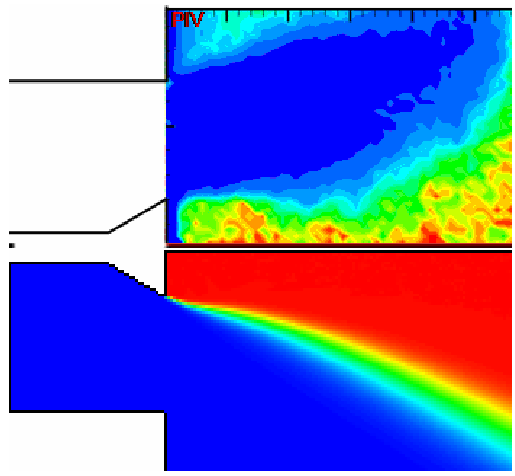
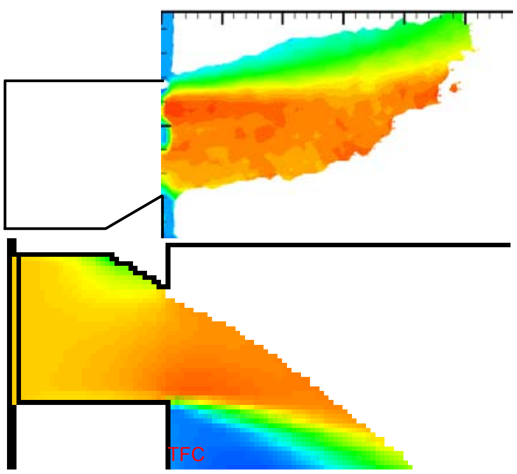


Figure 8. Comparison of predicted and measured contours of the Favre averaged progress variable (TFC, SOFIE).

Figure 9. Comparison of predicted and measured contours of the Favre averaged progress variable (TFC, Fluent™).



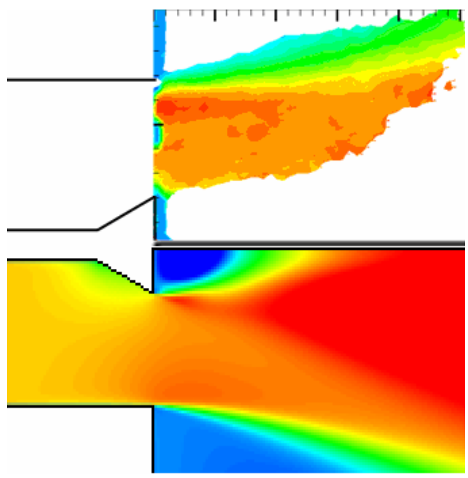


Figure 10. Comparison of predicted and measured contours of the reactant velocity (TFC, SOFIE).

Figure 11. Comparison of predicted and measured contours of the reactant velocity (TFC, Fluent™).

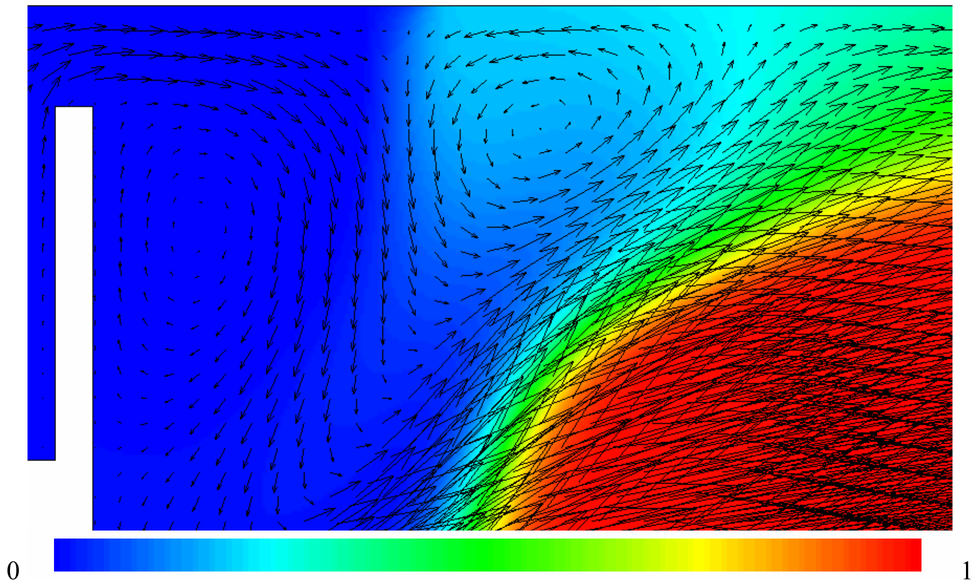


Figure 12. Velocity vector displayed over progress variable contour.

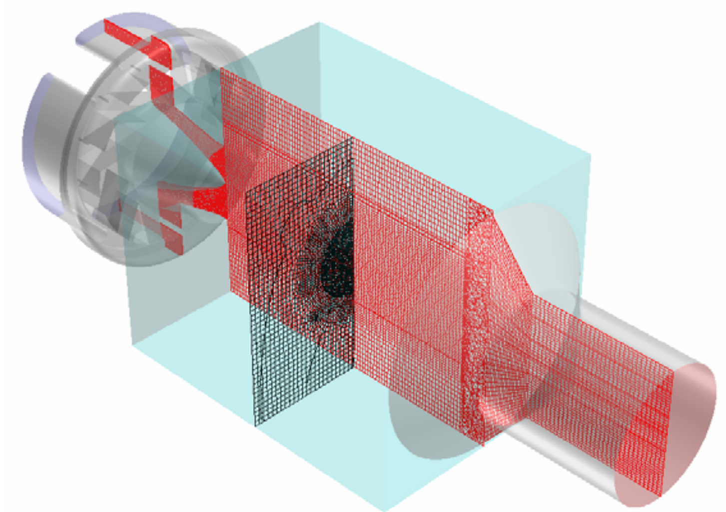


Figure 13. Complete simulation domain and computational grid.

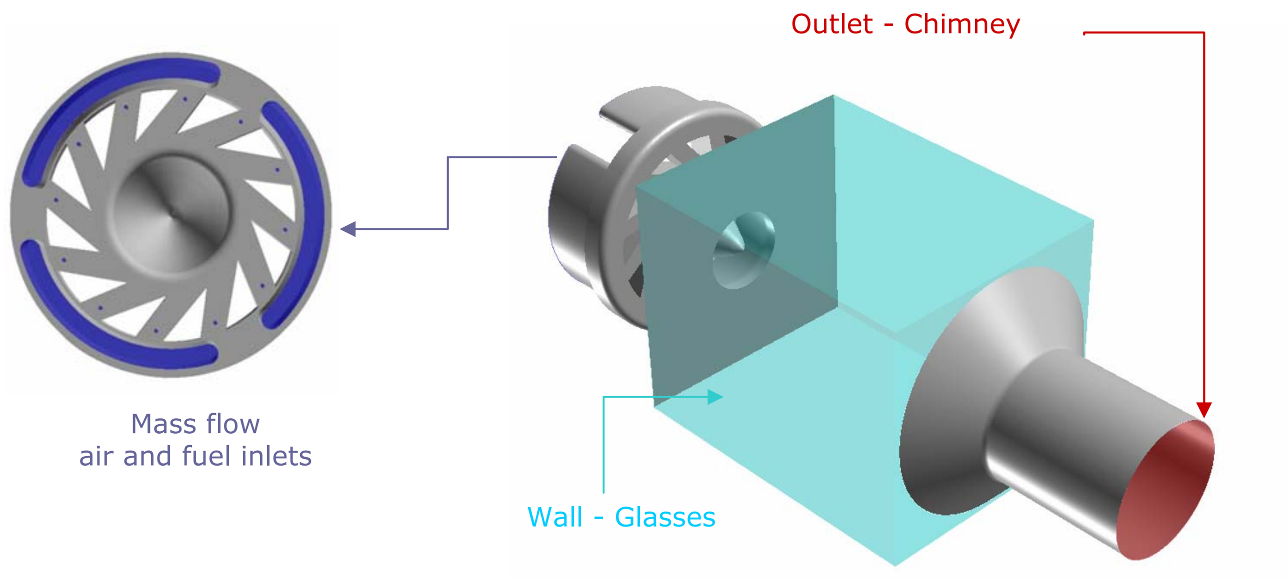


Figure 14. Boundary Conditions.

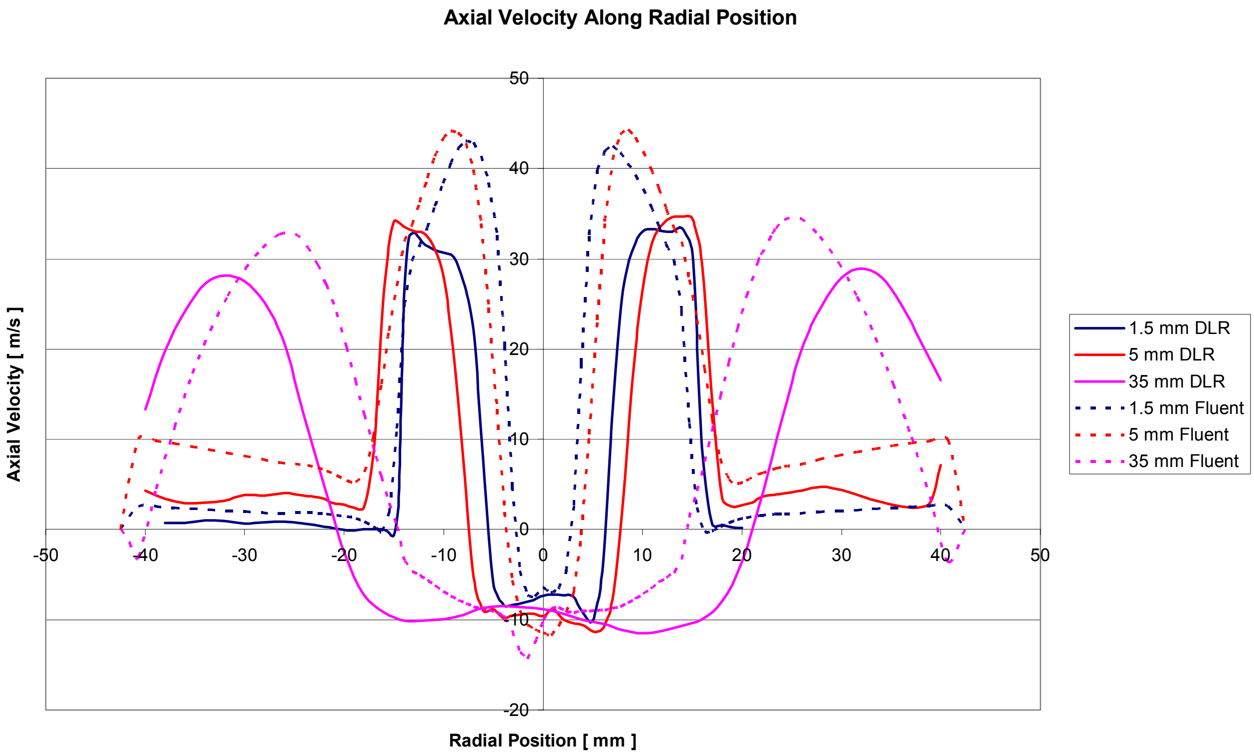


Figure 15. Predicted axial velocity profiles compared to experimental measurements (Fluent™).

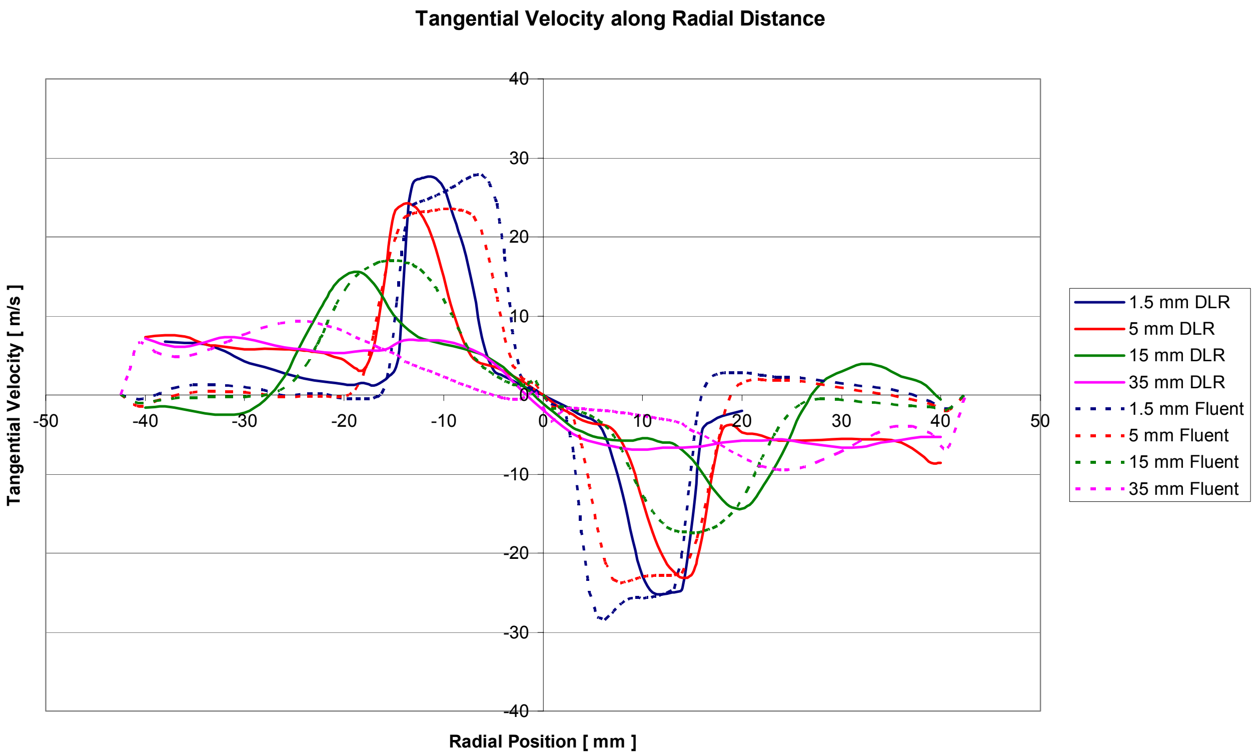


Figure 16. Predicted tangential velocity profiles compared to experimental measurements (Fluent™).

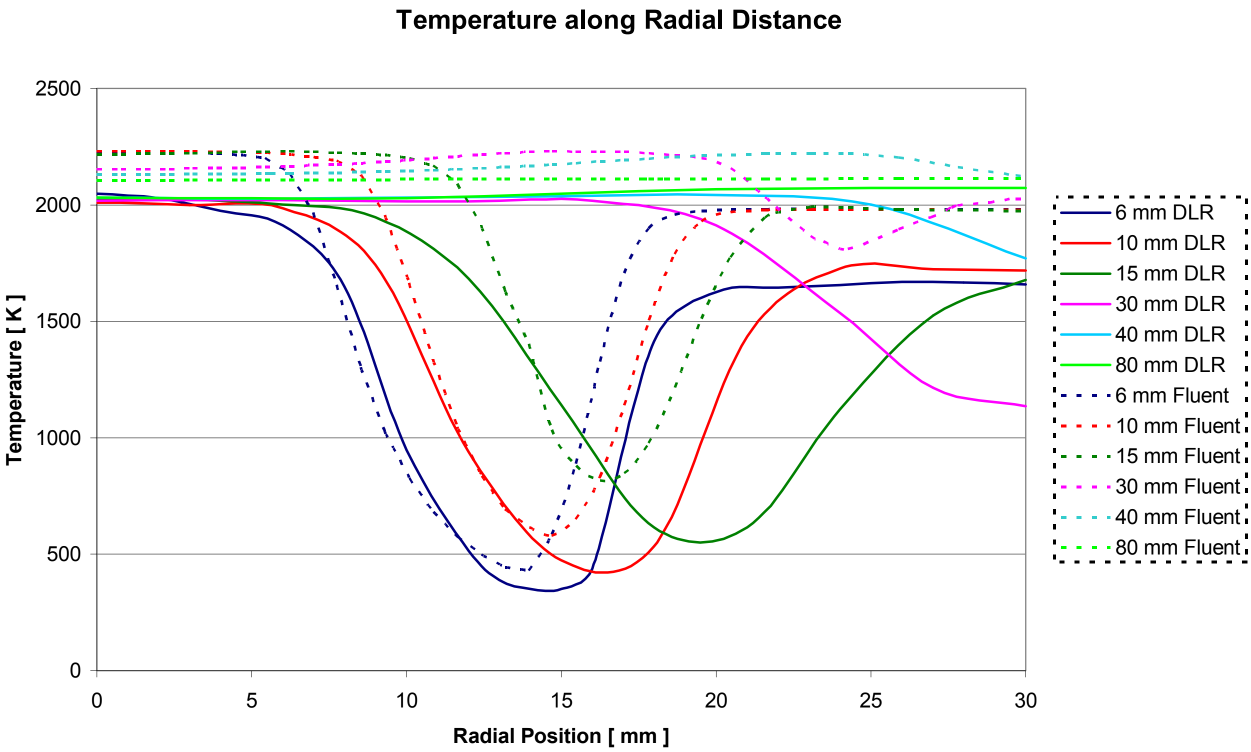
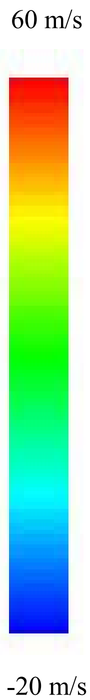


Figure 17. Predicted static temperature profiles at different distances from the burner's nozzle compared to experimental measurements (Fluent™).



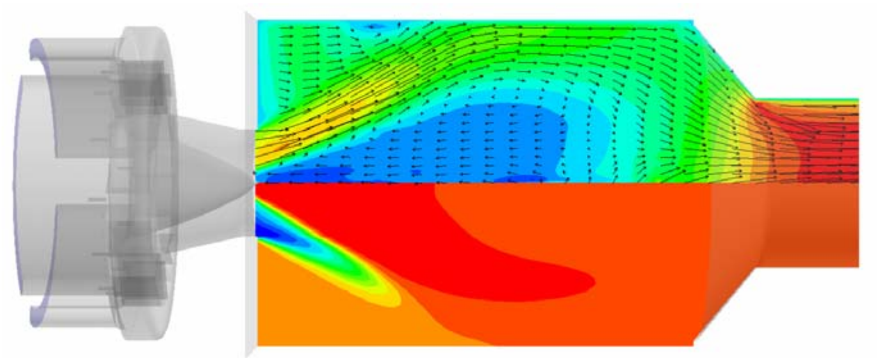
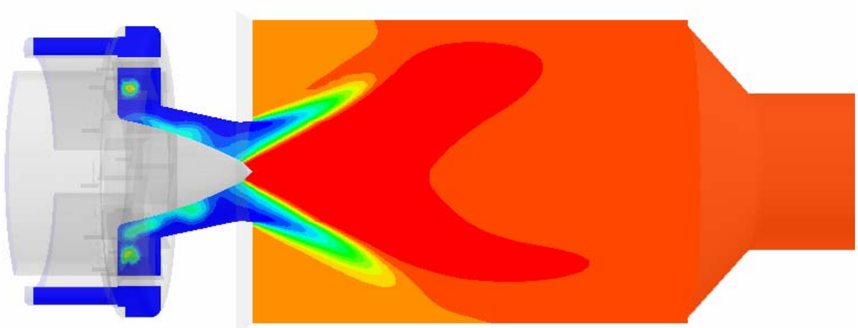


Figure 18. Aerodynamic and temperature field. Axial velocity vectors show the recirculation pattern inside the combustion chamber.



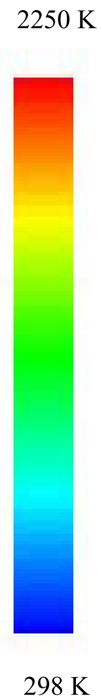


Figure 19. Contour of static temperature (Fluent™).

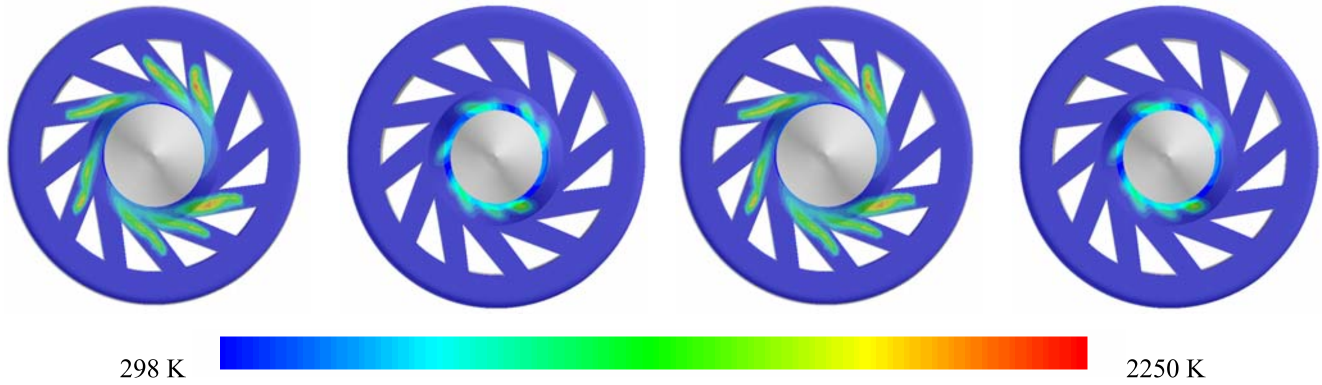


Figure 20. High temperature pockets proceeding through the injection cone.

Figure 21. Laminar flame velocity contour displayed inside swirler and injector.

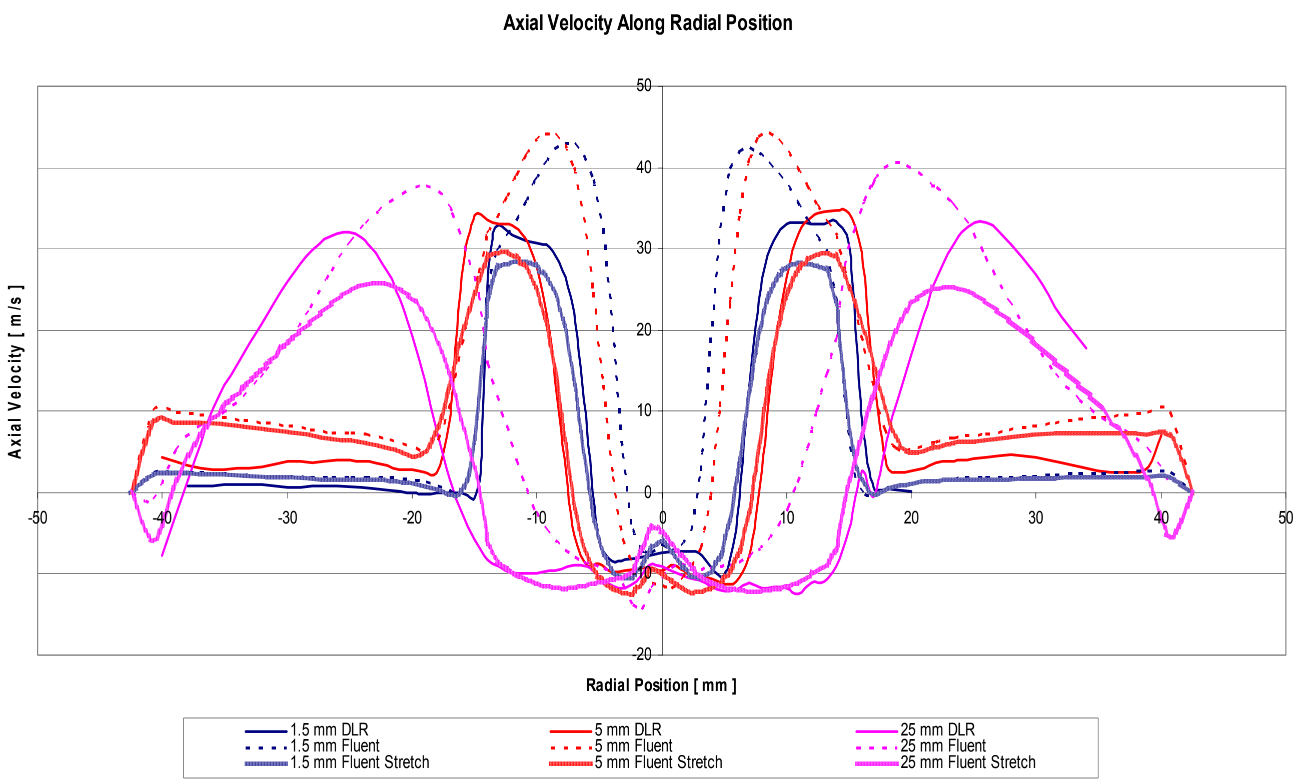


Figure 22. Predicted axial velocity profiles compared to experimental measurements implementing the flame stretching correction (Fluent™).

Variable	Reactants Inlet	Shielding Air Inlet
Axial velocity	9,227 m/s	0.463 m/s
Turbulence intensity	20%	1%
Turbulence length scale	3.5 mm	3.5 mm
Temperature	293 K	293 K
Equivalence ratio	0.8	0
Burner exit	Outlet	
Fuel	Propane	
Centre body diameter	15 mm	
Reactant dynamic viscosity	$1.789 \cdot 10^{-5}$ kg/ms	
Pressure	1.013 bar absolute	

Table 1. Boundary condition for the propane burner simulation.

Variable	Air Inlet	Fuel Inlets
Mass flow	0.01221 kg/s	$4.96 \cdot 10^{-5}$ kg/s
Turbulence intensity	2 %	2 %
Hydraulic diameter	0.05 m	0.000987 m
Inlet Temperature	298 K	298 K
Equivalence Ratio	0.83	
Fuel	Methane	

Table 2. Boundary condition for the methane burner simulation.