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*Research Article*

# Theory Comparison between Propane and Methane Combustion inside the Furnace

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***Abstract***

*This study used ANSYS FLUENT to model the transport, mixing, and reaction of chemical species. The reaction system was defined by using and modifying a mixture-material entry in the ANSYS FLUENT database. The study used propane $C_3H_8$ for simulation of hydrocarbon combustion and comparison the results with another study for methane $CH_4$combustion for find the difference in combustion temperature and effect of change in specific heat as a function of temperature. The study found that the maximum temperature for propane is less than methane for both states in constant and change of specific heat, and the reason for this attribute because of methane has octane number higher than propane and this effects on flame propagation speed and flame temperature also we note the distribution of maximum temperature is mostly near to wall and axis region as shown in the results . This distribution helps to know where will be the maximum temperature for varies applications. Also the NOx production in this study was dominated by the thermal NO mechanism. This mechanism is very sensitive to temperature. Every effort should be made to ensure that the temperature solution is not over predicted, since this will lead to unrealistically high predicted levels of NO. Because of all this the emission of NOx for methane is more than propane as result for high temperature for methane combustion*

***Keywords:*** *Propane, Methane Combustion etc.*

## Background

Propane has been tested in fleet vehicles for a number of years. It's a good high octane number for SI engine fuel and produces less emission than gasoline about 60% less co, 30%less HC, and 20%less NOx **(Pulkrabek).**Propane stored as a liquid under pressure and delivered through a high pressure line to the engine. In this study, you will use the generalized eddy-dissipation model to analyze the methane-air combustion system. The combustion will be modeled using a global one step reaction mechanism, assuming complete conversion of the fuel to CO2 and H2O. The reaction equation is

$$C_3H8 + 5O2 \rightarrow 3CO2 + 4H2O \quad (1)$$

This reaction will be defined in terms of stoichiometric coefficients, formation enthalpies, and parameters that control the reaction rate. The reaction rate will be determined assuming that turbulent mixing is the rate-limiting process, with the turbulence-chemistry interaction modeled using the eddy-dissipation model.

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## Problem Description

The cylindrical combustor considered in this study **(Ansys inc.)** is shown in **Figure 1**.

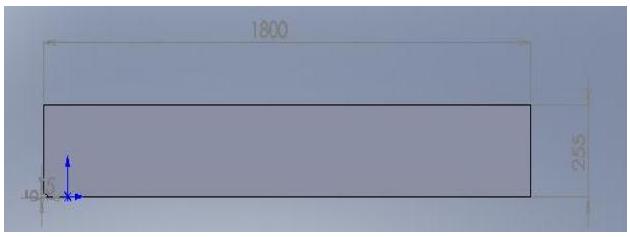



**Figure 1** Problem description

The flame considered is a turbulent diffusion flame. A small nozzle in the center of the combustor introduces propane ($C_3H_8$) at 80 m/s. Ambient air enters the combustor coaxially at 0.5 m/s. The overall equivalence ratio is approximately 0.76 (approximately 28% excess air). The high-speed methane jet initially expands with little interference from the outer wall, and entrains and mixes with the low-speed air. The Reynolds number based on the methane jet diameter is approximately $5.7 \times 10^3$.

**Creating the cylindrical combustor and mesh generation**

The shape of cylindrical combustor is formed by solid program and exports it to workbench of Ansys 12 the shape will be plane for two dimension and the dimension be in SI units (m). Then the ansys program will mesh the shape and It is a good practice to check the mesh after you manipulate it (i.e., scale, convert to polyhedra, merge, separate, fuse, add zones, or smooth and swap.)This will ensure that the quality of the mesh has not been compromised **Figure 2**.

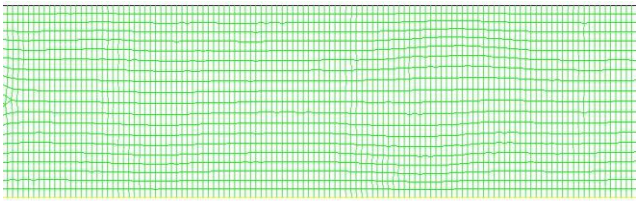


**Figure 2** Mesh generation

**Model Species Transport and Finite-Rate Chemistry**

ANSYS FLUENT can model the mixing and transport of chemical species by solving conservation equations describing convection, diffusion, and reaction sources for each component species. Multiple simultaneous chemical reactions can be modeled, with reactions occurring in the bulk phase (volumetric reactions) and/or on wall or particle surfaces, and in the porous region. Species transport modeling capabilities, both with and without reactions. Note that you may also want to consider modeling your turbulent reacting flame using the mixture fraction approach (for non-premixed systems) or the reaction progress variable approach (for premixed systems, the partially premixed approach, or the composition PDF Transport approach. The study will use to solve conservation equations for chemical species, ANSYS FLUENT predicts the local mass fraction of each species, Yi, through the solution of a convection, diffusion equation for the ith species. This conservation equation takes the following general form:

$$\frac{\partial}{\partial t}(\rho Yi) + \nabla.(\rho v Yi) = -\nabla.Ji + Ri + Si \quad (2)$$

**Mass Diffusion in Turbulent Flows**

In turbulent flows, ANSYS FLUENT computes the mass diffusion in the following form:

$$Ji = \left(\rho Di, m + \frac{\mu t}{Sct}\right)\nabla Yi - DT, i\frac{\nabla T}{T} \quad (3)$$

The default Sct is 0.7. Note that turbulent diffusion generally overwhelms laminar diffusion, and the specification of detailed laminar diffusion properties in turbulent flows is generally not necessary.

**Treatment of Species Transport in the Energy Equation**

For many multi component mixing flows, the transport of enthalpy due to species diffusion **Magnussen**

$$\nabla.\sum_{i=1}^{n} hiJi \quad (4)$$

can have a significant effect on the enthalpy field and should not be neglected. In particular, when the Lewis number

$$Lei = \frac{k}{\rho CpDi,m} \quad (5)$$

for any species is far from unity, neglecting this term can lead to significant errors. ANSYSFLUENT will include this term by default.

**The Eddy-Dissipation Model**

Most fuels are fast burning, and the overall rate of reaction is controlled by turbulent mixing. In non-premixed flames, turbulence slowly convects /mixes fuel and oxidizer into the reaction zones where they burn quickly. In premixed flames, the turbulence slowly convects/mixes cold reactants and hot products into the reaction zones, where reaction occurs rapidly. In such cases, the combustion is said to be mixing-limited, and the complex, and often unknown, chemical kinetic rates can be safely neglected, ANSYS FLUENT provides a turbulence-chemistry interaction model, based on the work of **(Magnussen and Hjertager)**, called the eddy-dissipation model. The net rate of production of species *i* due to reaction r, *Ri,r*, is given by the smaller (i.e., limiting value) of the two expressions below:

$$R_{i,r} = v'_{ir} M_{w,i} A\rho \frac{\epsilon}{k} \min\left(\frac{Y_R}{v'_{R,r} M_{w,R}}\right) \quad (6)$$

$$R_{i,r} = v'_{ir} M_{w,i} AB\rho \frac{\epsilon}{k} \frac{\sum PY_P}{\sum_j^N v_{j,r} M_{w,j_{R,r}}} \quad (7)$$

Reaction rates are assumed to be controlled by the turbulence, so expensive Arrhenius chemical kinetic calculations can be avoided. The model is computationally cheap, but, for realistic results, only one or two step heat-release mechanisms should be used.

**Results and discussions**

The study will discuss mainly the static temperature in case of constant specific heat and variation of specific heat as function to temperature and distribution of temperature and outlet temperature and comparisons it with static temperature for methane combustion for validation to another study. Also the emission for NOx and the difference between methane as fuel and propane in our study.

**Iteration and residuals**

The initial calculation will be performed assuming that all properties except density are constant. The use of constant transport properties (viscosity, thermal conductivity, and mass diffusivity coefficients) is acceptable because the flow is fully turbulent. The molecular transport properties will play a minor role compared to turbulent transport. The assumption of constant specific heat, however, has a strong effect on the combustion solution. **Figure (3)** shows the solution will converge in approximately 250 iterations. Then the study will change the specific heat property definition in step with varying heat capacity as a function of temperature (polynomial equation) and the solution will be converge in approximately 375 iterations **Figure (4)**. The residuals will jump significantly as the solution adjusts to the new specific heat representation. The solution will converge after approximately 125 additional iterations.

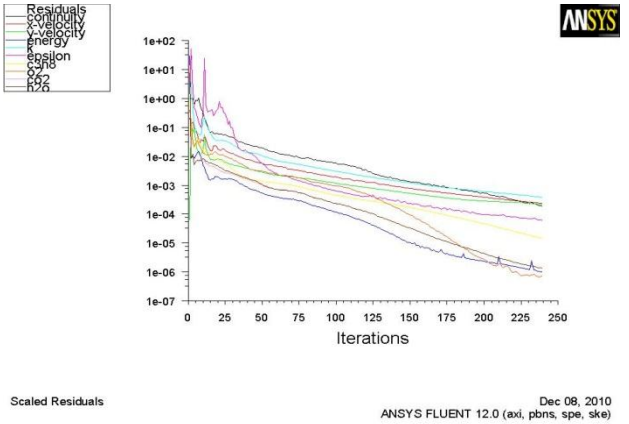



**Figure 3** Converge history for constant Cp

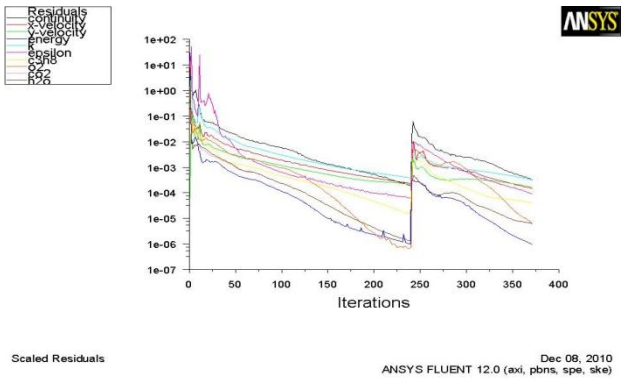


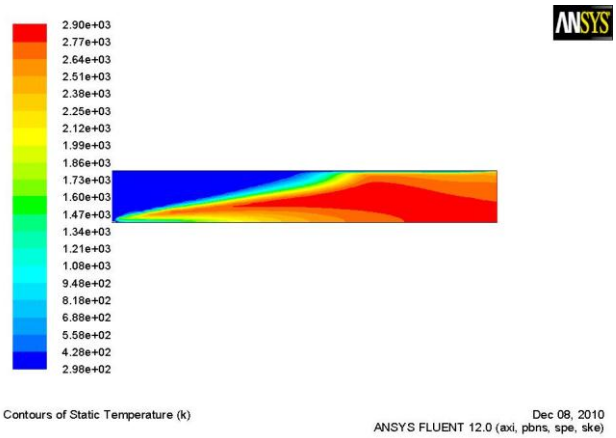

**Figure 4** Converge history for variable Cp

**Temperature of reaction**

In **Figure (5)** we observe the static temperature for combustion of propane at constant heat capacity is 2900 K and is less than for methane combustion for another study **(Ansys inc)** which is above of 3000 K the reason is attribute to octane number for methane is higher than propane and this effect on flame propagation speed which will be more in methane so that increase the reaction speed and temperature of the reaction. Also the molecular weight for propane is more than methane which effect on the generation of water molecular, also the heating value for methane is higher than propane this is a more reason for this differences. The peak temperature, predicted using a constant heat capacity of 1000 J/kg − K, is over 2900 K. This over prediction of the flame temperature can be remedied by a more realistic model for the temperature and composition dependence of the heat capacity, as illustrated in the **Figure (6)**.

The peak temperature has dropped to approximately 2160K as a result of the temperature and composition-dependent specific heat **(Ruud Beerkens & Adriaan Lankhorst)**. The strong temperature and composition dependence of the specific heat has a significant impact on the predicted flame temperature. The mixture specific heat is largest where the $C_3H_8$ is concentrated, near the fuel inlet, and where the temperature and combustion product concentrations are large. The increase in heat capacity, relative to the constant value used before, substantially lowers the peak flame temperature **Figure (7)**.

Present study (Propane combustion)




Comparison study (methane combustion)

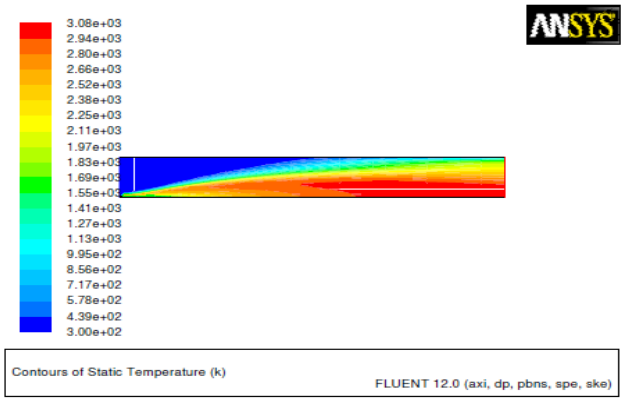
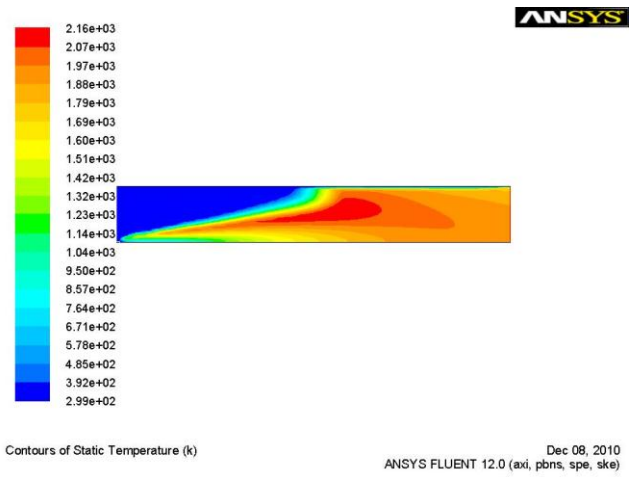



**Figure 5** Contours of static temperature- constant Cp

Present study (Propane combustion)




Comparison study (methane combustion)

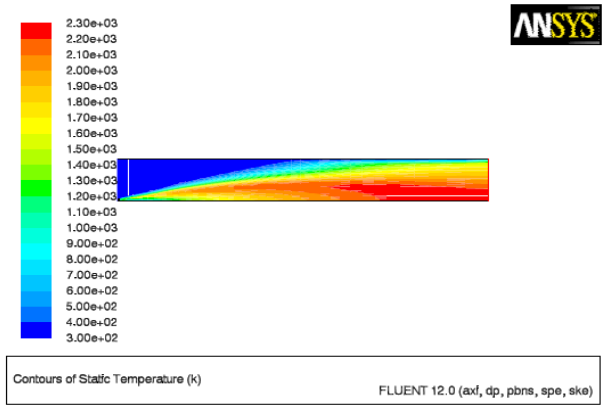



**Figure 6** Contours of static temperature- variable Cp

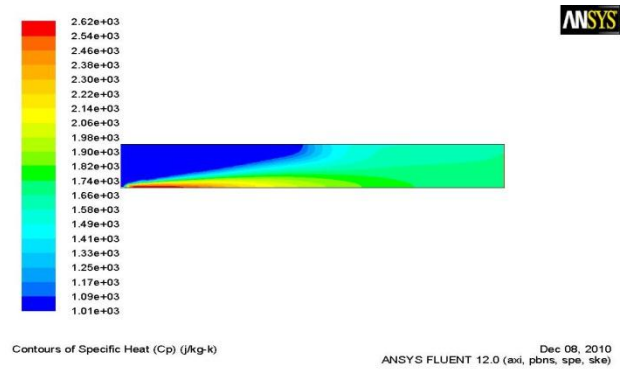



**Figure 7** Contours of specific heat Cp

## Mass fraction

The Figure (8,9,10, and 11) are show the contours of mass fraction for the remaining species $C_3H_8$, $H_2O$,$O_2$,$CO_2$, respectively , the amount and distribution of these species is useful for prediction of how the reaction will end and how we can change this way to improvement performance of design of furnaces. So the **Figure (12)** appoint to the temperature on length of furnaces which is start in minimum near the nozzle and maximum further of it.


**Figure 8** Contours of $C_3H_8$ mass fraction

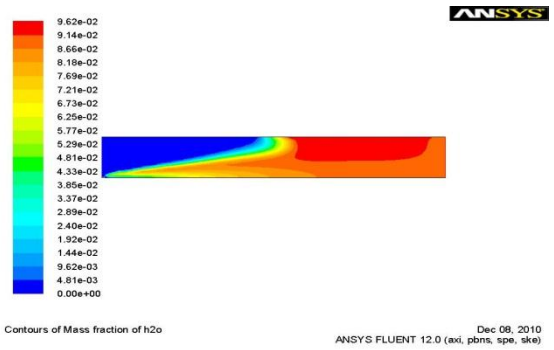



**Figure 9** Contours of $H_2O$ mass fraction

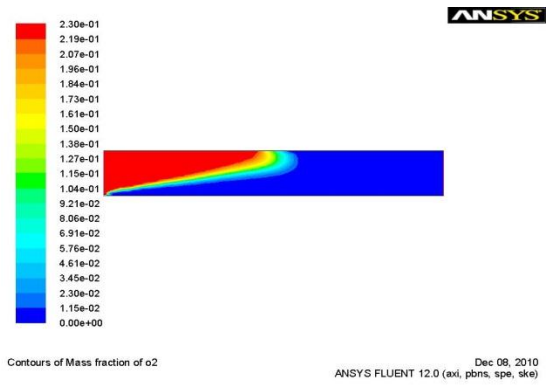



**Figure 10** Contours of $O_2$ mass fraction

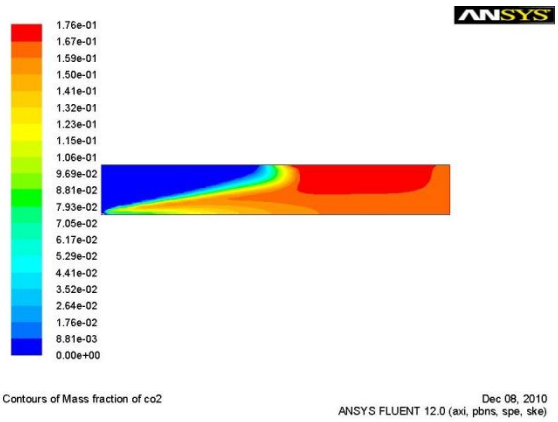



**Figure 11** Contours of $CO_2$ mass fraction

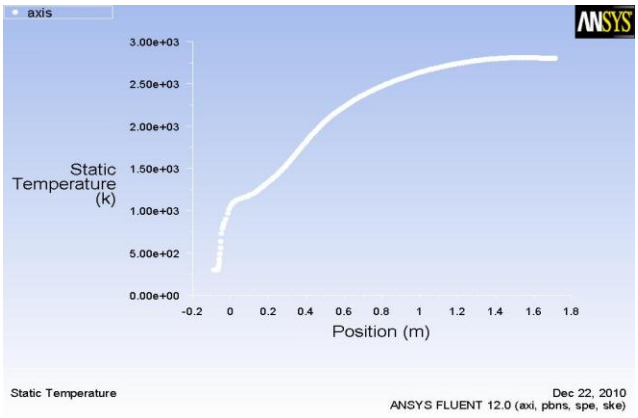



**Figure 12** The relation between axis static temperature and the length of furnace

## NOx Prediction

In this section you will extend the ANSYS FLUENT model to include the prediction of NOx.

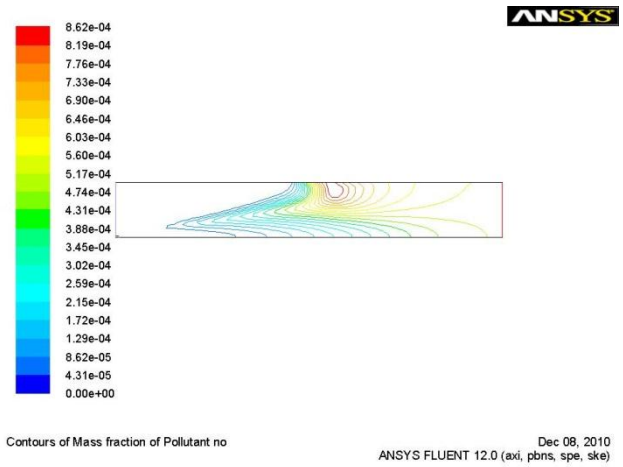



**Figure 13** Contours of NO mass fraction –Prompt and Thermal NOx formation

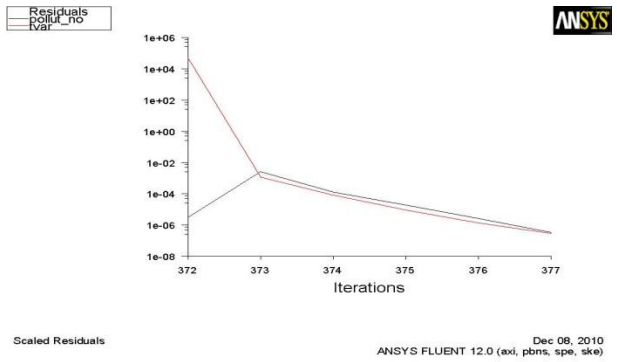



**Figure 14** Converge history for NOx model

The study will calculate the formation of both thermal and prompt NOx, the peak concentration of NO is located in a region of high temperature where oxygen and nitrogen are available **(Ronald A. Jordan)** and less than in methane combustion because of lowering of flame temperature and distribution of mass fraction for species. **Figure (13)**. The prediction of NOx formation in a postprocessing mode, with the flow field, temperature, and hydrocarbon combustion species concentrations fixed. Hence, only the NO equation will be computed. Prediction of NO in this mode is justified on the grounds that the NO concentrations are very low and have negligible impact on the hydrocarbon combustion prediction. The solution will converge in approximately 7 iterations **Figure (14)**.

## Combustion kinetics

Due to the high local Reynolds Numbers occurring in combustion in furnaces, the flow, in general, is highly turbulent **Figure (15)**, meaning that eddies of different sizes lead to random fluctuations (in time & space) of flow velocity **Figure (16)**, temperature and species concentrations. A typical important aspect of turbulent flows is the increased level of mixing of momentum, heat and mass, as compared to laminar flows. In turbulence modeling this usually is described by the eddy viscosity concept and a typical model frequently used in engineering is the two-equation k-turbulence model **(Launder & Spalding)**.

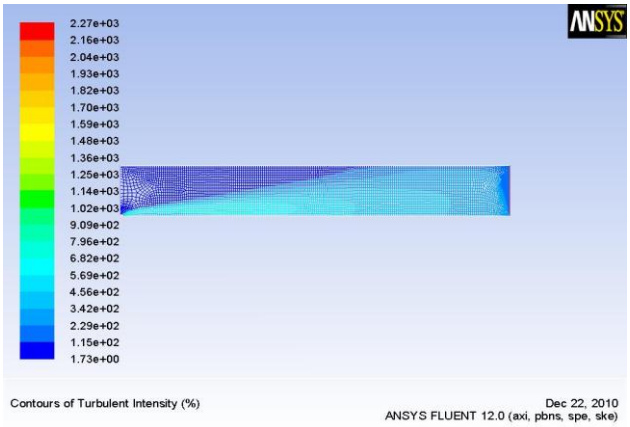



**Figure 15a** Contours for turbulent intensity

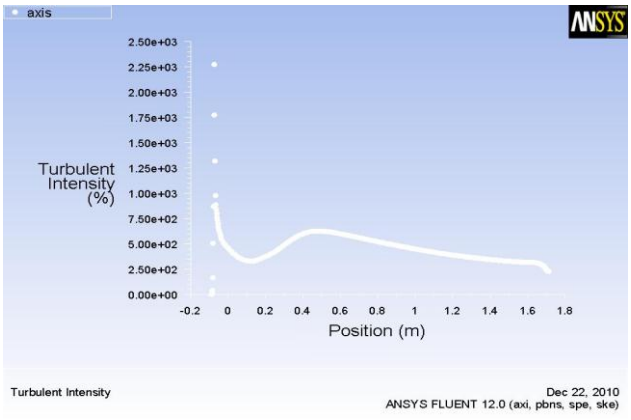



**Figure 15b** Plot for turbulent intensity of axis'

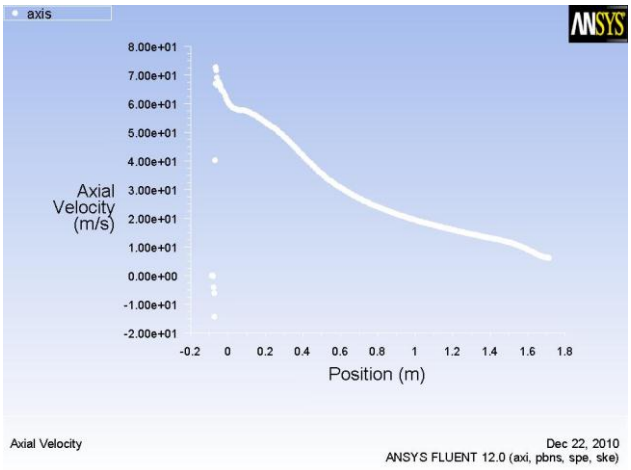



**Figure 16** Plot for axial velocity of axis

**Table 1** Summarizing results

| Peak temperature K | Outlet temperature (K) | Outlet velocity (m/s) | Outlet mass fraction of Pollutant NO |
|---|---|---|---|
| 2900 (constant Cp)<br>2160 (variable Cp) | 2637.7017<br>1878.1829 | 4.95788<br>3.5646446 | 0.00049750332 |

## Conclusion

1. There is possibility for using propane as fuel for furnaces and reduce the emission of NOx with gotten the desired temperature.
2. The use of a constant Cp results in a significant over prediction of the peak temperature. The average exit velocity and temperature are also over predicted
3. The variable Cp solution produces dramatic improvements in the predicted results.

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| Symbols | Meaning |
|---|---|
| $i$ | Species |
| $Yi$ | Local mass fraction of each species |
| $Ri$ | Net rate of production of species $i$ |
| $Si$ | Rate of creation |
| $Ji$ | Diffusion flux of species $i$ |
| $D_{i,m}$ | Mass diffusion coefficient for species $i$ |
| $D_{T,}i$ | Thermal diffusion coefficient |
| $Sct$ | Turbulent Schmidt number |
| $_t\mu$ | Turbulent viscosity |
| $hi$ | Enthalpy of species |
| $Lei$ | Lewis number |
| $Y_P$ | Mass fraction of any product species |
| $Y_R$ | Mass fraction of a particular reactant |
| $A$ | Empirical constant equal to 4.0 |
| $B$ | Empirical constant equal to 0.5 |
| P and R | Products and Reactants |
| $\epsilon/_k$ | Turbulent mixing rate |
| $Mw,i$ | Molecular weight of species $i$ |
| $Dt$ | Turbulent diffusivity |
| $v'i,r$ | Stoichiometric coefficient for reactant $i$ in reaction $r$ |
| $v''i,r$ | Stoichiometric coefficient for product $i$ in reaction $r$ |