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RANS studies of hydrogen-enrichment premixed turbulent flames

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Abstract: In this study, we show numerical predictions of the Zimont and Peter's turbulent flame speed models for low-swirl Methane/Air/Hydrogen flames [1]. These models are contained as default options within the ANSYS Fluent Premixed reaction model. Two distinct simulation tasks as part of the present study are – non-reacting and reacting flows, for with three different methane mixtures in compositions added with – 0, 40 and 60% hydrogen. The results show that the RANS approach provides a reasonable prediction of the cold flow conditions, whilst the reacting flow conditions, good agreement is reached up to 40% enrichment, except near the recirculation region,.

Keywords—Combustion, Hydrogen Flame, Enrichment, Numerical Analysis

Nomenclature

l_*^q = Ewald's corrector

α = Thermal diffusivity

Subscript l = Laminar

Subscript u = Unburnt

μ_i = Viscosity (material i)

δ = Laminar flame brush thickness

l_f = Flame brush thickness

l_t = Turbulence length scale

Subscript t = Turbulent



\bar{c} = Mean progress variable

U = Velocity

∇ = Gradient

S_c = Schmitt number

\hat{u} = RMS velocity

ρ = Density

1. Introduction

Hydrogen is a practical solution to the worldwide drive to reduce polluting emissions. The methods of ‘green’ hydrogen production provide relatively low yields that would be inadequate for widespread 100% hydrogen combustion; however, it would be suitable for lower levels of hydrogen enrichment of hydrocarbons as an intermediate compromise. As hydrogen enrichment offers a number of the benefits of hydrogen combustion, namely reduced emissions, this provides a stepping-stone towards pure hydrogen combustion.

With the recent advances in computer technology, the use of computational fluid dynamics as a tool to study reacting flows has become more feasible. This study seeks to extend the scope of this approach via the validation of two commercially available turbulent flame speed closures; within the ANSYS Fluent premixed reaction model as applied to enrichment of hydrogen combustion. The low-swirl flame examined as part of this study was generated using a model of the low-swirl injector seen in Figure 1. The flame itself relies on the divergent nature of the flow to facilitate aerodynamic stabilization rather than utilizing a bluff body as in some flames. The flame stabilizes where the local fluid velocity equals the turbulent flame speed (approximately 2 m/s).



Figure 1 - Low Swirl Injector [12]

2. Flame background

The hydrogen doping of methane significantly affects the structure of the resulting flame with a shift from a wrinkled, continuous flame front to a discontinuous, cellular structure. This discontinuous cellular structure poses the greatest challenge for reaction models. Figure 2 shows the concentrations of the OH radical identifies the reacting regions of the flame, clearly the hydrogen flame has extinguished at each of the wrinkled indents. This is where the strain rate has exceeded 1061 s^{-1} . Extinguished regions do not reignite because when a section of the flame front extinguishes the fuel diffuses towards the reactions on either side of the region. In the study by Bell, et al. [2] finds that almost 97% of the hydrogen had diffused out of the extinguished region preventing re-ignition.

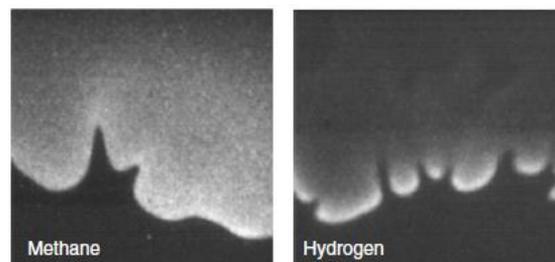


Figure 2 - PLIF images of methane and hydrogen flames [2]

In addition to the visible increase in wrinkling (seen by the human eye as a thickening of the flame brush) the turbulent flame speed also increases; this in turn decreases the time-scale of the flame that means the flame is more robust. This is because the flame is able to react to changes in strain more often, which minimizes the occurrence of the large-scale changes in strain that cause extinction; this then means that hydrogen flames have a greater flame area.

3. Literature Review

To date the RANS approach to turbulence modelling has been one of the most prevalent due to the simple, efficient use of resources; in particular, the k - ϵ model is widely used. Eldrainy, et al. (2009) uses, with a reasonable agreement

with experimental data [5]. Mameri and Golkalp [9] and Mardani, et al. [10] who used the Pope correction with good agreement found in each case, took a modified approach. Saqr, et al., [14] compared the performance of the unmodified k- ϵ with the Realizable k- ϵ model and found the Realizable model to be a significant improvement [14]. This was also observed by Shih, et al [16] where the modified model ‘performed better than the standard k- ϵ in almost all the cases tested’ [16]. This observation was noted by Rohani and Saqr who employed this model, however they stated that because of the way ‘the dissipation of turbulence energy is calculated’ [13] this model should be teamed with a flamelet model to obtain the best results. The improvement noted in regards to this model was to be expected as this model was designed to mitigate a number of the issues with the standard model, particularly the way in which the eddy dissipation was modelled. This was addressed in the Realizable model via a ‘new eddy-viscosity formula and a new dissipation equation’ [15]. As a final note regarding two equation models the study by Engdar and Kingmann [5] considered all the common two equation models including the k- ω and SST k- ω models. At the most relevant swirl value they found the best performing model to be the SST k- ω however this still performed poorly, significantly over-predicting the axial velocity [6]. This study also highlighted that neither the standard k- ϵ or the curvature modified k- ϵ models properly predicted the recirculation region [6].

Both Jawarneh & Vatista [7] and Su, et al., [17] used the RSM model and achieved good agreement with experimental data. However, in the works of Meier, et al., poor agreement with experimental data was found with the recirculation region significantly over-predicted [11]. Shamami and Birouk [15] assess the performances of all previously mentioned models. This study applied the models to a swirling flow with a sudden expansion at the swirl values 0.4 and 0.81, the former of which is of interest here. “One may conclude that amongst the two-equation eddy viscosity models, the k- ϵ and SST show the worst and best predictions of the mean swirl velocity profiles, respectively” [15]. Conversely, however the k- ϵ model provided the most accurate prediction of the central recirculation region size. The RSM and RSM SSG models produced “the best predictions of the mean velocity profiles” [15] and the closest measurements of the corner recirculation regions though these were not especially accurate [15].

In terms of general numerical geometry, the dimensions are given in both validation studies. Reacting validation: *Laboratory investigations of a low-swirl injector with H₂ and CH₄ at gas turbine conditions* [3] and non-reacting validation: *Fuel effects on a low-swirl injector for lean pre-mixed gas turbines* [8]. As non-reacting results were not available from the core study [3] in order to validate the non-reacting model the geometry and flow conditions were altered slightly to allow the cold results from [8] to be utilised.

The possibility of not modelling the swirler and merely applying a swirl value was examined, however Day, et al. [4] completed a detailed study into the possibility and “considerably better agreement was found between simulated and measured profiles when the flow generated inside the nozzle was included” [4].

4. Numerical Analysis

Initially, using an optimal meshing approach, a hybrid mesh with the combustor and pre-swirl sections are fully structured. Because of the conflicting approaches taken in literature, we consider a full turbulence model and a solver set up as part of this numerical work, the final settings are given in Table 1.

Table 1 - Fluent solver settings

Setting / Scheme	Value
Momentum	1 st order upwind
Pressure	PRESTO!
Pressure-Velocity coupling	SIMPLE
Turbulence dissipation	1 st order
Turbulence energy	1 st order
Reynolds stress	1 st order

Table 2- Mesh statistics

Entity	Value (mm)
Combustor (Max/wall)	2.0 / 0.5
LSI (Max/wall)	0.9 / 0.6
Pre-Swirl (Max/wall)	2.0 / 0.5
Shear layer	0.5
Core	0.9
Total no of elements	3892722

All of the turbulence models tested as part of this study utilized the standard model constants and for those that contained wall functions uses the scalable wall function on each occasion [1].

Mean Reaction rate, premixed model: $\frac{\partial}{\partial t}(\rho \bar{c}) + \nabla * (\rho \bar{v} \bar{c}) = \nabla * \left(\frac{\mu_i}{Sc_i} \nabla \bar{c} \right) + \rho S_c$

The turbulent flame speed model: $U_t = 0.52 * (\dot{u})^{\frac{3}{4}} U_l^{\frac{1}{4}} \alpha^{-\frac{1}{4}} l_t^{\frac{1}{4}}$

Peters Flame Speed Model: $U_t = U_l(1 + \sigma_t)$ and $\sigma_t = -\frac{a_4 b_3^2 l_f}{4 b_1 \delta} l_*^q + \left[\left(\frac{a_4 b_3^2 l_f}{4 b_1 \delta} l_*^q \right)^2 + \frac{c_s b_3^2 \dot{u} l_f^2}{2 U_l \delta l_t} \right]^{\frac{1}{2}}$

for constant values, see [1].

5. Results and Discussion

Addressing the cold results first, we validate the results against [8], only the positive X values are shown here. The flow conditions for this section of the study were as per the validation study [8]. All the models under predict the velocity in the core region (Figure 3). This is attributed to assumptions made during the geometry generation stage and not due to prediction errors, given the correlation between the different models. Unfortunately, time did not permit revisiting the geometry to address this. The reacting region is reasonably well predicted, except with a slight over prediction at the peak and approaching the wall, and the two RSM models producing asymmetric results. Therefore, we employ Realizable k-ε model for all simulations here.

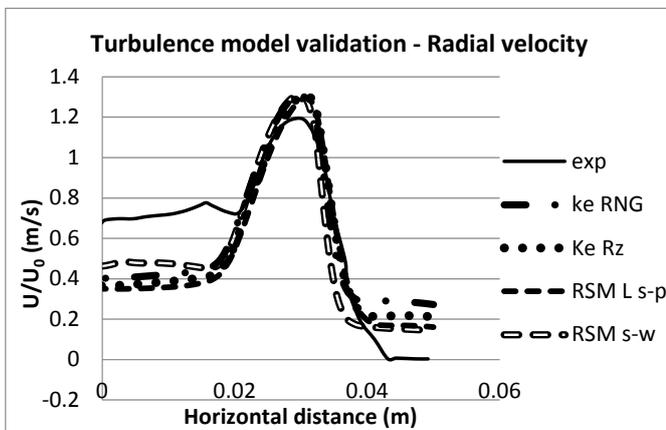


Figure 3 - Turbulence model validation, radial velocity plot: k-ε RNG, Realizable k-ε, RSM Linear Pressure-Strain, RSM Stress-Omega

As an additional comparison, the velocity plot from this study compares well with the findings of [12] with good agreement found between the two studies. Please note this contour plot refers to the flow conditions as per the reacting validation study [3].

The first reacting results presented here are from the pure methane case for both turbulent flame models. For validation purposes, we chose experimental data by Cheng, et al. [3]. The results given in Figure 5 show some correlation particularly pre 30mm and within the reaction region, however the flame front has been predicted at 46mm vs the experimental 40mm. Limited correlation can also be

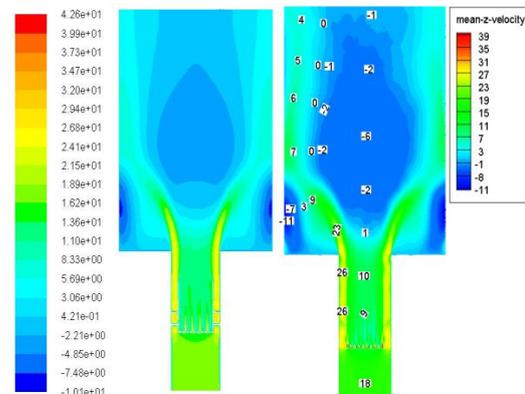


Figure 4 - Left Axial velocity plot, Right axial velocity plot from [12]

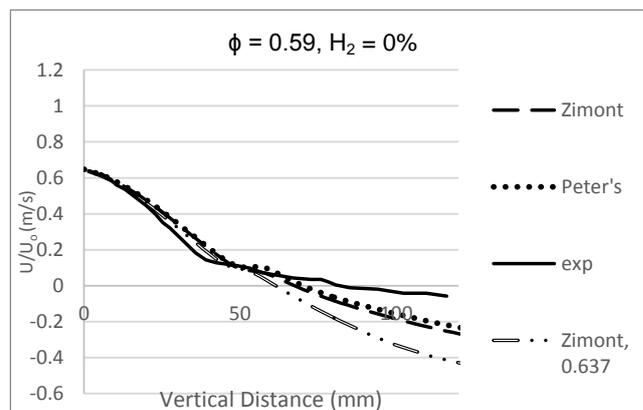


Figure 5 - Axial profile for 100% methane, both flame models, modified Zimont results and experimental

seen beyond 65mm.

The Zimont modification, turbulent flame speed constant = 0.637 given in [1] can be seen to cause further deterioration in the results; so this is not taken further. Whilst the numerical predictions show significant correlation with each other it can be said that beyond 65mm Peters flame speed model produced slightly yield more accurate results. However, the difference was marginal.

Figures 6 and 7 show the numerical predictions and experimental results for 40% and 60% hydrogen respectively. Once again, the predictions beyond 60mm show significantly deteriorated correlation. As this can be seen across all of the results including 0% hydrogen it is this studies opinion that this error was likely to be due to an over prediction of the axial velocity in the recirculation region on the part of the RANS model, as in a number other studies, for example

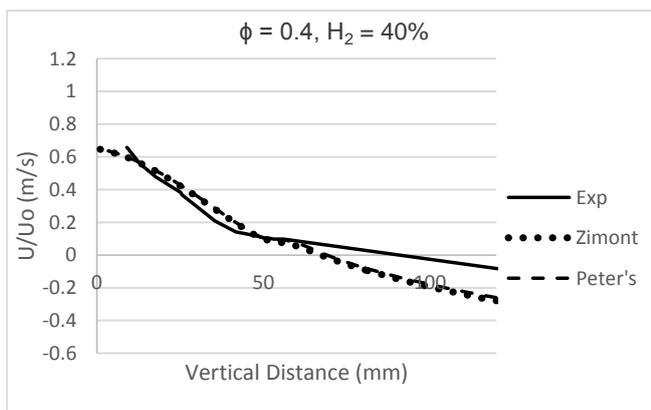


Figure 6 - Axial profile for 40% hydrogen, both flame models and experimental ($U_0=18$)

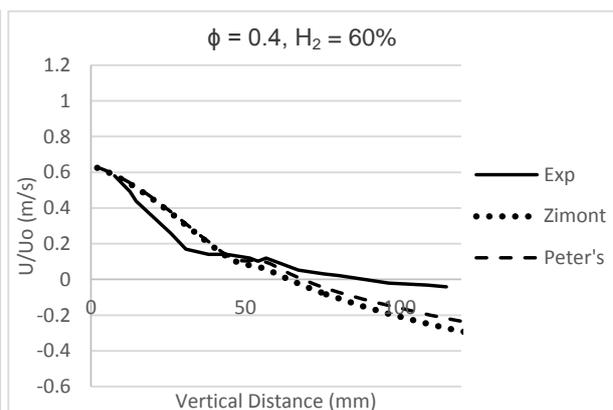


Figure 7 - Axial profile for 60% hydrogen, both flame models and experimental ($U_0=18$)

[18]. An interesting is that the difference in magnitude increases with the level of enrichment, with additional deterioration in the 60% hydrogen predictions pre 50mm of both reaction models.

6. Conclusions

This study highlights a viable stepping-stone towards pure hydrogen combustion through hydrogen enrichment. Given the feasibility of this approach and the rising cost of experimental testing, numerical predictions is a solution. Here, we assess the validity of two turbulent flame models contained within the ANSYS Fluent premixed combustion model applied to enriched hydrogen combustion. We find that the accuracy of the numerical predictions would deteriorate with increase in levels of hydrogen enrichment. An additional point worth noting is that the RSM turbulence model group (seven-equation models) is significantly less sensitive to solver set up than the two-equation models.

In all simulations cases, there is every prediction of the axial velocity in the recirculation region, and we attribute this consistent error to the performance of the Realizable $k-\epsilon$ turbulence model and not so much to the reaction model. The additional deterioration in this region at levels of enrichment greater than 40% is due to the performance of the reaction model. The effect of the RANS simplification on the flow conditions needs further assessment using the LES approach to turbulence modelling. The results through LES would allow for the accurate detailing of the errors and cause of these errors with greater confidence.

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