VSB -Technical University of Ostrava Faculty of Mechanical Engineering Department of Energy Engineering

# SIMULATION OF THE GASEOUS SPECIES TRANSPORT AND COMBUSTION OF THE METHANE IN THE DROP TUBE USING ANSYS

Simulace přenosu plynných látek a spalování methanu v pádové trubce pomocí ANSYSU

Student:

Manjesh Ramakrishnaiah

Diploma thesis supervisor:

Doc. Ing. Marian Bojko, Ph.D.

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2) Application of CFD model for air flow in the tube.

3) Characteristics of combustion of gaseous fuels.

4) Defining a CFD model for combustion of gaseous species.

5) Application of methane combustion with air in a tube.

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Supervisor:

#### doc. Ing. Marian Bojko, Ph.D.

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HOULS

Head of Department

doc. Ing. Stanislav Honus, Ph.D. OSTRAN

prof. Ing. Ivo Hlavatý, Ph.D. Dean

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## Abstract

The main goal of the project to study the gaseous species transport and combustion of methane in the drop tube by using ANSYS FLUENT. The problem is divided into three steps such as in first step we are going to do CFD modelling of the air flow without heat transfer in the drop tube. In second step CFD modelling of air flow by gaseous species  $(O_2, H_2O, CO_2 AND N_2)$  without heat transfer in the drop tube. In third step CFD modelling of air flow by gaseous species and combustion of the methane with oxygen in the drop tube. Combustion of methane will be calculating for different models such Finite-rate/tci, Finite-rate /Eddy dissipation, Eddy dissipation and Eddy-dissipation concept.

The geometry of drop tube is created in design modeller and mesh is generated in ANSYS meshing which is read to fluent where simulation of the gaseous species and combustion of methane is calculated for different models.

#### Keywords

CFD, meshing, combustion, methane, rate parameters, nitrogen, oxygen, hydrogen, carbon dioxide

### Abstrakt

Hlavním cílem diplomové práce je CFD výpočet plynných látek a spalování methanu v pádové trubce s využitím Software ANSYS Fluent. Problematika je rozdělena do tří kroků. V prvním kroku je realizováno CFD modelování proudění vzduchu bez přestupu tepla v pádobé trubce. V druhém kroku se jedná o CFD modelování proudění vzduchu pomocí plynných příměsí ( $O_2$ ,  $H_2O$ ,  $CO_2$  a  $N_2$ ) bez přestupu tepla v pádobé trubce. Třetím krokem je CFD modelování proudění vzduchu pomocí plynných příměsí a spalování metanu s kyslíkem v pádové trubce. Spalování metanu je definováno pomocí různých modelů jako jsou "Finite-rate/tci, Finite-rate /Eddy dissipation, Eddy dissipation and Eddy-dissipation concept".

Geometrie pádové trubky je vytvořena v programu DesignModeler a výpočetní síť je vygenerována v ANSYS Meshingu s následným načtením do Fluentu, kde jsou provedené simulace proudění plynných látek včetně spalování metanu pro různé modely spalování.

#### klíčová slova

CFD, spalování, Metan, rychlostní parametry, dusík, kyslík, vodík, oxid uhličitý

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# List of variables

Α	Pre exponential factor	(s <sup>-1</sup> )
A	Area	(m²)
$A_{b,r}$	Pre-exponential factor for backward reaction	(s <sup>-1</sup> )
c <sub>p</sub>	Heat capacity	(J.kg <sup>-1</sup> k <sup>-1</sup> )
C <sub>P</sub>	Specific heat capacity at constant pressure	(J.kg <sup>-1</sup> k <sup>-1</sup> )
C <sub>v</sub>	Specific heat capacity at constant volume	(J.kg <sup>-1</sup> k <sup>-1</sup> )
C <sub>j,r</sub>	Molar concentration of species in reaction	(Kmol.m <sup>-3</sup> )
$d_h$	Hydraulic diameter	(m)
E <sub>a</sub>	Activation energy	(J.kmol <sup>-1</sup> )
E <sub>b,r</sub>	Activation energy in backward reaction	(J.kmol <sup>-1</sup> )
Ē	Force	(N)
$ec{g}$	Acceleration due to gravity	(m.s <sup>-2</sup> )
h	Enthalpy	(kJ.kg <sup>-1</sup> )
L, l	Length	(m)
Ν	Number of chemical species in the system	(1)
р	Pressure	(Pa)
$Q_m$	Mass flow rate	(kg.s <sup>-1</sup> )
$Q_v$	Volume flow rate	(m <sup>3</sup> .s <sup>-1</sup> )
R	Universal gas constant	(J.kmol <sup>-1</sup> K <sup>-1</sup> )
R <sub>e</sub>	Reynolds number	(1)
S	Entropy	(kJ.kg <sup>-1</sup> K <sup>-1</sup> )

Sct	Turbulent Schmidt number	(1)
t	Time	(s)
Т	Temperature	(°C)
T <sub>abs</sub>	Absolute temperature	(K)
$\vec{u}$	Velocity	(m.s⁻¹)
u <sub>i</sub>	i-th velocity component	(m.s <sup>-1</sup> )
$\overline{u}_i$	i-th mean velocity component	(m.s⁻¹)
V	Volume	(m³)
X <sub>i</sub>	Coordinate in Cartesian system $[X_1, X_2, X_3]$	(m)
Y	perpendicular distance from wall	(m)

#### Greek alphabet

α	heat transfer coefficient	(W.m <sup>-2</sup> K <sup>-1</sup> )
β	Temperature exponent	(1)
$\beta_{b,r}$	Temperature exponent for backward reaction	(1)
ε	rate of dissipation	(m².s-³)
η	dynamic viscosity	(Pa.S)
θ	kinematic viscosity	(kg.m <sup>-1</sup> s <sup>-1</sup> )
$\vartheta_t$	turbulent kinematic viscosity	(m <sup>2.</sup> s <sup>-1</sup> )
λ	Thermal conductivity	(W.m <sup>-1</sup> k <sup>-1</sup> )
μ	Dynamic viscosity	(kg.m <sup>-1</sup> s <sup>-1</sup> )
$\mu_t$	Turbulent viscosity	(m <sup>2</sup> .s <sup>-1</sup> )
$\overline{\pi}$	total stress tensor	(Pa)

ρ	density	(kg.m⁻³)
$\sigma_{\varepsilon}$	empirical constant	(1)
$\sigma_k$	empirical constant	(1)
τ	Stress tensor	(N.m <sup>-2</sup> )
$ au_t$	Turbulent stress	(Pa)

## **1. Introduction**

Computational Fluid Dynamics (CFD) simulation provides a virtual laboratory results to perform experiments in early stages of design without building the physical apparatus. Virtual results decease the unit of design costs as number of unsatisfactory experimental devices that ends to scrap decrease drastically. Otherwise, the cost of experimental and its until obtain satisfactory results can be become very huge. Simulations can be done by CFD modelling using commercial or own software with same base "CFD simulations use mathematical models which represents the different phenomena occurring in the system". The most used software to calculate the flow is ANSYS FLUENT. And in my thesis i used this software for CFD calculation.

The accuracy of CFD simulation to the real solution depends on the appropriated selections of the models and boundary conditions. The geometry can be created in the program Design Modeller and mesh is generated in ANSYS meshing. After generated mesh in the ANSYS meshing is read to the ANSYS FLUENT to perform the simulation as per the model selected and boundary conditions applied. (chapter 3.3 and 3.4)

In my diploma thesis problem is divided into three steps. For first and second step geometry remains same but in the first modelling of air flow without heat transfer in the drop tube and second step its same as first but modelling of air flow by gaseous species such as  $N_2$ ,  $O_2$ ,  $CO_2$  and  $H_2O$  without heat transfer in the drop tube. In the last step CFD numerical modelling of flow mixture of air and methane including the combustion of methane with oxygen. Combustion of methane takes inside the drop tube (Chapter 5). In this problem the model of turbulence is defined as k- $\mathcal{E}$  standard model (chapter 2.3)

Combustion is a process of burning of fuel in presence of oxygen. In this problem fuel is defined as methane which enters to the drop tube with different velocities and CFD calculations are performed for all different velocities and results are compared with each other. In this problem the defined model is K- $\mathcal{E}$  standard model (chapter2.3) and the boundary conditions are velocity inlets, pressure outlet wall and axis. The inlet for  $O_2$  and  $CH_4$  are defined as velocity inlet and outlet is defined as pressure outlet. The problem is calculated for all the turbulent model of volumetric reactions such Finite rate /No TCI model, Finite rate/eddy dissipation, eddy dissipation and eddy dissipation concept model. From postprocessing the static temperature and mass fractions of the species are

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evaluated. Static temperature is evaluated by contours in all region and by plot in of the tube. Evaluation is done for all models of volumetric and velocities of methane. Mass fractions of oxygen and methane are evaluated by plot the graph with respect to axis of the drop tube. Results are compared with each other.

## 2. Characterisation of the flow

The characterises of flow depends on Reynolds number. It is an important dimensionless quantity in fluid mechanics used to predict flow patterns in different fluid flow situations.

Reynolds number is defined by the ratio of inertia force to viscous force.

$$R_e = \frac{ud_h}{\vartheta} \tag{2-1}$$

Where,

u = velocity in m.s<sup>-1</sup>

 $d_h$ =hydraulic diameter in m

 $\vartheta$ =kinematic viscosity in m<sup>2</sup>.s<sup>-1</sup>

Depending on Reynolds number there are two types of flow. They are

- Laminar flow
- Turbulent flow

For flow in the pipe critical Reynolds number determine the type of flow. If Reynolds number is less than 2320 then the flow is laminar, if its more, then the flow is turbulent flow.[1]

At low Reynolds numbers, flows which tend to be by laminar (sheet-like) flow, while at high Reynolds numbers turbulence results from differences in the fluid's speed and direction, which may sometimes intersect even move counter to the overall direction of the flow.

#### 2.1. Turbulent flow

Turbulence is commonly observed in daily phenomena such as surf, fast flowing rivers, billowing storm clouds (or) smoke from a chimney. Most of fluid flow occurring in nature is turbulent flow. It is a complex process, mainly because it's three dimensional, unsteady and consists of many scales. Turbulence is caused due to excessive kinetic energy in part of fluid flow, which overcomes the damping effect of fluids viscosity. For this reason, it's easier to create in low viscosity fluid, but more difficult in highly viscous fluids. If Reynolds number is higher, then the flow is turbulent flow. It is a type of flow occurs in liquid or gases in which the fluid undergoes irregular fluctuations. The flow of fluid is speed at a point which is continuously undergoing changes in both magnitude and direction. Smoke rising from a cigarette is a turbulent flow. However, for the first few centimetres the flow is laminar. The smoke plume becomes turbulent as is Reynolds number increases, due to flow velocity and characteristic of the length increasing.[2]&[3]

The numerical solution of the Navier –strokes equations for turbulent flow is extremely difficult, and it does not require any additional information. Due to high significantly different mixing –length scales that involved in turbulent flow, for stable solution it requires to have a fine mesh resolution that the computational time becomes significantly infeasible for calculation or direct numerical simulation.

A large amount of CFD research has concentrated on methods which can make use of turbulence models. Turbulence models have been specifically developed for the effects of turbulence without recourse to a prohibitively fine mesh and direct numerical simulation. Most turbulence models are statistical turbulence model. This approach is computationally more expensive in time and in computer memory, but produces better results, because it explicitly resolves the larger turbulent scales.[4]



Figure 1 shows the illustration of turbulent [5]

## 2.2 Models of turbulence in ANSYS FLUENT

It is a universally fact that there is no single turbulence model as being superior for classes of problems which should be accepted. The choice of turbulence model will depend on considerations of physics encompassed in the flow and, level of accuracy requited to available computational resources, and the amount of time required for the simulation. To make the most appropriate choice of model for our application, we need to understand the capabilities and limitations of the various options.[6]

The purpose of above section is to give an overview issues for the turbulence models provided in ANSYS FUENT. The computational time and memory required for the individual models discussed. By this it is impossible to state categorically which model is best for a specific application. So, general guidelines help us to choose the appropriate turbulence model for the flow.[6]

To describe the effects of turbulent fluctuations for various velocities and scalar quantities in a single phase, FLUENT uses various types of closure models which are listed below.

- > Spalart-Allmara model
- ➢ K-E models
  - Standard k-E model
  - Renormalization-group (RNG) k-E model
  - Realizable k-E model
- > K-ω models
  - Standard k -ω model
  - Baseline (BSL) k-ω model
  - Shear-stress transport (SST) k-ω model
- V<sup>2</sup>-f model
- Transition k-kl-ω model
- Transition SST model
- Reynolds stress models (RSM)
  - Linear pressure-strain RSM
  - Quadratic pressure-strain RSM
  - Stress-Omega RSM
  - Stress-BSL RSM

- Scale-Adaptive Simulation (SAS) model
  - SST k-ω model
  - Standard k-ω model
  - BSL k-ω model
  - Transition SST model
  - W-based Reynolds stress models (RSM)
- Detached eddy simulation (DES) model
  - Spalart-Allmaras RANS model
  - Realizable k-E RANS model
  - SST k-ω RANS model
  - BSL k-ω RANS model
  - Transition SST model

## 2.3. Description of Standard k-E model

It is of the simplest "complete models" of turbulence for two-equation models. In which gives the solution for two separate transport equations which allows the turbulent velocity and length of scales to be independently determined.

The standard k- $\varepsilon$  model in FLUENT falls within this class of turbulence model and has become the workhorse of all practical engineering flow calculations in the time since it was proposed by Launder and Spalding. This model is robustness, economy, and reasonable accuracy for a wide range of turbulent flows which is widely popular in industrial flow and heat transfer simulations. It is a semi-empirical model, in which the derivation of the model equations relies on phenomenological considerations and empiricism.[6]

As the strengths and weaknesses of the standard k- $\varepsilon$  model have become known, improvements have been made to the model to improve its performance. Apart from this there is other two variants, which are available in FLUENT. They are available, RNG k- $\varepsilon$  model and the realizable k- $\varepsilon$  model.[6]

The standard k- $\varepsilon$  model is a semi-empirical model based on model transport equations for the turbulence kinetic energy (k) and its dissipation rate ( $\varepsilon$ ), continuity equations and Navier-strokes equation. The model transport equation for k is derived from the exact equation, while the model transport equation for  $\varepsilon$  was obtained using physical reasoning and bears little resemblance to its mathematically exact counterpart.

In the derivation of the k- $\varepsilon$  model, the assumption is that the flow is fully turbulent, and the effects of molecular viscosity are negligible. The standard k- $\varepsilon$  model is therefore valid only for fully turbulent flows.[6]

The turbulence kinetic energy k, and rate of dissipation,  $\varepsilon$ , are obtained from the following transport equations[6]

$$\frac{\partial}{\partial t}(\rho k) + \frac{\partial}{\partial x_j}(\rho k u_i = \frac{\partial}{\partial x_j} \left[ \left( \mu + \frac{\mu_t}{\sigma_k} \right) \frac{\partial k}{\partial x_j} \right] + G_k + G_b + \rho \in -Y_M + S_k$$
(2.3-1)

And

$$\frac{\partial}{\partial t}\rho\epsilon + \frac{\partial}{\partial x_i}(\rho\epsilon u_i) = \frac{\partial}{\partial x_j}\left[\left(\mu + \frac{\mu_t}{\sigma_\epsilon}\right)\frac{\partial\epsilon}{\partial x_j}\right] + C_{1\epsilon}\frac{\epsilon}{k}(G_{1k} + G_{3\epsilon}G_b) - G_{2\epsilon}\rho\frac{\epsilon^2}{k} + S_\epsilon$$
(2.3-2)

Where,

 $C_{1\epsilon}$ ,  $G_{2\epsilon}$ , and  $G_{3\epsilon}$  are constants.  $\sigma_k$  And  $\sigma_{\epsilon}$  are the turbulent Prandtl numbers for k and  $\epsilon$ , respectively.  $S_k$  and  $S_{\epsilon}$  are user-defined source terms.

 $G_k$ = turbulence kinetic energy generated due to the mean velocity gradients.

 $G_b$ = turbulence kinetic energy generated due to buoyancy.

 $Y_M$ = contribution of the fluctuating dilatation in compressible turbulence to the overall dissipation rate

All velocity values are time averaged.

The turbulent viscosity,  $\mu_t$ , is computed by combining k and  $\varepsilon$  as follows:

$$\mu_t = \rho C_\mu \frac{k^2}{\epsilon} \tag{2.3-3}$$

Where,

 $C_{\mu}$  = constant

## 3. Numerical modelling of fluid flow

The basic equations for the flow predict and fluid behavior are continuity equation, Navierstroke equations and energy equations.

#### 3.1. The mass conservation equation (Continuity equation)

Continuity equation is used in ideal and real fluid which are identical. According to law of conservation of mass. The sum of the temporal and convective flow change is equal to zero eventually to source member.[7]

General equations of continuity for spatial unsteady flow of compressible fluid.

$$\iiint \frac{\partial(\rho)}{\partial t} dV + \iint \vec{u}\vec{n} \, dS = S_Z \tag{3.1-1}$$

In differential vector form

$$\frac{\partial(\rho)}{\partial t} + \nabla(\rho\vec{u}) = S_Z \tag{3.1-2}$$

In differential form

$$\frac{\partial(\rho)}{\partial t} + \frac{\partial(\rho u_X)}{\partial X} + \frac{\partial(\partial(u_Y)}{\partial Y} + \frac{\partial(u_Z)}{\partial X} = S_Z$$
(3.1-3)

With steady flow of an incompressible fluid the continuity equation is expressed by the relationship in the form.

$$\nabla \vec{u} = 0 \tag{3.1-4}$$

#### **3.2. Momentum conservation equation**

Navier-stroke equation express the relationship, when inertia forces is equal to the sum of the mass and surface (pressure and friction) forces.[7]

$$\overrightarrow{F_S} = \overrightarrow{F_O} + \overrightarrow{F_P}$$
(3.2-1)

In real fluid flow choose elementary volume dV. To that fluid volume the external volume force  $d\vec{F_o}$  is applied

Differential of mass force and consequently total mass force is given by

$$d\overline{F_o} = \vec{a}dm = \rho \vec{a}dV = \overline{F_o} = \iiint \vec{a}\rho dV$$
(3.2-2)

Similarly, inertial force is determined by the fluid acceleration by substantial derivative.

$$d\vec{F_s} = \frac{D\vec{u}}{Dt}dm = \frac{D\vec{u}}{Dt}\rho dV = \vec{F_s} = \iiint \frac{D\vec{u}}{Dt}\rho dV$$
(3.2-3)

Surface force that includes both pressure and friction force can be written using molecular stress factor  $\overline{\pi}$ , (for both shear and normal stress)

$$\bar{\pi} = -p\bar{\delta} + \bar{\tau} \tag{3.2-4}$$

Where,

p = is the normal component of the stress (static pressure), which specified the pressure force in the direction of inner normal in hydromechanics, and so that a pressure force is defined with a minus sign.[7]

 $ar{ar{ au}}=$ is the shear stress tensor

 $\overline{\delta}$  =is a unit tensor with components.

Let us illustrate the mathematical expression of the friction forces for the simplified Newton relationship applied in the coordinate system shown in below figure



*Figure 2 shows the velocity profile depending on coordinate y*[7]

$$\tau = \eta \frac{dV}{dY} \tag{3.2-5}$$

The above equation which is expressing the relation between viscous stresses and velocity derivative according to one direction perpendicular to the movement.

Vector-tensorial formulation of shear stress in space is given by

$$\vec{\tau} = \eta \left[ \left( \nabla \vec{V} + \left( \nabla \vec{V} \right)^T \right) - \frac{2}{3} \left( div(\vec{V}) \right) \vec{\delta} \right]$$
(3.2-6)

Where,

 $\nabla \vec{V}$  is tensor velocity gradients with components  $\left(\frac{\partial}{\partial X_i}\right) V_j$ ,  $\left(\nabla \vec{V}\right)^T$  is transposed tensor of velocity gradients with components  $\left(\frac{\partial}{\partial X_j}\right) V_i$  and div  $(\vec{V})$  is the divergence of velocity vector.

For incompressible fluid there is  $div(\vec{V}) = 0$ . Then the differential of surface forces is

$$d\overrightarrow{F_{P}} = \overline{\pi}\overrightarrow{n}dS = (-\rho\overrightarrow{\delta} + \overrightarrow{\tau})\overrightarrow{n}dS = (-\rho\overrightarrow{\delta} + \eta\left[\nabla\overrightarrow{V} + (\nabla\overrightarrow{V})^{T}\right])\overrightarrow{n}dS$$
(3.2-7)

Where,

 $\vec{n}$ =is the outer normal vector to element of closed surface dS.

The balance of all forces using vector notation for general compressible fluid in a rectangular coordinate system has the form

$$\iiint \frac{Dp\vec{u}}{Dt}dV = \iiint \frac{\partial(p\vec{u})}{\partial t}dV + \iint p\vec{u}(\vec{u}\vec{n})\,dS = -\iint p\vec{n}dS + \iint \tau dS + \iiint \vec{f}\,dV \quad (3.2-8)$$

respectively

$$\frac{\partial(p\vec{u})}{\partial t} + \nabla(\rho\vec{u}\vec{u}) = -\nabla p + \rho\vec{a} + \nabla(\tau) + S_m$$
(3.2-9)

Where  $\vec{u}\vec{u}$  is also called dyadic product of vectors and the equation is called Navier-stroke equation. This equation can be illustrated in the three coordinate forms, *X*, *Y* and *Z* are the coordinate incompressible flow.[7]

$$\frac{\partial u_x}{\partial t} + u_x \frac{\partial u_x}{\partial x} + u_y \frac{\partial u_x}{\partial y} + u_z \frac{\partial u_x}{\partial z} = a_x - \frac{1}{\rho} \frac{\partial p}{\partial x} + V \left( \frac{\partial^2 u_x}{\partial x^2} + \frac{\partial^2 u_x}{\partial y^2} + \frac{\partial^2 u_x}{\partial z^2} \right)$$
(3.2-10)

$$\frac{\partial u_Y}{\partial t} + u_X \frac{\partial u_Y}{\partial X} + u_Y \frac{\partial u_Y}{\partial Y} + u_Z \frac{\partial u_Y}{\partial Z} = a_Y - \frac{1}{\rho} \frac{\partial p}{\partial Y} + V \left( \frac{\partial^2 u_Y}{\partial X^2} + \frac{\partial^2 u_Y}{\partial Y^2} + \frac{\partial^2 u_Y}{\partial Z^2} \right)$$
(3.2-11)

$$\frac{\partial u_Z}{\partial t} + u_X \frac{\partial u_Z}{\partial X} + u_Y \frac{\partial u_Z}{\partial Y} + u_Z \frac{\partial u_Z}{\partial Z} = a_Z - \frac{1}{\rho} \frac{\partial p}{\partial Z} + V \left( \frac{\partial^2 u_Z}{\partial X^2} + \frac{\partial^2 u_Z}{\partial Y^2} + \frac{\partial^2 u_Z}{\partial Z^2} \right)$$
(3.2-12)

For one-dimensional flow, the above continuity equation is reduced into a simple form which is written below

$$\frac{\partial u_X}{\partial t} + u_X \frac{\partial u_X}{\partial X} = a_X - \frac{1}{\rho} \frac{\partial p}{\partial X} + V \left( \frac{\partial^2 u_X}{\partial X^2} \right)$$
(3.2-13)

In the system of differential Navier - Stokes equations and continuity equation there are four unknowns, they are three velocities  $u_X$ ,  $u_Y$  and  $u_Z$  and pressure. To solve these equations the external acceleration  $\vec{a}$ , fluid density  $\rho$  and boundary conditions must be known. Navier - Stokes equations are among the non-linear partial differential equations and are not generally solvable. The analytical solution is available for simpler cases of laminar flow. Nowadays even complex cases of laminar and turbulent flow are solved using numerical methods, of finite volume method and finite element method.[7]

#### 3.3. The Energy equations

It is derived from the Navier-Stroke equation. By scalar multiplication of velocity vector and a coefficient factor of 0.5. Then the equation will be complemented by other members and expresses the internal energy.[7]

$$\iiint \frac{D(\rho E)}{Dt} dV = \iiint \frac{\partial(\rho E)}{\partial t} dV + \iint \rho E(\vec{u}\vec{n}) dS$$
$$= \iint \lambda \nabla T dS - \iint \vec{\tau} dS + \iiint S dV$$
(3.3-1)

$$\frac{\partial(\rho E)}{\partial t} + \nabla \left( \vec{u} (\rho E + p) \right) = \nabla (\lambda \nabla T) - \nabla (\vec{\tau} \vec{u}) + S_h$$
(3.3-2)

Where,

Total energy is the sum of internal and kinetic energy. It is given by

$$E = U + \frac{1}{2}\vec{u}\vec{u} \tag{3.3-3}$$

 $\lambda$  is the coefficient of molecular thermal conductivity.

 $S_h$  is the heat generated due friction involves in chemical reaction and other heat sources. h is the enthalpy which is equal to the heat generated in system at constant pressure. It is given by[7]

$$h = U + \frac{p}{\rho} \tag{3.3-4}$$

then

$$E = h - \frac{p}{\rho} + \frac{1}{2}\vec{u}\vec{u}$$
(3.3-5)

Change in enthalpy for ideal gas is given by

$$h = \int_{T_{ref}}^{T} C_p dT \tag{3.3-6}$$

Change in enthalpy for incompressible fluid is given by

$$h = \int_{T_{ref}}^{T} C_p dT + \frac{p}{\rho}$$
(3.3-7)

where,

 $T_{ref}$  is 298.15k, which can be change according to situation.

S is the entropy and it is given by

$$S = \int_{T_{ref}}^{T} \frac{dQ}{T} = \int_{T_{ref}}^{T} \frac{c_{\nu}}{T} dT$$
(3.3-8)

Finally, mathematical model of flow without chemical reaction is defined by equations are below

- Continuity equation
- Navier-stroke equation
- Rate of dissipation
- The turbulence kinetic equation
- > The energy equation

#### 3.4. Species transport with chemical reactions

Using ANSYS FLUENT we can model mixing and transport chemical species of a model by solving conservation equations which describes convection, diffusion and reaction sources for each of the species component. Multiple simultaneous chemical reactions can be modelled with the reactions occurring in the bulk phase (volumetric reactions) or on wall surface or particles surfaces and in the porous region. In this chapter we will discuss about species transport and finite -rate chemistry as related to volumetric reactions.[6]

#### The Generalized Finite-Rate Formulation for reacting modeling

The reaction rates for the species transport in ANSYS FLUENT for turbulent flows, by one of three models are.

- Direct use of finite-rate kinetics: The effect of turbulent fluctuations on kinetics is neglected and reaction rates are determined by general finite-rate chemistry directly.
- Eddy-dissipation model: Reaction rates are assumed to be controlled by the turbulence with the ignoring the effect of chemistry timescales, which avoids the expensive Arrhenius chemical kinetic calculations. The model is computationally cheap for realistic results, only one or two step heat release mechanisms should be used. This approach should be used only when the chemistry times scales to be known fast relative to the turbulence timescales throughout the domain.
- Eddy –dissipation-Concept (EDC) model: In this detail chemical kinetics can be incorporated in turbulent flames, with considering timescales of both turbulence and kinetics. Note that detailed chemical kinetic calculation can be computationally expensive.

Generally finite-rate formulation is suitable for wide range of applications including laminar or turbulent reaction system and it's also suitable for combustion system with premixed, non-premixed or partially premixed flames.[6]

#### 3.4.1 Species transport equations

In this section is related to theoretical information about species transport and finite rate chemistry to volumetric reactions which is important for combustion of methane.

When we choose to solve conservation equation for chemical species, ANSYS FLUENT predicts local mass fraction for each species, and find  $Y_i$ , through solution of convection – diffusion equation for i<sup>th</sup> species. The general form of conservation equation is shown below[6]

$$\frac{\partial}{\partial t}(\rho Y_i) + \nabla \cdot (\partial \vec{v} Y_i) = -\nabla \cdot \vec{J}_i + R_i + S_i$$
(3.4.1-1)

Where,

 $R_i$  is net rate of production of species.

*i* is by chemical reaction (described in this chapter below).

 $\mathcal{S}_i$  is rate of creation by addition from dispersed phase any user defined sources.

An equation of the above form will be solved for N - 1 species. Where N is the total number of fluid phase chemical species present in system. Since, the mass fraction of the species must be sum to unity; the  $N^{th}$  mass fraction is determined by one minus the sum of the N - 1 solves mass fractions. To minimize numerical errors, the  $N^{th}$  species should be selected as that species with overall largest mass fraction, such as  $N_2$  when the Oxidizer is air.[6]

#### 3.4.2 Finite-Rate kinetics (no TCI)

When there is no turbulence chemistry interaction (TCI), then the finite rate kinetics model is used with incorporated by computing the chemical source terms using the general reaction-rate expressions, without attempting any account of explicitly for the effects of turbulent fluctuations for the calculations of source term. This approach is recommended mainly for laminar flows, where the formulation is exact, or for turbulent flows using complex chemistry where either the turbulence time-scales are expected to for the fast relative to the chemistry time scales or where the chemistry is sufficiently for that complex chemistry timescales is important for highly disparate.[6]

The net source for the chemical species due to reaction is computed as the sum of the reaction sources to over the reactions that the species participate in[6]

$$R_i = M_{w,i} \sum_{r=1}^{N_R} R_{i,r}$$
(3.4.2-1)

Where,

 $M_{w,i}$  is the molecular weight of species i.

 $R_{i,r}$  is the molar rate of creation or destruction of species in reaction r.

Consider the  $r^{th}$  reaction written in general form as follows:

$$\sum_{N}^{i=1} v_{i,r}' M \xrightarrow{\underset{kfr}{\longrightarrow}} \sum_{N}^{i=1} v_{i,r}'' M_i$$
(3.4.2-2)

Where,

N= number of chemical species in the system

 $v'_{i,r}$ =stoichiometric coefficient for reactant i in reaction r

 $v_{i,r}^{"}$  = stoichiometric coefficient for product i in reaction r

M<sub>i</sub>= symbol denoting species i

 $k_{f,r}$ =forward rate constant for reaction r

 $k_{b,r}$  = backward rate constant for reaction r

The above equation is valid for both reversible and irreversible reactions. For irreversible reactions the backward rate constant  $k_{b,r}$  is zero.

The summations for all chemical species in the system, but only species that appear as reactants or products will have non zero stoichiometric coefficients.

The molar rate of creation/destruction of species i in reaction r is given by[6]

$$R_{i,r} = \Gamma(v_{i,r}^{"} - v_{i,r}^{\prime}) \left( K_{f,r} \prod_{f=1}^{N} [C_{j,r}]^{n_{i,r}^{\prime}} - k_{b,r} \prod_{j=1}^{N} [C_{j,r}]^{v_{j,r}^{\prime}} \right)$$
(3.4.2-3)

Where,

 $C_{i,r}$  = molar concentration of species i in reaction r (Kmol.m<sup>-3</sup>)

 $\eta'_{i,r}$ =rate exponent for reactant species j in reaction r

 $\eta'_{i,r}$ =rate exponent for product species j in reaction r

For information about inputting the stoichiometric coefficients and rate exponents within the ANSYS Fluent user interface, for both global forward (irreversible) reactions and elementary (reversible) reactions, see Inputs for Reaction definition in the Fluent User's Guide. The information referred below for the mechanisms manually entered in ANSYS Fluent.[6]

 $\Gamma$  represents the net effect of third bodies on the reaction rate. The term is given by

$$\Gamma = \sum_{j}^{N} Y_{j,r} C_j \tag{3.4.2-4}$$

Where,

 $Y_{j,r}$  is the third-body efficiency of the j<sup>th</sup> species in the r<sup>th</sup> reaction. By default, ANSYS FLUENT does not include third-body effects in the reaction rate for calculation. However, you can opt to include the effect of third-body efficiencies if you have data for them.[6]

The constant for forward rate reaction, is computed using the Arrhenius expression[6]

$$K_{f,r} = A_r T^{\beta} e^{\frac{-E_r}{RT}}$$
(3.4.2-5)

Where,

 $A_r$  = pre-exponential factor (consistent units)

 $\beta$  = temperature exponent (dimensionless)

 $E_r$ =activation energy for the reaction (J. kmol<sup>-1</sup>)

R=universal gas constant. (Jkmol<sup>-1</sup>K<sup>-1</sup>)

ANSYS FLUENT data base also provides the values of  $V'_{i,r}$ ,  $V''_{i,r}$ ,  $\eta'_{j,r}$ ,  $\eta''_{j,r}$ ,  $\beta_r$ ,  $A_r$  and optionally  $Y_{j,r}$  during the problem definition.

ANSYS FLUENT also provides the option to explicitly specify the reversible reaction rate parameters such as preexponential factor, temperature exponent, and activation energy for the reaction if it is desired. In this case of backward rate constant of the reversible reaction is computed using the relationship similar to Arrhenius equation.[6]

It is given by

$$K_{b,r} = A_{b,r} T^{\beta_{b,r}} e^{\frac{-E_{b,r}}{RT}}$$
(3.4.2-6)

Where,

 $A_{b,r}$  = pre-exponential factor for backward reaction (consistent units)

 $\beta_{b,r}$ =temperature exponent for backward reaction (dimensionless)

 $E_{b,r}$ =activation energy for the backward reaction. (J. kmol<sup>-1</sup>)

#### 3.4.3. Eddy -Dissipation model

During the combustion process, some fuels burns quickly and chemical reaction is controlled by turbulent mixing. In high-temperature non-premixed flames, for example, turbulence slowly converts or mixes fuel and oxidizer into the reaction zones where they burn quickly. In certain premixed flames, the turbulence slowly converts or mixes cold reactants and hot products into the reaction zones, where reaction occurs rapidly. In such cases, one approximation is to assume the combustion is mixing limited, allowing neglect of the complex chemical kinetic rates and instead assuming instantaneous burn upon mixing.[6]

ANSYS FLUENT provides a turbulence-chemistry interaction model based on the Magnussen and Hjertager (two of reactions) called eddy-dissipation model. The average rate of production of species i in the reaction k is given by the smaller of the two expressions given below.[6]

$$R_{i,r} = V'_{i,r} M_{w,i} A \rho \frac{\epsilon}{k} min_R \left( \frac{Y_R}{V'_{R,r} M_{w,R}} \right)$$
(3.4.3-1)

$$R_{i,r} = V'_{i,r} M_{w,i} AB \frac{\epsilon}{\kappa} \frac{\sum_{P} Y_{p}}{\sum_{J}^{M} V''_{J,r} M_{w,j}}$$
(3.4.3-2)

Where,

 $Y_P$  = mass fraction of any product species, P

 $Y_R$ =mass fraction of a particular reactant, R

A=an empirical constant equal to 4.0

$$B$$
=an empirical constant equal to 5.0

In the above equations, the chemical reaction rate is governed by large eddy mixing time scale/£, as in the eddy-breakup model of Spalding. However, the combustion proceeds whenever turbulence is present (K/E>O), and an ignition source is not required to initiate combustion. This is usually acceptable for non-premixed flames, but in premixed flames, the reactants will burn as soon as they enter the computational domain, upstream of the flame stabilizer. To remedy this, ANSYS FLUENT provides the finite-rate or eddy-dissipation model, where both the finite-rate reaction rates and eddy-dissipation rates are calculated.

The net reaction rate is chosen as the minimum of these two rates. In practice, the finite rate kinetics acts as a kinetic "switch", preventing reaction before the flame holder. The eddy-dissipation rate is generally smaller than the Arrhenius rate when the flame is ignited and mixing of the reactions is limited.[6]

Also eddy-dissipation model requires products to initiate reaction. When you initialize the solution for steady flows, ANSYS FLUENT sets all species mass fractions to a maximum in the user-specified initial value and 0.01. This is usually sufficient to start the reaction. However, if you converge a mixing solution first, where all product mass fractions are zero, you may then have to patch products into the reaction zone to ignite the flame.[6]

#### 3.4.4. Finite-rate/Eddy dissipation model

It is combined of finite-rate and eddy-dissipation model. In this model, rate of reaction is determined by Arrhenius and also by eddy-dissipation equation. Local reaction rate is given by the minimum value from these two equations.

Although ANSYS FLUENT allows multi-step reaction mechanisms for the eddy-dissipation model and finite-rate /eddy-dissipation model, these will likely produce incorrect solutions. This is the reason that multi-step chemical mechanisms are based on Arrhenius rates and these chemical mechanisms are differing for each reaction. In eddy-dissipation model every reaction has the same rate and therefore model will be used only for one-step or two step global reactions.[6]

#### 3.4.5. Eddy-dissipation -concept (EDC) model

The eddy-dissipation-concept (EDC) model is an extension of the eddy-dissipation model that allows inclusion of detailed chemical mechanisms in turbulent flows and also multistep chemical kinetics mechanism is included. It assumes that reactions occur in small turbulent structures called Fine scales.[6]&[8]

The length fraction of the fine scales is obtained as below equation.[6]

$$\xi^* = C_{\xi} \left(\frac{v\epsilon}{k^2}\right)^{1/4} \tag{3.4.5-1}$$

Where

 $\xi^*$  is the fine-scales quantiles.

 $C_{\xi}$  is the volume fraction constant .and the value is 2.137

 $\nu$  is the kinematic viscosity.

The volume fraction of the fine scales is calculated as  $\xi^*$ . Reacted species are assumed to be in the fine structures over a time scale.

$$\tau^* = C_\tau \left(\frac{\nu}{\varepsilon}\right)^{1/2} \tag{3.4.5-2}$$

Where

 $C_{\tau}$  is a time scale constant equal to 0.4802

The source term in the conversation equation for the mean species i, is modeled as below.

$$R_i = \frac{\rho(\xi)^2}{\tau^* [1 - (\xi^*)^3]} [Y_i^* - Y_i]$$
(3.4.5-3)

Where,

 $Y_i^*$  is the fine-scale species mass fraction after reacting over time  $au^*$ 

The EDC model can incorporate detailed chemical mechanisms into turbulent reacting flows. However, this mechanism is invariably stiff and their numerical integration is costly for computational. Hence, the model should be used only when the assumption of fast chemistry is invalid, such as modeling low temperature or high-pressure combustion, the slow CO burnout in rapidly quenched flames, or the NO conversion in selective noncatalytic reduction (SNCR).[6]

#### 3.5. Characteristics of boundary conditions

In ANSYS FLUENT boundary conditions are associated with zones, not with individual faces or cells. According to combining of two or more zones that will have the same boundary conditions.

The boundary conditions that are available in ANSYS FLUENT are

- Inlet boundary conditions (velocity inlet, mass flow inlet, pressure inlet etc)
- > Outlet boundary conditions (pressure outlet, mass flow outlet etc)
- Wall boundary conditions
Symmetric, periodic, axis boundary conditions

#### Velocity inlet boundary conditions

Velocity inlet boundary conditions are used to define the flow velocity along with relevant scalar properties of the flow in the inlet. This velocity boundary conditions is applicable for both compressible and incompressible flow.[9]

#### Pressure inlet boundary conditions

Pressure inlet boundary conditions are used to define the fluid pressure at inlet flows along with all other scalar properties of flow. They are suitable for both compressible and incompressible flow calculations. Pressure inlet boundary conditions can be used when the inlet pressure is known as flow rate or velocity. Pressure inlet boundary conditions can also use to define a" free" boundary in an external or unconfined flow.[9]

#### Mass flow rate inlet boundary condition

A mass flow inlet is more important to match the total pressure for the inflow stream. Mass flow in inlet can be varies, then there will be change in the outlet pressure. An example is the case off small cooling jet that is bled into the main flow at fixed mass flow rate, while the velocity of main flow is governed by pressure inlet and outlet conditions.[9]

# Pressure outlet boundary condition

The boundary conditions are requiring to specific the static pressure at the outlet boundary. The value of specified static pressure is used only the flow is subsonic. If the flow become locally supersonic, the specified pressure will no longer to use. In the interior flow Pressure will be extrapolated. All other flow quantities are extrapolated from the interior.

A set of "backflow" conditions is also specified, that should be flow reverse direction at the pressure outlet during the solution process. Convergence difficulties will minimize the specific realistic values for the backflow quantities.[9]

# **Outlet flow boundary conditions**

Outlet flow boundary conditions are used in ANSYS FLUENT to model flow exits for the details of the flow velocity and pressure are not known to solve the flow problem.[9]

#### Mass- flow outlet boundary conditions

Mass-flow outlet boundary conditions are used in ANSYS FLUENT to out flow the pump domain to a prescribed mass flow rate or mass flux distribution. A mass-flow outlet is often used when it is more important to match a prescribed mass flow rate than to match the static pressure of the outflow stream.[9]

#### Wall boundary

Wall boundary conditions are used to bound between fluid and solid (wall) regions. In viscous flows there is no-slip boundary condition which is enforced by default, but you can specify a tangential velocity component in terms of translational or rotational motion of the wall boundary or a "slip "wall by specifying shear. If can also slip wall with zero shear using the symmetry boundary type, but we should apply symmetry conditions for all the equations.[9]

# Symmetry boundary conditions

This boundary conditions are used, when the physical geometry of interest and the expected pattern of flow /thermal solution, having mirror symmetry. They can also use to model zero-shear slip walls in viscous flows. This section describes the treatment of flow at symmetry planes and provides the use of symmetry. There is no need to define any boundary conditions at symmetry boundaries, but we must define correct symmetry boundary locations.[9]

#### Fluid zone

A fluid zone is a group of cells which are used to solve active equations. The required input is only fluid zone of the fluid material. We must indicate which material the fluid zone contains and for the materials appropriate properties are used.[9]

# 3.6. Computational grid (Mesh)

In order to conduct an analysis of a problem, the solution domain is splitted into number of sub-domains which are called cells. The combination of these cells in Computational Fluid Dynamics is called Mesh.

For 2D model we can define cells in rectangular and triangular elements and for 3D model we can define cells shape in hexahedral, tetrahedral and pyramid elements.



Figure 3 shows a simple mesh of rectangular

The above *Figure 3* shows the generation of mesh, in which it is possible to solve the mathematical model under the assumption of linearity. To know the behavior of the variables it is necessary to solve for assumed to be linear within each cell. It also implies a finer mesh, which is needed for areas in the domain where the physical properties to be predicted are suspected to be highly volatile.[10]&[11]

The failure of the simulation can be predicated by errors on mesh. Because the mesh is too coarse and doesn't cover all effects that happen in single element one by one, but if it covers multiple effects that changes the mesh, which gets finer. Therefore, it is necessary to study independency of cells. The accuracy of solution depends on the mesh structure. To get accurate solutions and obtaining reliable results, the analyst has to be extremely careful on the type of cell and computation time.[10]&[11]

# 4.Description of drop tube

Drop tube is equipment used for testing of pulverized coal combustion (shown in *Figure 5*), but for my thesis we just used only geometry of the drop tube.

The air flow, species transport and gaseous combustion of methane take place in the drop tube.



Figure 4 shows the drop tube

The 2-D model of the above drop tube is shown below



Figure 5 shows the 2-D of the drop tube

Where,

1-inlet

2-outlet

3-wall

The above *Figure 5* shows the 2-D of the drop tube which is having length of 4.9m with diameter of 0.066m. The air and species of air will pass from the inlet from starting of tube and methane will passes 0.6m from the inlet of the tube, where wall is stationary.

In this project firstly air is flow to the drop tube without heat transfer after air will be flow by gaseous species such as  $CO_2$ ,  $H_2O$ ,  $N_2$  and  $O_2$  but without heat transfer to the drop tube. Finally, air will be by gaseous species and combustion of methane takes place in inside the drop tube while oxygen is supplied to the drop tube.

# 5. Numerical solutions 5.1. CFD modelling of the air flow without heat transfer

In this modelling air is flow through the drop tube without heat transfer. First, as per the dimensions, geometry is created in Design Modeler and generate the mesh in the ANSYS Meshing. Then generated mesh should be read to the ANSYS FLUENT. When mesh is read in FLUENT, as per the requirement of the problem define the model of turbulence, boundary conditions are applied and finally calculation will be started and post processing will be done.

# Description

The design tube is in shown in the *Figure 6*. The boundary conditions will be provided for this study. There is defined inlet, outlet, wall and axis boundary condition. The geometry and boundary conditions are created in the "ANSYS" (18.2). The detailed boundary conditions are applied in the ANSYS FLUENT.

This problem can be defined using 2D model, since the geometry is axis symmetry. In 2D model time required for the solving is less.



*Figure 6 shows the air flow and pressure outlet in the drop tube.* 

# **Creation of mesh**

The mesh is created in the ANSYS Meshing and generated the rectangular mesh which is readied in ANSYS FLUENT.

Once mesh is read in the ANSYS fluent. Check for the dimensions and note down the size of mesh. Keep the dimensions as per you're convenient in meter or millimeters.

Table 1 The below table shows the number of cells, faces and nodes

Cells	Faces	Nodes
40000	82020	42021



Figure 7 shows the mesh generated in FLUENT

# Calculation of Reynolds number for air on the inlet

Density of air =1. 225kg.m<sup>-3</sup>

Kinematic viscosity of air =1.46E-05 m<sup>2</sup>.s<sup>-1</sup>

Hydraulic diameter =0.066m

Mass flow rate =0.004079 kg.s<sup>-1</sup>

Velocity of air =0.973 m.s<sup>-1</sup>

Dynamic viscosity =1.79E-05 kg.m<sup>-1</sup>s<sup>-1</sup>

$$R_e = \frac{u d_h}{\vartheta}$$
$$R_e = \frac{0.973 * 0.066}{1.46E - 05}$$
$$R_e = 4.40E + 03$$

Reynolds number for the flow is higher than 2320, hence the flow is turbulent flow.

#### **Definitions of models**

In this problem, we defined K-E standard model with pressure-based solver and absolute velocity with steady time and with axis symmetric. (for more information about k-E standard model see in chapter 2.3)

#### **Definition of Boundary conditions**

The defined boundary conditions are:

- > Wall boundary condition is defined as stationary wall.
- Inlet boundary condition is defined a mass-flow-inlet.
- Outlet boundary condition is defined as pressure outlet.
- Axis boundary condition, defined as axis.

#### Mass flow inlet

In this model mass flow rate is 0.00479 kg.s<sup>-1</sup> which pass through the hydraulic diameter of 0.066 m.

The mass flow is given by 
$$Q_m = \rho A u \text{ kg.s}^{-1}$$
 (5.1-1)

Calculation of velocity

$$Q_m = \rho A u$$

$$Q_m = \rho \frac{\pi d^2}{4} u$$

Finally, velocity is given by

$$u = \frac{4Q_m}{\rho \pi d^2} \tag{5.1-2}$$

$$u = \frac{4 * 0.004079}{1.225 * 3.14 * 0.066^2}$$

$$u = 0.973 \text{ m.s}^{-1}$$

#### wall

In this wall is stationary means fluid is flowing the stationary drop tube, where it is possible the increase or decrease the velocity, pressure and mass flow rate of the fluid.

# Outlet

In this case outlet is defined as pressure outlet. The value of relative pressure outlet is zero.

# Definition of physical properties of air

The physical properties of air are density, specific heat, thermal conductivity, viscosity and molecular weight.

Physical properties	Values
Density (kg.m <sup>-3</sup> )	1.225
Specific heat (J.kg <sup>-1</sup> k <sup>-1</sup> )	1006.43
Thermal conductivity (w.m <sup>-1</sup> k <sup>-1</sup> )	0.0242
Viscosity (kg.m <sup>-1</sup> s <sup>-1</sup> )	1.7894e-05
Molecular weight (kg.kmol <sup>-1</sup> )	28.966

Table 2 The below table shows the physical properties of air

# 5.1.1. Results from the CFD calculations

Solution is converged and you can see residuals in the Figure 8



Figure 8 shows the residuals plotted

We can see the velocity vectors from the *Figure 9* and we can see that maximum velocity of air is 1.36m.s<sup>-1</sup>.



Figure 9 shows the velocity vector

We can see Individual vectors from the *Figure 10*, where the maximum velocity of air is 1.36m.s<sup>-1</sup> (In the position 0.5m from the inlet of the tube)



Figure 10 shows the induvial vectors

#### Contour of velocity magnitude



Figure 11 shows the contours of velocity magnitude

From the *Figure 11* shows the velocity of the inlet air will be increasing as the air flow through the drop tube which is velocity of outlet air is higher than inlet air and maximum velocity of air is 1.36m.s<sup>-1</sup>.



# Contour of static pressure

#### Figure 12 shows the contour of static pressure

From the *Figure 12* we got the results as pressure of the inlet will be greater than the outlet pressure, which indicates the pressure goes on decreasing as the air flow through the tube.

#### 1,4000 1.2000 1.0000 0.8000 0.6000 0.4000 0.2000 0.0000 0.0350 0.0400 0.0000 0.0050 0.0100 0.0150 0.0200 0.0250 0.0300 Position (m)

#### Velocity profiles in the different sections of the computational domain

Figure 13 shows the velocities profiles in different sections

The *Figure 13* shows the graph plotted for different velocity of air passes through the tube with respect to the position of the tube(X=0,0.5,1,1.5,2,2.5,3.5,4.5m)

# 5.2. CFD Modelling of air flow by gaseous species $(O_2, CO_2, H_2O \text{ and } N_2)$ without heat transfer

In this modelling air will be flow by gaseous species such as  $N_2$ ,  $H_2O$ ,  $CO_2$  and  $O_2$  through the drop tube without heat transfer.

# Description

This problem is same as the previous problem only the air is flow through the drop tube in form of gaseous species such  $O_2$ ,  $H_2O$ ,  $N_2$  and  $CO_2$ . For more information its described in the previous chapter 5.1

# **Definition of models**

In this problem, we defined K-E standard model with pressure-based solver and absolute velocity with steady time and with axis symmetric. (for more information about k-E standard model see in chapter 2.3)

#### Define of mixture

In this problem mixture is defined as  $N_2$ ,  $H_2O$ ,  $O_2$  and  $CO_2$  species. We need to define composition of the mixture by mass fraction.

Table 3 The below table shows the mass fraction of the species on the inlet of the drop tube

Species	Mass fraction (Y)
Nitrogen ( $N_2$ )	0.78
Carbon dioxide ( $CO_2$ )	0.0004
Hydrogen ( $H_2O$ )	0.0128
Oxygen ( $O_2$ )	0.2317

# Types of Boundary conditions

Boundary conditions for this are same as the previous chapter (5.1)

# Mass flow inlet

In this model mass flow rate is 0.00479 kg.s<sup>-1</sup> which is passes through the hydraulic diameter of 0.066m.

# Outlet

In this case outlet is defined as pressure outlet. The value of relative pressure outlet is zero.

# 5.2.1 Results from the CFD calculation

Solution is converged and you can see residuals in the Figure 14



Figure 14 shows the residuals plotted

We can see the velocity vectors from the *Figure 15* and we can see that maximum velocity of air is 1.39m.s<sup>-1</sup>.



Figure 15 shows the velocity vector

We can see Individual vector from the *Figure 16*, where the maximum velocity of air is 1.39m.s<sup>-1</sup> (In the position 2.5m from the inlet of the tube)



Figure 16 shows the individual vectors

#### Contour of velocity magnitude

anataur 1		ANSYS
Velocity Magnitude		Academic
1.39e+00 1.32e+00 1.25e+00 1.18e+00 1.11e+00 1.04e+00 9.70e-01 9.00e-01 8.31e-01 7.52e.04		
7.024-01 6.93e-01 6.23e-01 5.54e-01 4.16e-01 3.46e-01 2.77e-01 2.08e-01 1.39e-01 6.93e-02 0.00e+00		
	P ((n)	

*Figure 17 shows the contour of velocity magnitude* 

From the *Figure 17* shows the velocity of the inlet air will be increasing as the air flow through the drop tube which is velocity of outlet air is higher than inlet air and maximum velocity of air is 1.39m.s<sup>-1</sup>.



#### Contour of static pressure

*Figure 18 shows the contour static pressure* 

From the *Figure 18 we* got the results as pressure of the inlet will be greater than the outlet pressure, which indicates the pressure goes on decreasing as the air flow through the tube.



#### Velocity profiles in the different sections of the computational domain

Figure 19 shows the velocities profiles in different sections

The *Figure 19* shows the graph plotted for different velocity of air passes through the tube with respect to the position of the tube(X=0,0.5,1,1.5,2,2.5,3.5,4.5m). Results obtain from both air passes through model and species passes through model are similar in velocity maximum in both the case is 1.36 and 1.39m.s<sup>-1</sup> and We can see pressure maximum is 3.04 Pa and 3.14 Pa and outlet pressure in both is equal to zero.

# 5.3. CFD modelling of air flow by gaseous species and combustion of methane with oxygen

To enhance the performance of methane combustion in the drop tube by using ANSYS FLUENT. Combustion is a process of burning the fuels in presence of oxygen and it occurs in a low-pressure and high temperature combustion chamber. Here oxygen and methane are injected to drop tube.

# **Chemical reaction**

In this problem we want analyse the combustion of methane. The combustion will be modelled using a global one-step reaction mechanism, assuming the complete conversion of the fuel.[15] The reaction is shown below.

 $CH_4+2O_2\rightarrow CO_2+2H_2O$ 

The above reaction will be defined the stoichiometric coefficients, formation values 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 models.

Here, we are going to study the combustion of methane in drop tube by using four different models such as,

- Finite- rate model /No TCI
- Finite-rate/Eddy-Dissipation model
- Eddy-Dissipation model
- Eddy-Dissipation -concept model

#### Description

A model is shown in the *Figure 20*. A methane enters to the drop tube by small nozzle at different velocity like 5,7,9,10,12,14,16 and 20 m.s<sup>-1</sup>. Ambient air as the mixture of  $N_2$ ,  $O_2$ ,  $H_2O$  and  $CO_2$  enters the combustors at 1 m.s<sup>-1</sup>. The overall equivalence ratio is approximately 0.76(approximately 28 excess air). The methane enters to combustion chamber and mixes with air and combustion takes place with initially expand with little interference from outer wall.



Figure 20 shows the air flow and Methane flow in the draft tube

# **Creation of mesh**

The mesh is created in the ANSYS Meshing by rectangular elements and generated. After mesh which is readied in ANSYS FLUENT.

Once mesh is read in the ANSYS fluent. Check for the dimensions and note down the size of mesh. Keep the dimensions as per you're convenient in meter or millimeters.

Table 4 The below table shows the mesh size

Cell	Faces	Nodes
54400	110828	56429



Figure 21 Fig shows the mesh generated in ANSYS Meshing

# **Defined Models**

For the given problem, we are going to use the K-E standard model with pressure-based solver and absolute velocity with steady time with the axisymmetric. In case of the combustion problem it is necessary to define model as the volumetric reaction, as per the problem required it is necessary to use the four different Turbulence -chemical interaction.

# **Mixture Materials**

The mixture materials concepts have been implemented in ANSYS Fluent to facilitate the species transport set up and flow reacting. A mixture material may be thought of as a set of species and a list rules governing their interaction. The mixture material carries with it the following information below.[12]

> A list of the constituent species, referred to as "fluid materials"

- A list of mixing laws dictating how mixture properties (density, viscosity, specific heat, and so on) are to be derived from the properties of individual species if composition-dependent properties are desired.
- A direct specification of mixture properties is a composition of independent properties.
- > Diffusion coefficients for the mixture of species is individual.
- Other material properties (for example, absorption and scattering coefficients) are not associated with individual species
- A set of reactions, including a reaction type (finite-rate, eddy-dissipation, and so on) and stoichiometry and rate constants.[12]

Significant effect of the results has mainly constant activation energy and pre-exponential factor. In this problem we used ZC model, In the below values of Pre-exponential factor and Activation energy are given.

Model	Pre-exponential	Activation energy	Temperature factor
	factor	(cal/mol)	
	(cm <sup>3</sup> /mol) <sup>2</sup> /s		
Z-C model	1.35e+20	30000	0

Table 5 The below given the Activation energy and pre-exponential factor for Z-C model[13]

In our problem, we are using methane, carbon -dioxide, oxygen nitrogen and hydrogen. In fluent data base there is default values for the mixtures has per your problem required we need to copy the values of the mixtures.

Table 6 The	below table shows	physical	properties of	f species of	air and methane
-------------	-------------------	----------	---------------	--------------	-----------------

Physical	Methane	Hydrogen	Nitrogen	Oxygen	Carbondioxide
properties	$(CH_4)$	(H <sub>2</sub> O)	$(N_2)$	( <i>O</i> <sub>2</sub> )	( <b>CO</b> <sub>2</sub> )
Density (kg/m <sup>3</sup> )	0.6679	0.5542	1.138	1.299	1.7878
Thermal	0.0332	0.0261	0.0242	0.0246	0.0145
conductvity					
(w/mk)					
Viscosity (kg/m-s)	1.087e-	1.34e-05	1.663e-	1.91e-05	1.37e-05
	05		05		

Molecular weight	16.04	18.01	28.013	31.99	44.009
(kg/kmol)					
Standard state of	-7.4e+07	-2.4e+08	0	0	-3.93e+08
enthaply					
(j/kgmol-k)					
Standard state of	186040.1	188696.4	191494.8	205026.9	213720.2
entropy (j/kgmol-					
k)					

#### **Boundary conditions**

#### Air mixture as velocity inlet

We define velocity inlet as air inlet which is the mixture of  $O_2$ ,  $H_2O$ ,  $N_2$  and  $CO_2$ . The mixture of air is passes through the drop tube with the velocity of 1m.s<sup>-1</sup> and turbulence intensity of 0.5% and hydraulic diameter of 0.066m with temperature of 300k

Table 7 The below table shows the mass fraction of species inlet to the drop tube

Species	Mass	
	fraction(Y)	
Nitrogen (N <sub>2</sub> )	0.78	
Carbon dioxide (C $O_2$ )	0.0004	
Hydrogen ( $H_2O$ )	0.0128	
Oxygen ( $O_2$ )	0.2317	

# Velocity inlet for Methane

We define velocity inlet as methane inlet which passes through the drop tube with different velocities like 5,7,9,10,12,14,16 and 20m.s<sup>-1</sup> with turbulence intensity of 0.5% and hydraulic diameter 0.0025m and with temperature 300k.

Table 8 The below table shows the methane and species mixtures passes to drop tube

Methane ( $CH_4$ )	1
Nitrogen (N <sub>2</sub> )	0
Carbon dioxide ( $CO_2$ )	0

Hydrogen ( $H_2O$ )	0
Oxygen ( $O_2$ )	0

## Outlet

We defined outlet as pressure outlet. The value of relative gauge pressure outlet is zero with back flow turbulence intensity of 0.5% and back flow diameter of 0.066m with temperature of 300k.

#### Wall bottom and wall top

Wall bottom is defined as stationary wall without slip and standard roughness models with roughness height is equal to zero and roughness constant 0.5.

#### **Initial Reaction Solution**

The following steps should be followed to initialize the solution

1. Select the Coupled Pseudo Transient solution method.

The Pseudo Transient option enables the pseudo transient algorithm for the coupled pressure-based solver. This algorithm adds an unsteady term to the solution equations in order to improve the stability and behaviour of convergence. Use of this option is recommended for general fluid flow problems

- 2. Modify the solution controls.
- 3. Ensure the results of residuals during the calculation.
- 4. Initialize the field variables
- 5. Run the calculation by number of iterations required

# Graphical evaluation of results for different models

The aim of the work us to create a model of combustion of methane gaseous with supply of oxygen and then apply for four different models contained in the ANSYS FLUENT software. The graphs are plotted for 5,7,9,10,12,14,16 and 20 m.s<sup>-1</sup> methane with 1 m.s<sup>-1</sup> of oxygen.

5.3.1. Results obtain for Finite rate /No TCI model Static temperature for 1 m.s<sup>-1</sup> of  $O_2$  and 5 m.s<sup>-1</sup> of  $CH_4$ 



Figure 22 Static temperature inside drop tube for 1 m.s<sup>-1</sup> of  $O_2$  and 5 m.s<sup>-1</sup> of  $CH_4$ 



Static temperature evaluated along the axis of the tube

Figure 23 Graph of static temperature with respect to axis of the tube

Static temperature for 1 m.s<sup>-1</sup> of  $O_2$  and 7 m.s<sup>-1</sup> of  $CH_4$ 



Figure 24 Static temperature inside drop tube for 1 m.s<sup>-1</sup> of  $O_2$  and 7 m.s<sup>-1</sup> of  $CH_4$ 



Figure 25 Graph of static temperature with respect to axis of the tube

Static temperature for 1 m.s<sup>-1</sup> of  $O_2$  and 9 m.s<sup>-1</sup> of  $CH_4$ 



Figure 26 Static temperature inside drop tube for 1 m.s<sup>-1</sup> of  $O_2$  and 9 m.s<sup>-1</sup> of  $CH_4$ 



Figure 27 Graph of static temperature with respect to axis of the tube

Static temperature for 1 m.s<sup>-1</sup> of  $O_2$  and 10 m.s<sup>-1</sup> of  $CH_4$ 



Figure 28 Static temperature inside drop tube for 1 m.s<sup>-1</sup> of  $O_2$  and 10 m.s<sup>-1</sup> of  $CH_4$ 



Figure 29 Graph of static temperature with respect to axis of the tube

Static temperature for 1 m.s<sup>-1</sup> of  $O_2$  and 12 m.s<sup>-1</sup> of  $CH_4$ 



Figure 30 Static temperature inside drop tube for 1 m.s<sup>-1</sup> of  $O_2$  and 12 m.s<sup>-1</sup> of  $CH_4$ 



Static temperature evaluated along the axis of the tube

Figure 31 Graph of static temperature with respect to axis of the tube

Static temperature for 1 m.s<sup>-1</sup> of  $O_2$  and 14 m.s<sup>-1</sup> of  $CH_4$ 



Figure 32 Static temperature inside drop tube for 1 m.s<sup>-1</sup> of  $O_2$  and 14 m.s<sup>-1</sup> of  $CH_4$ 



Static temperature evaluated along the axis of the tube

Figure 33 Graph of static temperature with respect to axis of the tube

Static temperature for 1 m.s<sup>-1</sup> of  $O_2$  and 16 m.s<sup>-1</sup> of  $CH_4$ 



Figure 34 Static temperature inside drop tube for 1 m.s<sup>-1</sup> of  $O_2$  and 16 m.s<sup>-1</sup> of  $CH_4$ 



Static temperature evaluated along the axis of the tube

Figure 35 Graph of static temperature with respect to axis of the tube

Static temperature for 1 m.s<sup>-1</sup> of  $O_2$  and 20 m.s<sup>-1</sup> of  $CH_4$ 



Figure 36 Static temperature inside drop tube for  $1m.s^{-1}$  of  $O_2$  and 20  $m.s^{-1}$  of  $CH_4$ 



Static temperature evaluated along the axis of the tube

Figure 37 Graph of static temperature with respect to axis of the tube

Graph of Mass fraction of  $CH_4$  along the axis of the drop tube for different velocities of methane



Figure 38 Graph of Mass fraction of  $CH_4$  along the axis of the drop tube for all velocities of methane

Graph of Mass fraction of  $O_2$  along the axis of the drop tube for different velocities of methane



Figure 39 Graph of Mass fraction of  $O_2$  along the axis of the drop tube for all velocities of methane

Graph plotted static temperature for all methane velocities evaluated along the axis of the tube



Figure 40 Graph of static temperature along the axis of the drop tube for all velocities of methane

We can see from the *Figure 40* static temperature plotted for all the velocities evaluated along the position of the tube. The temperature will go on increasing along axis of the tube and remains constant once the combustion finished.

From the analysis of combustion of the methane for different velocities of methane like 5,7,9,10,12,14,16 and 20 m.s<sup>-1</sup>. The results are similar for the velocities, we got know that combustion of methane will be higher in starting then goes on decreasing, we can tell the temperature will goes on increasing as velocity increase and pressure will be goes on decrease through the drop tube and outlet pressure will zero. The maximum static temperature is 2300K.

5.3.2. Results obtain for Finite rate/Eddy dissipation model Static temperature for 1 m.s<sup>-1</sup> of  $O_2$  and 5 m.s<sup>-1</sup> of  $CH_4$ 



Figure 41 static temperature inside drop tube for 1 m.s<sup>-1</sup> of  $O_2$  and 5 m.s<sup>-1</sup> of  $CH_4$ 



Figure 42 Graph of static temperature with respect to axis of the tube

Static temperature for 1 m.s<sup>-1</sup> of  $O_2$  and 7 m.s<sup>-1</sup> of  $CH_4$ 



Figure 43 Static temperature inside drop tube for 1 m.s<sup>-1</sup> of  $O_2$  and 7 m.s<sup>-1</sup> of  $CH_4$ 



*Figure 44 Graph of static temperature with respect to axis of the tube* 

Static temperature for 1 m.s<sup>-1</sup> of  $O_2$  and 9 m.s<sup>-1</sup> of  $CH_4$ 



Figure 45 Static temperature inside drop tube for 1 m.s<sup>-1</sup> of  $O_2$  and 9 m.s<sup>-1</sup> of  $CH_4$ 



Static temperature evaluated along the axis of the tube

Figure 46 Graph of static temperature with respect to axis of the tube

Static temperature for 1 m.s<sup>-1</sup> of  $O_2$  and 10 m.s<sup>-1</sup> of  $CH_4$ 



Figure 47 Static temperature inside drop tube for 1 m.s<sup>-1</sup> of  $O_2$  and 10 m.s<sup>-1</sup> of  $CH_4$ 



Figure 48 Graph of static temperature with respect to axis of the tube

Static temperature for 1 m.s<sup>-1</sup> of  $O_2$  and 12 m.s<sup>-1</sup> of  $CH_4$ 



Figure 49 Static temperature inside drop tube for 1 m.s<sup>-1</sup> of  $O_2$  and 12 m.s<sup>-1</sup> of  $CH_4$ 



Figure 50 Graph of static temperature with respect to axis of the tube
Static temperature for 1 m.s<sup>-1</sup> of  $O_2$  and 14 m.s<sup>-1</sup> of  $CH_4$ 



Figure 51 Static temperature inside drop tube for 1 m.s<sup>-1</sup> of  $O_2$  and 14 m.s<sup>-1</sup> of  $CH_4$ 



Figure 52 Graph of static temperature with respect to axis of the tube

Static temperature for 1 m.s<sup>-1</sup> of  $O_2$  and 16 m.s<sup>-1</sup> of  $CH_4$ 



Figure 53 Static temperature inside drop tube for 1 m.s<sup>-1</sup> of  $O_2$  and 16 m.s<sup>-1</sup> of  $CH_4$ 



Figure 54 Graph of static temperature with respect to axis of the tube

Static temperature for 1 m.s<sup>-1</sup> of  $O_2$  and 20 m.s<sup>-1</sup> of  $CH_4$ 



Figure 55 Static temperature inside drop tube for 1 m.s<sup>-1</sup> of  $O_2$  and 20 m.s<sup>-1</sup> of  $CH_4$ 



Static temperature evaluated along the axis of the tube

Figure 56 Graph of static temperature with respect to axis of the tube

Graph of Mass fraction of  $CH_4$  along the axis of the drop tube for different velocities of methane



Figure 57 Graph of Mass fraction of  $CH_4$  along the axis of the drop tube for all velocities of methane

Graph of Mass fraction of  $O_2$  along the axis of the drop tube for different velocities of methane



Figure 58 Graph of Mass fraction of  $O_2$  along the axis of the drop tube for all velocities of methane

Graph plotted static temperature for all velocities of methane evaluated along the axis of the tube



Figure 59 Graph of static temperature along the axis of the drop tube for all velocities of methane

We can see from the *Figure 59* static temperature plotted for all the velocities evaluated along the position of the tube. The temperature will go on increasing along axis of the tube and remains constant once the combustion finished.

From the analysis of combustion of the methane for different velocities of methane like 5,7,9,10,12,14,16 and 20 m.s<sup>-1</sup>. The results are similar for the velocities, we got know that combustion of methane will be higher in starting then goes on decreasing, we can tell the temperature will goes on increasing as velocity increase and pressure will be goes on decrease through the drop tube and outlet pressure will zero. The maximum static temperature is 2250K.

# 5.3.3. Results obtain for Eddy dissipation model

Static temperature for 1 m.s<sup>-1</sup> of  $O_2$  and 5 m.s<sup>-1</sup> of  $CH_4$ 



Figure 60 Static temperature inside drop tube for 1 m.s<sup>-1</sup> of  $O_2$  and 5 m.s<sup>-1</sup> of  $CH_4$ 



Figure 61 Graph of static temperature with respect to axis of the tube

Static temperature for 1 m.s<sup>-1</sup> of  $O_2$  and 7 m.s<sup>-1</sup> of  $CH_4$ 



Figure 62 Static temperature inside drop tube for 1 m.s<sup>-1</sup> of  $O_2$  and 7 m.s<sup>-1</sup> of  $CH_4$ 



Figure 63 Graph of static temperature with respect to axis of the tube

Static temperature for 1 m.s<sup>-1</sup> of  $O_2$  and 9 m.s<sup>-1</sup> of  $CH_4$ 



Figure 64 Static temperature inside drop tube for 1 m.s<sup>-1</sup> of  $O_2$  and 9 m.s<sup>-1</sup> of  $CH_4$ 



Figure 65 Graph of static temperature with respect to axis of the tube

Static temperature for 1 m.s<sup>-1</sup> of  $O_2$  and 10 m.s<sup>-1</sup> of  $CH_4$ 



Figure 66 Static temperature inside drop tube for 1 m.s<sup>-1</sup> of  $O_2$  and 10 m.s<sup>-1</sup> of  $CH_4$ 



Figure 67 Graph of static temperature with respect to axis of the tube

Static temperature for 1 m.s<sup>-1</sup> of  $O_2$  and 12 m.s<sup>-1</sup> of  $CH_4$ 



Figure 68 Static temperature inside drop tube for 1 m.s<sup>-1</sup> of  $O_2$  and 12 m.s<sup>-1</sup> of  $CH_4$ 



Figure 69 Graph of static temperature with respect to axis of the tube

Static temperature for 1 m.s<sup>-1</sup> of  $O_2$  and 14 m.s<sup>-1</sup> of  $CH_4$ 



Figure 70 Static temperature inside drop tube for 1 m.s<sup>-1</sup> of  $O_2$  and 14 m.s<sup>-1</sup> of  $CH_4$ 



Figure 71 Graph of static temperature with respect to axis of the tube

Static temperature for 1 m.s<sup>-1</sup> of  $O_2$  and 16 m.s<sup>-1</sup> of  $CH_4$ 



Figure 72 Static temperature inside drop tube for 1 m.s<sup>-1</sup> of  $O_2$  and 16 m.s<sup>-1</sup> of  $CH_4$ 



Figure 73 Graph of static temperature with respect to axis of the tube

Static temperature for 1 m.s<sup>-1</sup> of  $O_2$  and 20 m.s<sup>-1</sup> of  $CH_4$ 



Figure 74 Static temperature inside drop tube for 1 m.s<sup>-1</sup> of  $O_2$  and 20 m.s<sup>-1</sup> of  $CH_4$ 



Static temperature evaluated along the axis of the tube

Figure 75 Graph of static temperature with respect to axis of the tube

Graph of Mass fraction of  $CH_4$  along the axis of the drop tube for different velocities of methane



Figure 76 Graph of Mass fraction of  $CH_4$  along the axis of the drop tube for all velocities of methane

Graph of Mass fraction of  $O_2$  along the axis of the drop tube for different velocities of methane



Figure 77 Graph of Mass fraction graph of  $O_2$  along the axis of the drop tube for all velocities of methane

Graph plotted static temperature for all velocities of methane evaluated along the axis of the tube



Figure 78 Graph of static temperature along the axis of tube for all velocities of methane We can see from the Figure 78 static temperature plotted for all the velocities evaluated along the position of the tube. The temperature will go on increasing along axis of the tube and remains constant once the combustion finished.

From the analysis of combustion of the methane for different velocities of methane like 5,7,9,10,12,14,16 and 20 m.s<sup>-1</sup>. The results are similar for the velocities, we got know that combustion of methane will be higher in starting then goes on decreasing, we can tell the temperature will goes on increasing as velocity increase and pressure will be goes on decrease through the drop tube and outlet pressure will zero. The maximum static temperature is 2250K.

5.3.4. Results obtain for Eddy dissipation concept Static temperature for 1 m.s<sup>-1</sup> of  $O_2$  and 5 m.s<sup>-1</sup> of  $CH_4$ 



Figure 79 Static temperature inside drop tube for 1 m.s<sup>-1</sup> of  $O_2$  and 5 m.s<sup>-1</sup> of  $CH_4$ 



Static temperature evaluated along the axis of the tube

Figure 80 Graph of static temperature with respect to axis of the tube

Static temperature for 1 m.s<sup>-1</sup> of  $O_2$  and 7 m.s<sup>-1</sup> of  $CH_4$ 



Figure 81 Static temperature inside drop tube for  $1m.s^{-1}$  of  $O_2$  and  $7m.s^{-1}$  of  $CH_4$ 



Static temperature evaluated along the axis of the tube

*Figure 82 Graph of static temperature with respect to axis of the tube* 

Static temperature for 1 m.s<sup>-1</sup> of  $O_2$  and 9 m.s<sup>-1</sup> of  $CH_4$ 



Figure 83 Static temperature inside drop tube for 1 m.s<sup>-1</sup> of  $O_2$  and 9 m.s<sup>-1</sup> of  $CH_4$ 



Static temperature evaluated along the axis of the tube

Figure 84 Graph of static temperature with respect to axis of the tube

Static temperature for 1 m.s<sup>-1</sup> of  $O_2$  and 10 m.s<sup>-1</sup> of  $CH_4$ 



Figure 85 Static temperature inside drop tube for 1 m.s<sup>-1</sup> of  $O_2$  and 10 m.s<sup>-1</sup> of  $CH_4$ 

Static temperature evaluated along the axis of the tube



Figure 86 Graph of static temperature with respect to axis of the tube

Static temperature for 1 m.s<sup>-1</sup> of  $O_2$  and 12 m.s<sup>-1</sup> of  $CH_4$ 



Figure 87 Static temperature inside drop tube for 1 m.s<sup>-1</sup> of  $O_2$  and 12 m.s<sup>-1</sup> of  $CH_4$ 



Figure 88 Graph of static temperature with respect to axis of the tube

Static temperature for 1 m.s<sup>-1</sup> of  $O_2$  and 14 m.s<sup>-1</sup> of  $CH_4$ 



Figure 89 Static temperature inside drop tube for 1 m.s<sup>-1</sup> of  $O_2$  and 14 m.s<sup>-1</sup> of  $CH_4$ 



Figure 90 Graph of static temperature with respect to axis of the tube

Static temperature for 1 m.s<sup>-1</sup> of  $O_2$  and 16 m.s<sup>-1</sup> of  $CH_4$ 



Figure 91 Static temperature inside drop tube for 1 m.s<sup>-1</sup> of  $O_2$  and 16 m.s<sup>-1</sup> of  $CH_4$ 



Static temperature evaluated along the axis of the tube

Figure 92 Graph of static temperature with respect to axis of the tube

Static temperature for 1 m.s<sup>-1</sup> of  $O_2$  and 20 m.s<sup>-1</sup> of  $CH_4$ 



Figure 93 Static temperature inside drop tube for 1 m.s<sup>-1</sup> of  $O_2$  and 20 m.s<sup>-1</sup> of  $CH_4$ 



Figure 94 Graph of static temperature with respect to axis of the tube

Graph of Mass fraction of  $CH_4$  along the axis of the drop tube for different velocities of methane



Figure 95 Graph of Mass fraction of  $CH_4$  along the axis of the drop tube for all velocities of methane

Graph of Mass fraction of  $O_2$  along the axis of the drop tube for different velocities of methane



Figure 96 Graph of Mass fraction of  $O_2$  along the axis of the drop tube for all velocities of methane

Graph plotted static temperature for all velocities of  $CH_4$  evaluated along the axis of the tube



Figure 97 Graph of static temperature along the axis of the tube for all velocities of methane

We can see from the *Figure 97* static temperature plotted for all the velocities evaluated along the position of the tube. The temperature will go on increasing along axis of the tube and remains constant once the combustion finished.

From the analysis of combustion of the methane for different velocities of methane like 5,7,9,10,12,14,16 and 20 m.s<sup>-1</sup>. The results are similar for the velocities, we got know that combustion of methane will be higher in starting then goes on decreasing, we can tell the temperature will goes on increasing as velocity increase and pressure will be goes on decrease through the drop tube and outlet pressure will zero. The maximum static temperature is 300K

# 6. Concussion

The main work of the problem is to transport the air and gaseous species transport to the drop tube without heat transfer and finally the combustion of methane for the four different turbulent model. The problem is focused on solving the equations for species transport with chemical reactions.

For CFD calculations i used software ANSYS. The geometry of the drop tube is created in Design modeller. Model of geometry is 2D model (discussed in chapter 5.1 and 5.3) and mesh is generated in program ANSYS Meshing. For air passes through drop tube and species ( $N_2$ ,  $H_2O$ ,  $CO_2$  and  $O_2$ ) passes through the drop tube having 40000 number of elements and for the combustion of methane with oxygen having 54400 number of elements. The generated mesh in ANSYS Meshing, will be read in ANSYS fluent to perform CFD calculations.

First part of my diploma thesis is CFD modelling of air flow without heat transfer and second part is CFD modelling of gaseous species ( $N_2$ ,  $H_2O$ ,  $CO_2$  and  $O_2$ ) flow without heat transfer. The result obtains from both air passes through the drop tube and gaseous species( $N_2$ ,  $H_2O$ ,  $CO_2$  and  $O_2$ ) passes through the drop tube are similar. The maximum of velocity for air passes and gaseous species ( $N_2$ ,  $H_2O$ ,  $CO_2$  and  $O_2$ ) transport is 1.35 and 1.39m.s<sup>-1</sup> and also maximum inlet pressure for both models is 3.04 and 3.14 Pa.

In this problem the results obtain for the combustion of methane for four different model for different velocities of methane passes through the drop tube are similar. The result mainly depends on the selection of models, boundary conditions and species transport with chemical reactions and the selection of pre-exponential factor and activation energy. It is got through know that the results for the same problem will be different for the activation energy and pre-exponential factor are different.

From the comparison of the all results from all the obtain from four models such as Finite rate/No TCI, finite rate /eddy dissipation, Eddy dissipation model and eddy dissipation concept it is evident that all of them are very similar results in static temperature which is having maximum value of 2300K.

Results obtain from the postprocessing of maximum static temperature for Finite rate /No TCI model is in the range of 2200-2300K for velocities from 5 to 20m.s<sup>-1</sup>.(Discussed in Chapter 5.3.1)

Results obtain from the postprocessing of maximum static temperature for Finite rate/Eddy dissipation model is in the range of 2100-2200K for velocities from 5 to 20m.s<sup>-1</sup>.(Discussed in Chapter 5.3.2)

Results obtain from the postprocessing of maximum static temperature for Eddy dissipation model is in the range of 2100-2250K for velocities from 5 to 20m.s<sup>-1</sup>.(Discussed in Chapter 5.3.3)

Results obtain from the postprocessing of maximum static temperature for Eddy dissipation concept model is in the range of 2200-2300K for velocities from 5 to 20m.s<sup>-1</sup>.(Discussed in Chapter 5.3.3)

We can see from postprocessing of mass fraction of methane passes through the drop tube with different velocities for different mode are similar. (Shown in *Figure 38,57,76 and 95*)

We can also see from postprocessing of mass fraction of oxygen passes through the drop tube with different velocities for different model are similar. (Shown in *Figure 39,58,77 and 96*)

We can also see higher value of mass fraction of oxygen in Eddy dissipation model and eddy dissipation concept model for all variants of methane velocities. (Shown in *figure 77 and 96*)

In conclusion, the results seem very satisfying because of its overall results of all four models for similar and also, I got to know that we can use all four different models for this type of problems or similar type of problems.

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