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Assessment of Turbulence Models for Simulating Internal Reacting Flows in a Ducted Rocket

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Abstract

A parametric computational modelling of flow, temperature and species field in a generic ducted rocket (DR) combustor has been undertaken. Calculations (3D) were performed on an unstructured mesh with approximately 150000 hexahedral cells that was selected following grid-independence testing. A segregated solver and a second order discretisation scheme were used for all equations. A comparative assessment of three turbulence models was performed, using: the Reynolds Stress Model-RSM (taken as a benchmark for comparison), the Realisable k-ε (RKE), and the Renormalised Group Theory model (RNG). The results showed that the RKE turbulence model performed only slightly better that the RNG model in regions of high swirl, however the RNG model showed closer predictions to the RSM in weaker swirl regions. The RKE model however converged more rapidly than the RNG hence was selected in all subsequent calculations.

For reacting flow modelling, turbulence-chemistry interaction was accounted for using a β-shaped PDF. The chemistry of the mixture was represented in the model using an Equilibrium Chemistry Model (ECM). A look-up table (in mixture-fraction space) was generated for gaseous air-ethylene mixture. This mixture was selected because it reasonably represents the chemistry of a particular DR solid-fuel, but is much easier to model. The effect of air-fuel momentum ratio on flow and combustion characteristics was investigated. It was found that increasing the air-fuel momentum ratio improves the thermal efficiency of the combustor, reduces unburnt fuel, lowers CO emission, but did not have a significant effect on flow structure.

Introduction

Ducted rockets are emerging as a potential candidate for powering existing and future high-speed missiles, particularly beyond visual range air-to-air missiles. Their primary advantages over conventional rocket-propelled systems are longer operational range and higher average velocity. The experimental testing of different DR designs is complex and expensive. An alternative option for assessing DR performance is to employ a Computational Fluid Dynamics (CFD) approach. It is a cost-effective tool that allows external and internal flow structure, temperature field, and chemical species distribution to be numerically simulated and visualised for various geometric configurations and flow conditions [3,4,7,8].

The prime objective of this study is to model the aerothermochemical processes in a ducted rocket combustor and to examine the effect of different turbulence models on the solution. The effect of air-fuel momentum ratio on the flow, temperature and chemical species fields is also examined.

Combustor Model

A generic DR geometry was selected as shown in Fig. 1. The combustor is 100 mm in diameter and 500 mm in length. It has dual air inlets each 38 mm in diameter, spaced 90° apart circumferentially and inclined 60° with respect to the centre line along the axial direction. This geometry configuration is believed to create a highly stable recirculating flow in the dome region [9,10]. The dome height is 57 mm. The fuel port is 27 mm in diameter with its centre-line aligns with the combustor's. The current model did not include details of the intake ducts or the booster nozzle. The geometry and dimensions of the intakes and the air and fuel flow rates do not necessarily represent realistic rocket motor configuration.

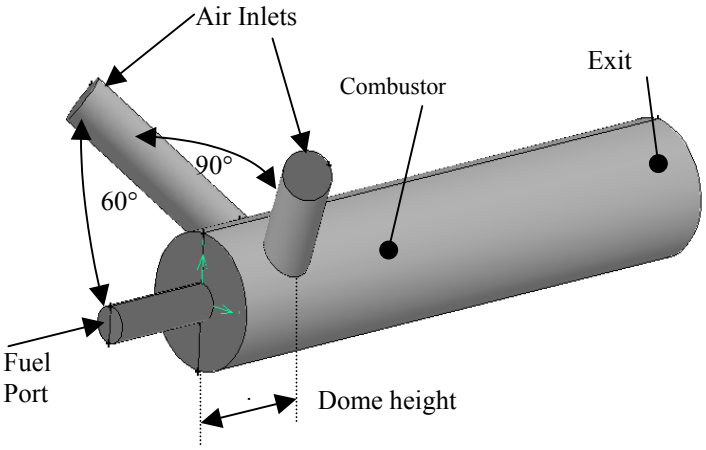

Figure 1. Basic geometry of a generic ducted rocket combustor.

Only half of the combustor is modelled due to the geometrical symmetry along the central longitudinal plane of the combustor. Three-dimensional calculations were performed for weakly compressible non-reacting as well as chemically reacting flows with different inlet mass flow rates. The air mass flow rate was kept constant at 0.25 kg/sec, and the fuel flow rate was adjusted (0.017 kg/s – 0.2 kg/s) to simulate various air-to-fuel momentum ratios. Whilst varying the fuel or airflow rates also changes the mass ratio, the air-to-fuel momentum ratio has been identified as a critical parameter for describing the flow field [10]. In all calculations the combustor pressure was kept unchanged at 0.5 MPa.

The commercial CFD code FLUENT (version 5) was used for all calculations. FLUENT is a finite-volume unstructured code that solves transport equations for mass, momentum, energy, turbulence and chemical species. A segregated solver (transport equations are solved sequentially) and a second order discretisation scheme were used for all equations. Solution convergence was determined by ensuring that the following

criteria are met. Firstly, the sum of the residuals of the solved equations drops below a predetermined value that was set separately for each equation, and secondly profiles of selected field variables (e.g. velocity or temperature) at critical locations are stabilised and no longer changing with iterations.

Results and Discussion

A mass-averaged swirl number ($\widetilde{S}$) is introduced to compare solutions of various grids and to assess the performance of different turbulence models. $\widetilde{S}$ is defined as the ratio between the mass-averaged tangential and axial velocities at a given plane and is evaluated by:

$$\widetilde{S} \equiv \frac{\int W \rho \vec{V} \bullet d\vec{A}}{\int U \rho \vec{V} \bullet d\vec{A}}, \qquad (2)$$

where U and W are the local axial and tangential velocity components, respectively. ρ is the mass density of the fluid, $d\vec{A}$ is a surface area of a grid element and $\vec{V}$, is the velocity vector.

Grid-Independence Analysis

The adequacy of the grid size is first evaluated. Five sets of calculations were carried out for a non-reacting flow using the RKE turbulence model for various meshes with 150000, 177000, 223000, 376000 and 500000 cells. Figure 2 shows the axial distribution of the mass-averaged swirl number for the different grids. It shows a similar $\widetilde{S}$ distribution and magnitude for all the meshes. Therefore all subsequent calculations were carried out using a grid with 150000 cells because it required a moderate computing time and memory without compromising the accuracy of the solution.

Turbulence Models & Flow Field Structure

The flow in a typical DR combustor is characterised by regions of recirculation, intense swirling and separated flows. It is therefore essential that an appropriate turbulence model be chosen. The weakness of the standard k-ε turbulence model in predicting swirling or recirculating flows is well documented and therefore it was not considered in this study. Three alternative turbulence models were evaluated; the Reynolds Stress Model (RSM), the Realisable k-ε (RKE), and the Renormalised Group Theory model (RNG). For the purpose of turbulence model assessment the calculations were carried out for non-reacting flow using air as the working fluid in all the inlets. The air mass flow rates through the air and fuel ports were set to 0.25 kg/s and 0.05 kg/s, respectively. The complexity of the flow structure is evident in Fig. 3, which shows plots of velocity vectors (for case C_4) in the dome region, identifying recirculation zones, and at lateral cross-sections Z/D=0.5 and Z/D=1, which illustrate the complex swirl patterns.

Figure 4, shows the mass-averaged swirl number distribution obtained for the three turbulence models. It indicates a strong swirling flow in the core region Z/D < 1.5, which then alters its rotational direction within a short distance of one combustor diameter creating intense mixing. Overall all three turbulence models predicted a similar swirl distribution but had a lesser agreement in predicting the magnitude of $\widetilde{S}$.

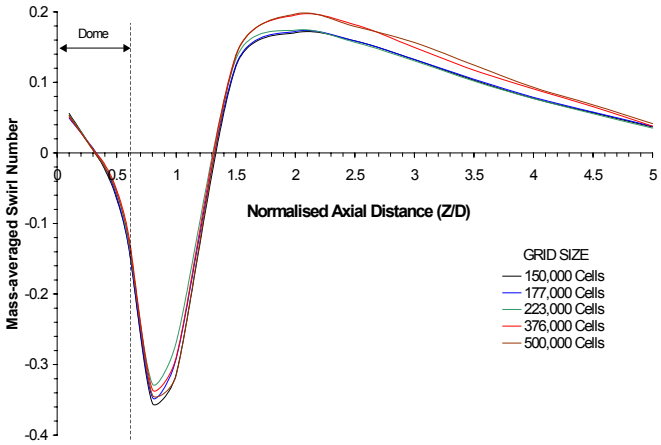

Figure 2. Effect of grid size on solution accuracy.

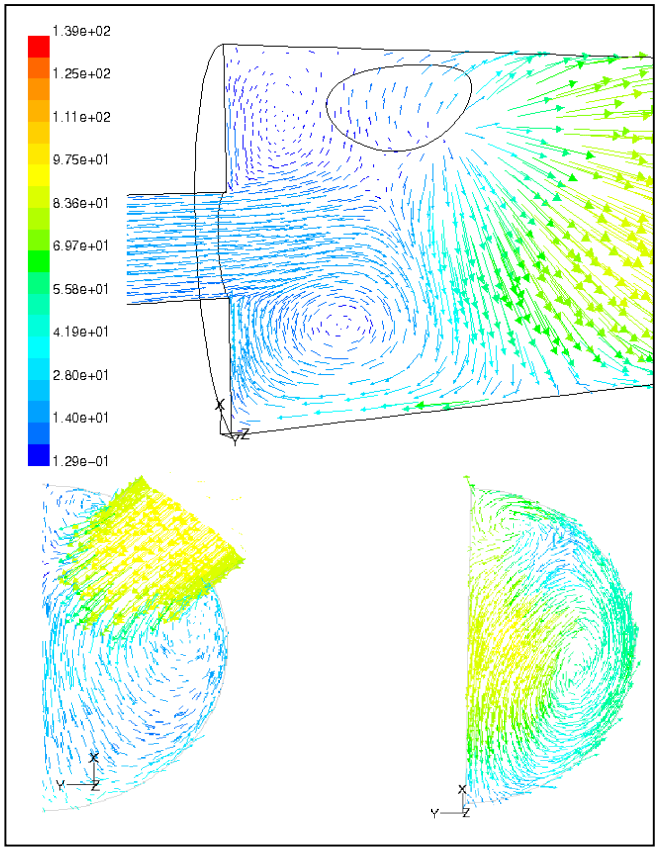

Figure 3. Velocity vectors (m/s) along the central longitudinal plane showing the recirculation zones in the dome region (top) and the swirling pattern at lateral cross-sections Z/D=0.5 (bottom left), and Z/D=1 (bottom right) for case C_4.

It is interesting to note that the discrepancies between the models are smaller in the core region (Z/D < 1.5) where the flow structure is more complex than in the downstream region (Z/D > 2). In the core region the RSM and RKE show similar predictions but both differ slightly from the RNG model. In the downstream region however, both the RKE and RNG predictions were different from the RSM solution.

All three turbulence models predicted similar flow structure in regions of high swirl, but had a lesser agreement in the weaker swirl regions downstream beyond Z/D > 2. With reference to the RSM (used as a benchmark model), the RKE model performs exceptionally well in the core (strong swirl) region Z/D < 1.5,

while the RNG results were closer to the RSM in the downstream region.

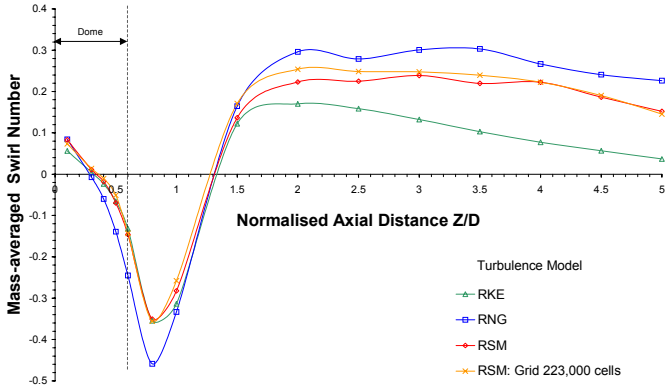

Figure 4. Swirl number distribution using various turbulence models (150000 cells, unless othewise stated).

Overall the RKE under-predicts the absolute magnitude of the swirl number while the RNG model always over-predicts it. For chemically reacting flows the region of intense mixing Z/D < 2, is also the region where turbulence-chemistry interaction is critical for flame stability. For this reason the RKE turbulence model was selected for modelling the chemically reacting flows. Calculations using the RSM model were also repeated using a finer grid with 223000 cells and showed similar predictions to those of the coarser grid (Fig. 4). This result reinforces the earlier conclusion on grid-independence.

Combustion Model

The combustion regime in a DR can be characterised as a non-premixed since the air and fuel streams are initially separated. Assuming that the chemical reaction time scale is much smaller than the turbulence mixing time scale, the fast chemistry assumption can be used to model the combustion process. An Equilibrium Chemistry Model (ECM) was used to represent the chemistry of the reacting mixture. The ECM implies local thermochemical equilibrium exists between the fuel and oxidiser at the molecular level. The model can predict the formation of intermediate species without implanting a detailed kinetic scheme. This model was selected because it offers a reasonable compromise between the computationally elaborate Flamelet Model and the simplistic Mixed-is-Burnt Model.

A combined PDF-mixture fraction (ξ) approach offers drastic simplifications for modelling the turbulence-chemistry interaction. In this approach only two additional transport equations (for the mixture fraction and its variance) are required instead of solving an additional transport equation for each chemical species. Linking the means and higher moments of the thermochemical properties is achieved using a predefined probability distribution function (PDF). A β-function PDF was selected because it most closely represents experimentally observed PDFs [1,5].

Calculations were carried out for a number of air-ethylene (C_2H_4) mixtures. This mixture reasonably represents the chemistry of a particular experimental DR solid-fuel, but its chemistry is much easier to model than that of the solid fuel. The inlet temperature of the ethylene and air was set to 400K and 700K, respectively. The chemistry of the mixtures (in ξ-space) was represented as follows: for each set of a given compositions defined in terms of the mean and variance of ξ, and mole fraction of C_2H_4, O_2, and N_2, the equilibrium temperature and concentrations of major species (C_2H_4, O_2, N_2, CO, CO_2, and H_2O) were calculated and stored in a look-up table that is accessible to the flow solver. Table 1 summarises the various conditions that were modelled and the maximum adiabatic flame temperature within the combustor obtained from the CFD calculations. In terms of an overall stoichiometry case C_4 (and C_8) represents a stoichiometric ratio while cases C_1-C_3 are fuel-rich mixtures and C_5-C_7 are fuel-lean mixtures.

Case	Fuel Mass Flow Rate (kg/s)	Air-to-fuel Momentum Ratio	Adiabatic Flame Temperature (K)
C_0	0.05	10	Mixing only
C_1	0.2	0.67	2494
C_2	0.1	2.5	2479
C_3	0.05	10	2408
C_4	0.017	86	2525
C_5	0.0135	136	2527
C_6	0.0101	243	2522
C_7	$6.7x10^{-3}$	542	2510
C_8	0.05	92	2529

Table 1. Summary of modelled operating conditions. In all cases, air and fuel inlet temperatures are fixed at 700K and 400K, espectively. Air flowrate is kept constant at 0.25 kg/s, except for C_8 where an air flowrate of 0.75 kg/s is used.

Table 2 lists the gas temperature, velocity and mole fractions of major species at the exit plane of the combustor. Comparing cases C_0 and C_1 in Fig. 5 clearly demonstrates that the combustion has significantly affected the flow field causing a noticeable reduction in flow swirl intensity particularly within the core region. Nevertheless the flow structure within the combustor remains largely unchanged. This result also indicates that using a RKE or RNG turbulence model is justified due to weakening in swirl intensity. The results in Table 2 indicate that increasing the air-fuel momentum ratio reduces the amount of unburnt C_2H_4 and lowers the exit CO concentration indicating enhanced turbulence mixing and completion of the fuel conversion.

Case	V_{exit} (m/s)	T_{exit} (K)	Exit Plane Mole Fraction (%)				
			C_2H_4	CO	CO_2	H_2O	O_2
C_0	25	650	(Mixing only)				
C_1	89	1574	29.5	11.4	1.21	7.86	0.52
C_2	88	1771	19.4	14.5	0.27	9.49	0.07
C_3	92	2101	7.82	16.9	0.12	10.9	0.01
C_4	95	2425	0.17	6.04	10.4	8.16	3.47
C_5	84	2366	0.07	2.92	12.8	6.88	5.12
C_6	66	2210	0.06	0.08	14.7	5.13	7.85
C_7	49	1919	0.11	0	13.8	3.49	11.3
C_8	272	2388	0.26	6.58	9.8	8.16	3.69

Table 2. Mean values of gas temperature, velocity, and mole fractions of major species at the exit plane of the combustor. In all cases, air and fuel inlet temperatures are fixed at 700K and 400K, respectively. Air flowrate is kept constant at 0.25 kg/s, except for C8 where flowrate of 0.75 kg/s is used.

Another useful indicator for the performance of the combustor that incorporates the effects of turbulent mixing and chemistry-turbulence interaction processes is the local thermal efficiency of the combustor. The mean local thermal efficiency η, (based on

mean local temperature T) is calculated at various lateral cross-sectional planes using:

$$\eta = \frac{(m_f + m_a)C_p(T - T_{ref})}{m_f H_c + H_a} \times 100 \quad (3)$$

where m_f and m_a are the fuel and air mass flow rates, respectively, C_p is the mean local specific heat, H_c is the heat of combustion of the fuel (50.4 MJ/kg) and H_a is the flow rate enthalpy (MJ/s) at the air inlet. The inclusion of H_a in Eq. (3) is to account for different air inlet conditions such as the effect of shock wave compression, altitude etc. T_{ref} is a reference temperature set to 650K (a representative average of the fuel and air inlet temperatures). The results, presented in Fig. 6, show that the thermal efficiency of the combustor is directly correlated with the air-fuel momentum ratio with higher efficiency achieved at higher momentum ratios. These conditions also correspond to fuel-lean and stoichiometric mixtures, while fuel-rich mixtures (C_1-C_3) yielded much lower thermal efficiencies. The irregularities in the curves within the dome region (Z/D < 0.5) are attributed to temperature variations due to the mixing of recirculated hot gases that are drawn backward from the flame zone with a colder incoming fuel stream.

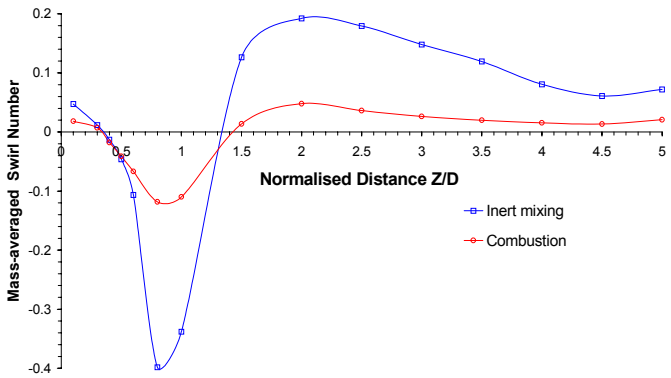

Figure 5. Effect of combustion on flow structure.

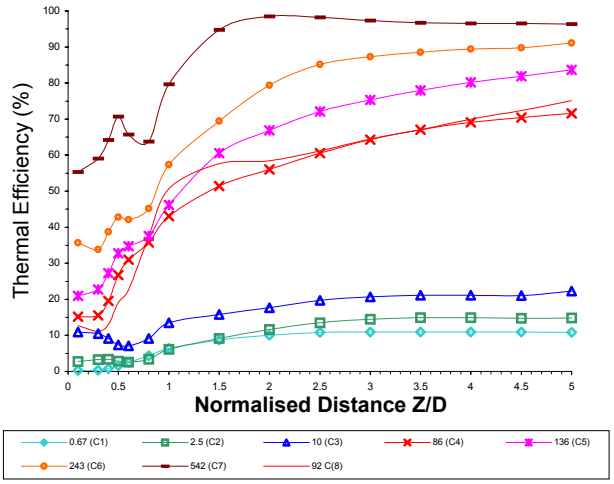

Figure 6. Mean thermal efficiency for various air-fuel momentum ratios.

To examine the effect of air mass flow rate (which is related to the flight speed of the DR) on flow structure and combustion characteristics, a mixture with fuel and air mass flow rates three times larger than in case C_4 is modelled. The momentum ratio however remained similar to that of C_4. The results denoted as C_8 (see Tables 1 and 2 and Fig. 6) showed similar exit species concentrations, temperature and thermal efficiency as case C_4, but had approximately three times higher exit velocity. The flow structure was largely kept unchanged retaining the main flow pattern observed in C_4 with only a minor change in the shape of the recirculation zone. Its elongated shape (observed in C_4) became shorter, more circular in shape and its centre was slightly shifted upstream.

Conclusions

Inert and chemically reacting flows are modelled in a generic ducted rocket combustor using three turbulence models. It is found that the RKE and the RNG models perform equally well when compared to the RSM results. Whilst the RKE model performed better than the RNG in predicting the flow structure in regions with strong swirl, it performed poorly in regions with weaker swirl intensity. This is an interesting outcome since the RKE formulation is intended to better represent the physics of turbulent flows involving recirculation. The effect of combustion on the flow is pronounced, significantly reducing the swirl intensity in the dome region though the bulk of the flow structure remained unchanged. The air-fuel momentum ratio has a strong influence on swirl intensity and on the thermal efficiency of the combustor.

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References

[1] Bilger, R.W., Turbulent Flows with Non-premixed Reactants, in *Turbulent Reacting Flows*, Editors P.A. Libby and F.A. Willimas, Springer-Verlag, Berlin, 1980.

[2] Buchanan, C.R., and Frame, M.J., "A Review of Supersonic Missile Intake Research at DERA", TTPC WPN TP4, Energetic Materials and Propulsion Technology Workshop, DSTO Salisbury, 6 April 2000.

[3] Chakravarthy, M.K., Sundararajan, T., Ganesan, V., and Natarajan, R., Numerical Investigation of Multi Dimensional Reacting Flow In A Dump Combustor, in *2nd Int. Seminar on Fluid Mechanics and Heat Transfer, pp. 85-91, Dec. 17-18, 1997, Dhaka, Bangladesh.*

[4] Cherng, D.L., Yang, V., and Kuo, K.K., Numerical Study of Turbulent Reacting Flows in Solid-Propellant Ducted Rocket Combustors, *J. Propulsion* Vol. 5, No. 6, pp. 678-685, Nov-Dec 1989.

[5] Jones, W.P., and Whitelaw J.H., Calculation Methods for Reacting Turbulent Flows; A Review. *Combust. Flames, 48:1-26, 1982.*

[6] Phillips, D. D., Hewitt, P., and Siebenhaar A., "Rocket Ramjet Boosters For Sustained High Speed Flight", AGARD Symposium on *Future Aerospace Technology in the Service of the Alliance*, Ecole Polytechnique, Palaiseau, France 14-17, April, Vol 3 C8 pp1-10, 1997.

[7] Ravichandran K., Sundararajan, T. , Ganesan, V., and Natarajan, R., Jet Mixing in a Three Dimensional Combustor, in *2nd Int. Seminar on Fluid Mechanics and Heat Transfer, pp. 583-591, Dec. 17-18, 1997, Dhaka, Bangladesh.*

[8] Ristori, A., Heid, G., Cochet, A., and Lavergne G., Experimental and Numerical Study of Turbulent Flow inside a Research SDR Combustor, *AIAA 99-2814, in the* 35th AIAA/ASME/SAE/ASEE Joint Propulsion Conference and Exhibit, 20-24 June 1999, LA, California.

[9] Stowe, R.A., De Champlain, A., and Mayer, A.E.H.J, Modelling Combustor Performance of A Ducted Rocket, *AIAA-2000-3728, 2000.*

[10] Stowe, R.A., De Champlain, A., Mayer, A.E.H.J, and Niemeijer, S.F., Modelling and Flow Visualization of Mixing in a Ducted Rocket Combustor, *AIAA-98-3768, 1998.*