
Final Project Documentation

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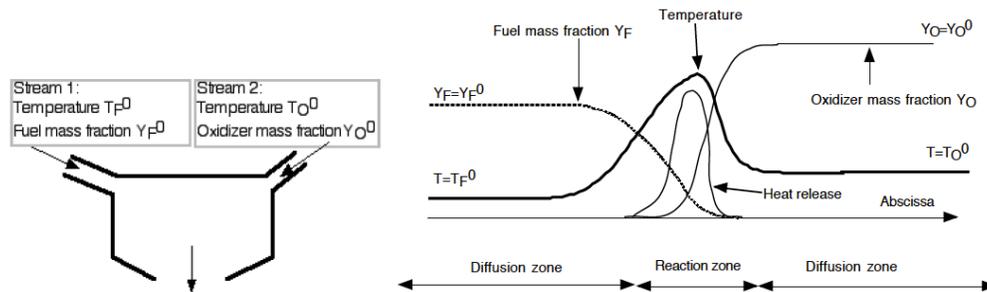
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1.1 Introduction

This project aims to develop a theoretical tool for diffusion flame. To clarify the combustion physics of diffusion flame, diffusion flame is a class of combustion study with a flame in which the oxidizer combines with the fuel in reactor. In other words, the fuel and oxidizer streams independently enter into the reactor and meet together forming an instantaneous mixture created in space. This type of burning process is thus mainly dominated by the diffusion process. Diffusion flames tend to burn slower and are known to produce more soot because of possible insufficient oxidizer concentration for the complete reaction to take place.

The figure shown below illustrates a simplified configuration of diffusion flame formation with separated fuel and oxidizer streams. The figure on the right shows the qualitative thermodynamic properties of mixture along the axis normal to the diffusion flame surface. This clarifies the diffusion flame structure and tells that the high-temperature flame zone is located at the position where the fuel and oxidizer streams meet together at a certain condition, which is a stoichiometric mixture that will be later discussed.



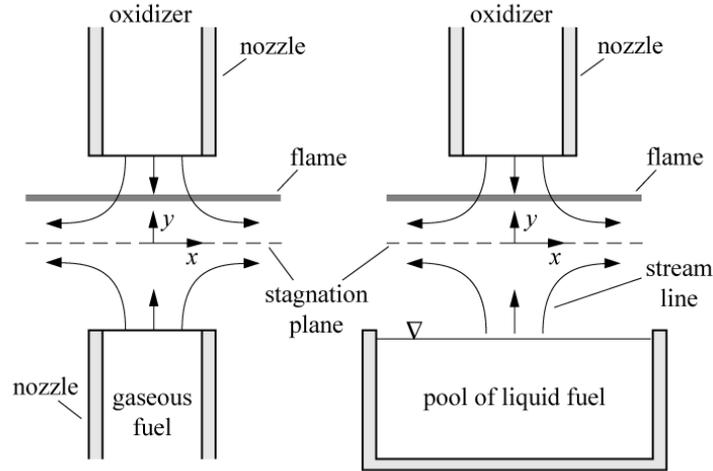
To simplify the theoretical analysis in the diffusion flame, many studies idealized situations of this type of flame by introducing the passive scalar concept that is mathematically manipulated variables from the physical properties of mixture. To introduce the passive scalar, several idealized assumptions need to be introduced and stated as listed below:

- Thermodynamic pressure is constant and Mach numbers are small.
- All the diffusion coefficients D_k of chemical species are equal to D . Fick's law, without velocity correction, is used for diffusion velocities.
- The heat capacities C_p of chemical species are all identical and independent of temperature, calorically perfect gas.

Introducing a passive scalar that well represents the flame properties allows us to solve a linear set of equations in a simplified form of a single transport equation. Then the resolved passive scalar contains all the information of the flame

properties and can be converted to desired quantities of interest.

In this project, a planar counterflow diffusion flame is employed to discuss. Counterflow diffusion flames are very often used experimentally because it is well representative of one-dimension diffusion flame structures. Following figure illustrates the diffusion flame configuration that fuel and oxidizer streams issues on opposite side facing to each other.



1.2 Formulations

Passive scalar transport analysis should start with the case where reaction involves only fuel, oxidizer, and products:



The mass fraction Y_k of each species follows a species conservation equation that can be expressed by:

$$\frac{\partial \rho Y_k}{\partial t} + \frac{\partial}{\partial x_i} (\rho u_i Y_k) = \frac{\partial}{\partial x_i} \left(\rho D \frac{\partial Y_k}{\partial x_i} \right) + \dot{\omega}_k$$

Species production rates $\dot{\omega}_k$ are all related to each species because their production and consumption are correlated in a single step reaction. Note that this approach works out for the single step reaction assumption. Let Q is the single-step reaction rate such that following relation can be introduced:

$$\dot{\omega}_k = W_k \nu_k Q$$

It enables to relate the oxidizer reaction rate to the fuel reaction rate given by:

$$\dot{\omega}_O = s \dot{\omega}_F \quad \text{with} \quad s = \frac{\nu_O W_O}{\nu_F W_F}$$

where s is the mass stoichiometric ratio. And the reaction rate for temperature is also obviously linked to the fuel reaction rate:

$$\dot{\omega}_T = -Q \dot{\omega}_F$$

Using the relation stated above, three conservation equation for all three species in the single step reaction can be formulated:

$$\begin{aligned}\frac{\partial \rho Y_F}{\partial t} + \frac{\partial}{\partial x_i} (\rho u_i Y_F) &= \frac{\partial}{\partial x_i} \left(\rho D \frac{\partial Y_F}{\partial x_i} \right) + \dot{\omega}_F \\ \frac{\partial \rho Y_O}{\partial t} + \frac{\partial}{\partial x_i} (\rho u_i Y_O) &= \frac{\partial}{\partial x_i} \left(\rho D \frac{\partial Y_O}{\partial x_i} \right) + s \dot{\omega}_F \\ \frac{\partial \rho T}{\partial t} + \frac{\partial}{\partial x_i} (\rho u_i T) &= \frac{\partial}{\partial x_i} \left(\frac{\lambda}{C_p} \frac{\partial T}{\partial x_i} \right) - \frac{Q}{C_p} \dot{\omega}_F\end{aligned}$$

As of now, we are still having three conservation equations in addition to continuity, momentum equations to solve the diffusion flame physics. Our goal is to reduce the number of balance equation by employing a new variable. To obtain this goal, we can simplify the given equation by combining above three equations two by two, assuming unity Lewis numbers ($Le = \lambda / \rho C_p D = 1$). This can be achieved by linking the dependent variables, Y_F , Y_O , and T :

$$Z_1 = s Y_F - Y_O ; \quad Z_2 = \frac{C_p T}{Q} + Y_F ; \quad Z_3 = s \frac{C_p T}{Q} + Y_O$$

These three quantities follow the same balance equation dropping the source terms:

$$\frac{\partial \rho Z}{\partial t} + \frac{\partial}{\partial x_i} (\rho u_i Z) = \frac{\partial}{\partial x_i} \left(\rho D \frac{\partial Z}{\partial x_i} \right)$$

Here Z is now introduced as a passive (or called conserved) scalar and changes only due to diffusion and convection. Without source term, this quantity is supposed to vary monotonically with properly setup of boundary condition. Now the three variables Z_1 , Z_2 and Z_3 follow the same balance equation stated above but have different boundary condition. It means these quantities still have to be resolved in their own transport equation. To finally reduce the set of equations, the quantities should be normalized such a way that they end up with same boundary condition as well as same balance equation. The normalized z_j variables can be achieved by defining:

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$$z_j = \frac{Z_j - Z_j^O}{Z_j^F - Z_j^O} \quad \text{for } j = 1, 2, 3$$

Now all reduced variables z_j follow the same transport equation expressed by:

$$\frac{\partial \rho z_j}{\partial t} + \frac{\partial}{\partial x_i} (\rho u_i z_j) = \frac{\partial}{\partial x_i} \left(\rho D \frac{\partial z_j}{\partial x_i} \right)$$

and have the same boundary conditions: $z_j = 1$ in the fuel stream and $z_j = 0$ in the oxidizer stream. And this z is now called the mixture fraction and measures the local fuel/oxidizer ratio. Again, this mixture fraction can also be converted to desired thermodynamic properties by formulating the following relations:

$$z = \frac{s Y_F - Y_O + Y_O^0}{s Y_F^0 + Y_O^0} = \frac{\frac{C_p}{Q} (T - T_O^0) + Y_F}{\frac{C_p}{Q} (T_F^0 - T_O^0) + Y_F^0} = \frac{\frac{s C_p}{Q} (T - T_O^0) + Y_O - Y_O^0}{\frac{s C_p}{Q} (T_F^0 - T_O^0) - Y_O^0}$$

Now we came up with the finalized form of reduced balance equation without source term such that is is easily to solve it numerically and analytically sometime. However, it is not sufficient to resolve the reacting field. The given form of equation only provides the mixing properties with no combustion. In order to simulate the reacting field, we need an additional assumption: infinitely fast chemistry.

In this assumption, the chemical kinetics goes much faster than all flow process such as mixing. Since our approach is based on the single step reaction, there should be no chance that fuel and oxidizer co-exist. It means that there will be a pure 'fuel' side with $Y_F = 0$ and a pure 'oxidizer' side with $Y_O = 0$. Based on this assumption, the solution can be classified into two separate zone:

- Fuel side ($z > z_{st}$):

$$Y_F(z) = zY_F^0 + (z - 1)\frac{Y_O^0}{s} = Y_F^0 \frac{z - z_{st}}{1 - z_{st}}$$
$$Y_O(z) = 0$$
$$T(z) = zT_F^0 + (1 - z)T_O^0 + \frac{QY_F^0}{C_p} z_{st} \frac{1 - z}{1 - z_{st}}$$

- Oxidizer side ($z < z_{st}$):

$$Y_F(z) = 0$$
$$Y_O(z) = Y_O^0 \left(1 - \frac{z}{z_{st}}\right)$$
$$T(z) = zT_F^0 + (1 - z)T_O^0 + \frac{QY_F^0}{C_p} z$$

where the flame position in the z -space, z_{st} is determined by expressing that the flame is located where both Y_F and Y_O are zero. At this location, z is equal to its stoichiometric value given by:

$$z_{st} = \frac{1}{1 + \frac{sY_F^0}{Y_O^0}}$$

Numerical solution method

In this project, arbitrary compressibility method (ACM) is employed to solve the set of balance equations. The ACM is supposed to solve the continuity and momentum equation in a way of compressible solution method by introducing pseudo time integration in continuity equation. Unlike the way of typical density based solution, this method is to solve the pressure that is manipulated with arbitrary compressibility in the continuity equation instead of density itself. So the algorithm is not proper for unsteady solution because of its pseudo time integration. However, it is very efficient to achieve steady solution with a very less computational effort because it does not come up with higher value of characteristic velocity in the convective terms. Therefore the time step for this method does not have to reach up to the level of time scale of wave propagation.

In this particular problem set, we need to add one additional balance equation with dependent variable of mixture fraction, z . This can be easily achieved by simply adding the variable into the state variable vector. Like the same way of original ACM approach, the flux vector only needs to contain additional element corresponding to the convection and diffusion terms of passive scalar transport equation.

For this reason, the solution method is pretty much similar with the previous homework problem. The brief introduction of ACM approach is summarized below and only additional description of modified state vector and flux vectors are listed after that.

- Continuity (incompressible)

$$\frac{\partial u_i}{\partial x_i} = 0$$

- Momentum equation:

$$\frac{\partial u_i}{\partial t} + \frac{\partial u_i u_j}{\partial x_j} = -\frac{1}{\rho} \frac{\partial p}{\partial x_i} + \nu \frac{\partial}{\partial x_j} \left(\frac{\partial u_i}{\partial x_j} \right)$$

- Non-dimensionalization of the Navier-Stokes equations

In some cases, it is beneficial to non-dimensionalize the given transport equation because it eases the analysis of problem of interest, and also may reduce the number of parameters. The non-dimensionalized form of the Navier-Stokes equation can be achieved by first normalizing the primitive variables as followings:

$$\tilde{u}_i = \frac{u_i}{U_{\text{ref}}}, \quad \tilde{x}_i = \frac{x_i}{L_{\text{ref}}}, \quad \tilde{\rho} = \frac{\rho}{\rho_{\text{ref}}}, \quad \tilde{P} = \frac{P}{\rho_{\text{ref}} U_{\text{ref}}^2}, \quad \tilde{t} = \frac{t}{L/U_{\text{ref}}}$$

For the final form of non-dimensionalized Navier-Stokes equation, tilda, $\tilde{\cdot}$, will be dropped out for brevity and a new non-dimensional physical parameter Re that represents the flow inertia against the fluid viscosity is introduced. Now we got:

$$\frac{\partial u_i}{\partial t} + \frac{\partial u_i u_j}{\partial x_j} = -\frac{1}{\rho} \frac{\partial p}{\partial x_i} + \frac{1}{Re} \frac{\partial}{\partial x_j} \left(\frac{\partial u_i}{\partial x_j} \right)$$

where the Reynolds number is defined as:

$$\text{Re} = \frac{U_{\text{ref}} L_{\text{ref}}}{\nu}$$

- Artificial Compressibility Method (ACM)

In the artificial compressibility method (ACM), the continuity equation is modified adding an unsteady term with artificial compressibility β . To have this new form of continuity equation, an artificial equation of state that relates pressure, P , to artificial density $\tilde{\rho}$ is employed as following form:

$$P = \frac{\tilde{\rho}}{\beta}$$

Finally, the modified continuity equation can then be recast as:

$$\frac{\partial P}{\partial t} + \frac{1}{\beta} \frac{\partial u_i}{\partial x_i} = 0$$

- Addition of passive scalar transport equation

In this project, the mixture fraction z field needs to be added to the equation set. Looking at given transport equation of mixture fraction, it looks pretty much similar to the above equation set in terms of having convection and diffusion terms in common. As opposed to the derived equation in the previous section, we need to drop density quantity out of the equation because of incompressible flow assumption. As a result, the mixture fraction transport equation is rewritten in the form:

$$\frac{\partial z}{\partial t} + \frac{\partial u_j z}{\partial x_j} = \frac{\partial}{\partial x_j} \left(\text{Re} D \frac{\partial z}{\partial x_j} \right)$$

- Vector form of transport equations

Rewriting the previously derived non-dimensionalized continuity and momentum equation in vector form generates a simple format that eases implementation of the numerical method. The above transport equation can be newly formed as shown below:

$$\frac{\partial \vec{U}}{\partial t} + \frac{\partial \vec{E}}{\partial x} + \frac{\partial \vec{F}}{\partial y} = \frac{1}{\text{Re}} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) \vec{U}$$

where the each of vector elements are summarized below:

$$\vec{U} = \begin{bmatrix} P \\ u \\ v \\ z \end{bmatrix}, \quad \vec{E} = \begin{bmatrix} \frac{u}{\beta} \\ uu + P \\ uv \\ uz \end{bmatrix}, \quad \vec{F} = \begin{bmatrix} \frac{v}{\beta} \\ uv \\ vv + P \\ vz \end{bmatrix}$$

Now this is good to go further for discretization because the given task is to solve explicit form of discretization equation. Even though the derived form of transport equation is not linearized, each of vectors above are easily discretized in terms of their elements that are combinations of each primitive variables. Thus, in this project, actual discretization has been done from the driven transport equation above.

- Finding time step algorithm

In order to find time step that may stabilize the numerical solution, we need to know system convecting velocity as we pick the coefficient of spatial derivative terms in Burger's and Euler equations as the convection velocity. The driven system of equation is not a single partial differential equation but a set of three different partial differential equation. To find the convection speed of numerical information in the time and space domains, we need to

first linearize the given system of equations and find the Eigen values. The linearization can be obtained by following process. The driven system of PDE should be reformulated in linearized set of equations:

$$\frac{\partial \vec{U}}{\partial t} + [A] \frac{\partial \vec{U}}{\partial x} + [B] \frac{\partial \vec{U}}{\partial y} = \frac{1}{\text{Re}} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) \vec{U}$$

Now we have found two coefficient matrices of convection terms and the spatial derivatives is now taken with respect to \vec{U} only. Despite the vector form, the PDE form is a identical with Burger's equation. The coefficient matrices are below listed:

$$[A] = \begin{bmatrix} 0 & \frac{1}{\beta} & 0 \\ 1 & 2u & 0 \\ 0 & v & u \end{bmatrix}, \quad [B] = \begin{bmatrix} 0 & 0 & \frac{1}{\beta} \\ 0 & v & u \\ 1 & 0 & 2v \end{bmatrix}$$

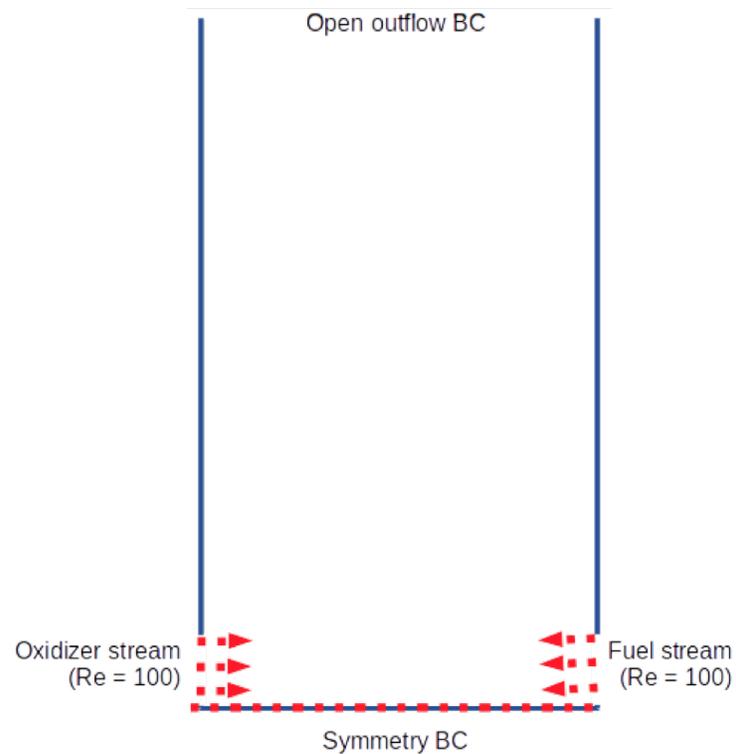
The resolved Eigen values of $[A]$ and $[B]$ matrices are $u, u + a, u - a$ and $v, v + a, v - a$, respectively. Taking $[A]$ for example, the maximum convection velocity that transmit the numerical information can then be $|u| + a$. Therefore, the Courant number for this case can also be determined by:

$$C = \frac{|u_x| + a}{\Delta x} + \frac{|u_y| + a}{\Delta y}$$

3.1 Computational domain

In this project, a simple square domain is employed to construct a counter flow stretched diffusion flame with two separate fuel and oxidizer streams as shown below. The fuel stream comes into the reactor on the right side and oxidizer stream is made on the opposite direction. Two streams are set with the same velocity and different temperature. In this configuration, the flow must be characterized perfectly with symmetrical shape across the centerline axis. An half of computational domain is redundant to run, accordingly it may delay the computational time to achieve steady solution. Thus, another half of domain is considered to run and symmetric boundary condition is employed along the centerline axis of two streams.

Grid resolution is set to 150x300 in x and y direction, respectively.



3.2 Boundary conditions

Two inlet streams size is as 10% as the height of the domain. And the height of the domain is set to be twice of the width such that the flow formation moving out of the domain is ensured to be align with the vertical direction. Note that when two streams mix together and form a stretched flow field (called counter-flow) and leads to another vortices on both side of the walls. Then it may create back-flow if the length of the side wall is not sufficiently long. This type of back-flow does not ensure the outflow boundary condition on the upper boundary and may cause the numerical inaccuracy due to lack of flow information of outer field.

- Inlet BC

To accomodate the pre-specified inlet stream during the simulation, velocity fixed boundary condition is applied to the inlet boundary nodes and the u and v velocity components remain constant. On the other hand, the pressure keeps changing according to the inlet pressure change. This can be achieved by applying extrapolated pressure computation from the inner point values.

- Symmetric BC

To achieve the symmetric boundary condition on the bottom nodes, v velocity and the gradient of u velocity and other state vector elements normal to the boundary are set to zero.

- No-Slip BC

Both side walls are set to no-slip boundary condition such that all components of velocity become zero and pressure and mixture fraction gradients are set to zero.

- Pressure boundary condition for open outlet

The outer domain pressure is set identical to the initial pressure of the inner domain. If there is difference between pressure on the upper nodes and inner pressure right next to them, there will be stiff pressure driven flow happening right at the boundary, resulting in critical numerical instability. Note that the characteristic boundary needs to be implemented to cope with this problem. However in this project, this type of numerical issue is neglected to make the implementation simple.

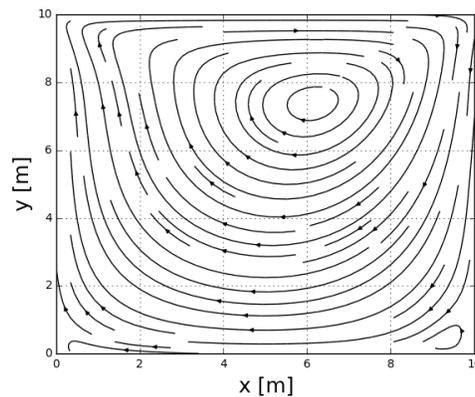
3.3 Initial condition

- Initial pressure = 1 atm
- Outlet pressure = 1 atm (fixed during the simulation)
- Initial temperature = 900 K
- Initial mixture fraction = 0 except for the inlet fuel stream nodes.

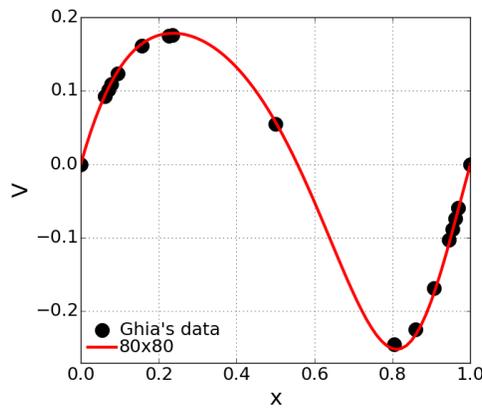
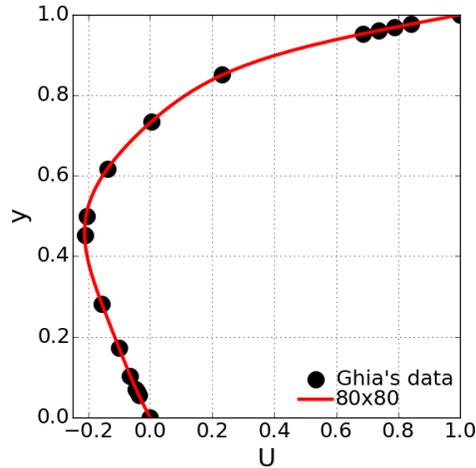
4.1 Validation

For this project, the Python script is newly created independent of the previous homework project. Thus the script needs to be assessed with a well-defined problem. Therefore, the lid-driven cavity problem for this validation step is chosen and performed with this new Python script. The test case is selected with $Re = 100$ and the calculated flow field is compared to the reference data produced by Ghia et al. Since all the simulation setup and initial and boundary conditions are identical with the previous ones, the details of simulation setups are skipped for brevity.

- Streamline of lid-driven cavity simulation with 60x60 grid spacing



- Measured u and v velocity along the centerline axes



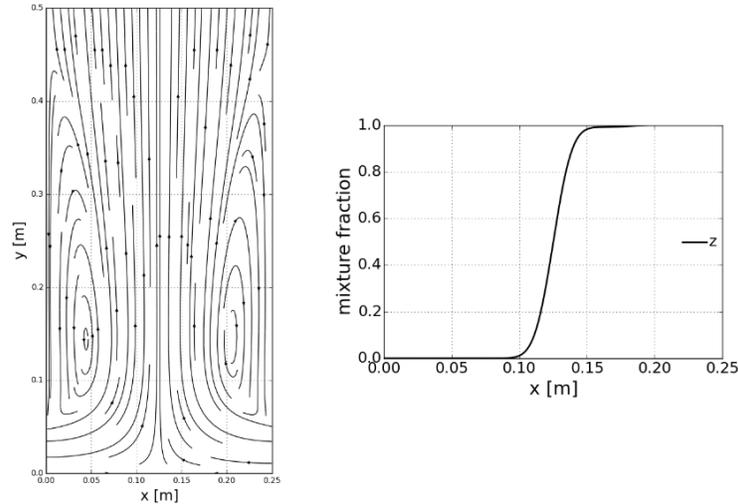
The RMS error obtained from the steady solution as compared to the reference data is 0.29% with convergence criteria set to 0.01%.

4.2 Discussion on non-reacting flow field / mixture fraction

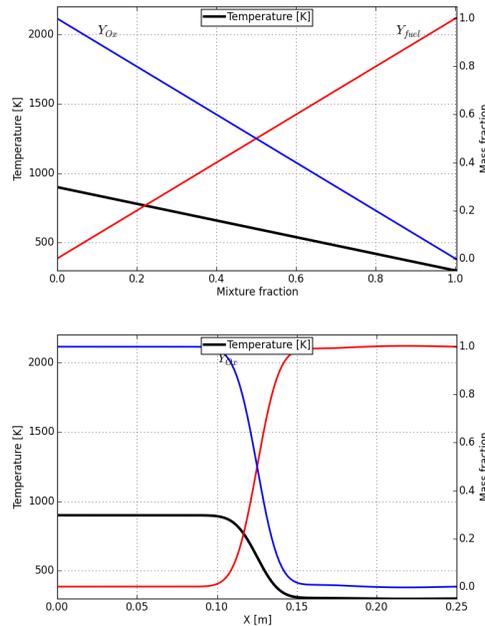
Following figure is showing the flow feature of the counter flow made by two fuel and oxidizer streams with $Re=100$. The shape of streamlines makes perfect symmetry and stagnation point at the center axis. Two vortices are formed at both side walls.

The figure on the right side describes the mixture fraction distribution along the centerline axis of the fuel and oxidizer streams. As well known, the mixture fraction goes from 0 of pure oxidizer to 1 of pure fuel jet. The significant mixture is noticeably formed at the center position.

- Steady flow streamline and mixture fraction distribution along the centerline axis



- Mixture temperature and mass fraction of fuel and oxidizer in the mixture fraction space (up) and physical space (bottom)



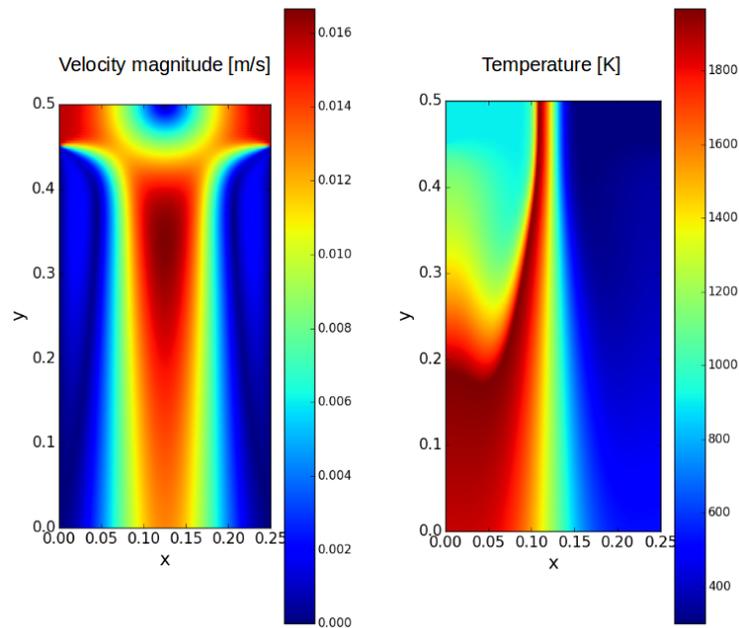
Both two figure above illustrates the mixture temperature and mass fractions of two non-reactive streams along the z space and x space. In mixture fraction space, all the mixture temperature and mass fraction draw linear lines, meaning linear composition of mixture is made. As already assumed in the previous section, the thermal properties is constant and so the temperature is also an outcome of linear mixture of two reactants.

If the mixture field lies on the spatial axis, the noticeable curve of the mixture fields is made in the region where the mixture fraction z changes as illustrated previously. Since the density and diffusivity of two streams are assumed identical to each other, exactly half of each mixture fraction is located at the stagnation point.

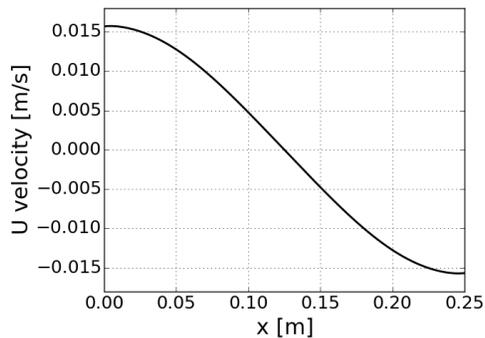
4.3 Reacting case (Re=100)

In this section, a simulation with consideration of infinitely fast chemistry is introduced. The following two snapshots illustrate the flow feature and temperature distribution in space. Note that for some reason the image is flipped from the original position of the domain. So the fuel stream seems to be issued from the right inlet and the resulting streamlines go down and exit the domain. As already illustrated in the non-reacting case, the velocity contour is formed symmetrically. The reacting case simulation enables to predict high temperature region near at the center position but slightly shifted to the oxidizer stream. This very well-known feature of typical diffusion flame because the diffusion flame is positioned at stoichiometric condition. Note that the stoichiometric mixture fraction is around 0.05 under this condition.

- **Velocity and temperature contour**

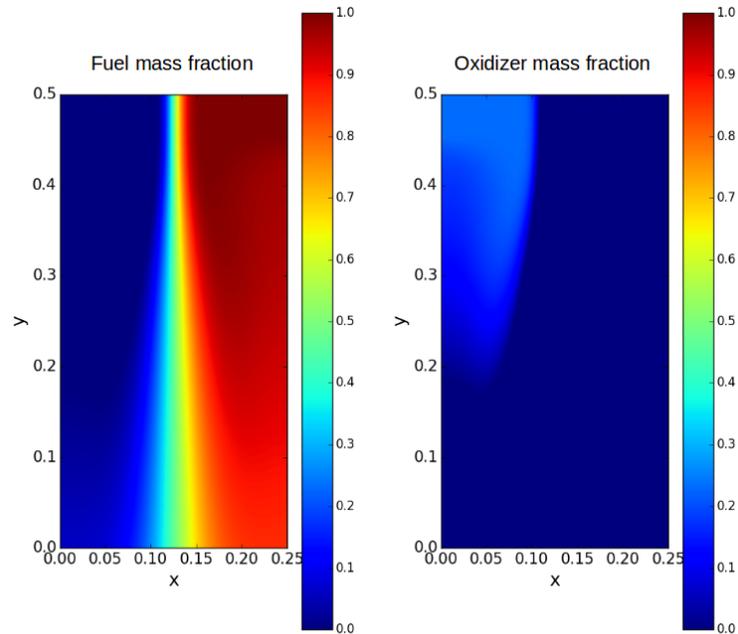


As identically to the non-reacting case, the velocity distribution is formed perfectly symmetry but by the opposite sign from each other's stream. The stagnation point is exactly located at $x=0$ position.



- **Mass fraction contour of fuel and oxidizer**

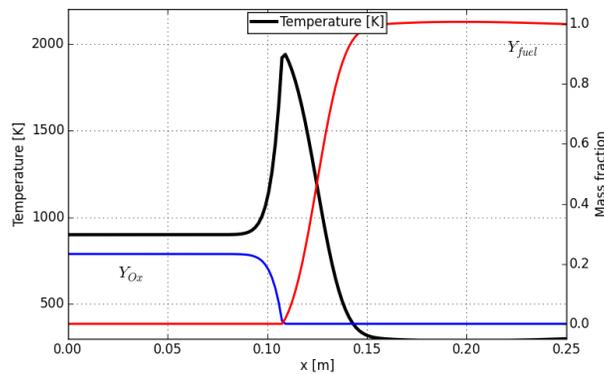
These images illustrate the formation of fuel and oxidizer in their mass fraction. Note that inlet condition of oxidizer is much leaner than the fuel stream: $Y_{O}^0 = 0.233$, which is overall unity equivalence ratio.



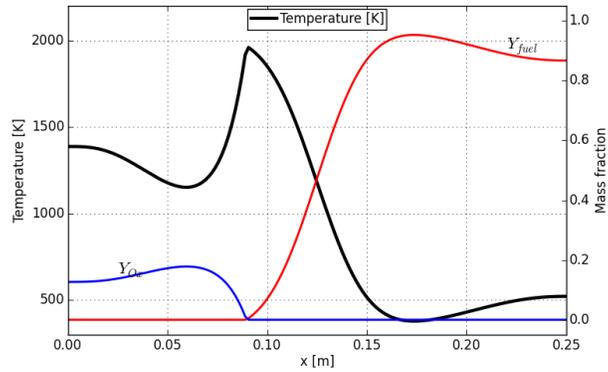
The figures shown below are outcomes of competition between mixture formation and chemical reaction. As compared to the non-reacting case, the fuel and oxidizer does not co-exist because of infinitely fast chemistry assumption. And the maximum temperature peak is positioned at the location where those two massfraction goes to zero. It means that complete combustion results in maximum flame temperature at the stoichiometry condition. The noticeable reaction zone is anchored over about 0.05 mm length in x direction when it is drawn along the centerline axis.

The following second figure was capture downstream at $y = 0.2$ m. Because of the flow development and diffusion process, the mixture fraction field is no more sharp and thus the flame thickness become bigger than at the centerline axis.

- **Flame structure at $y = 0$ m**



- **Flame structure at $y = 0.2$ m**

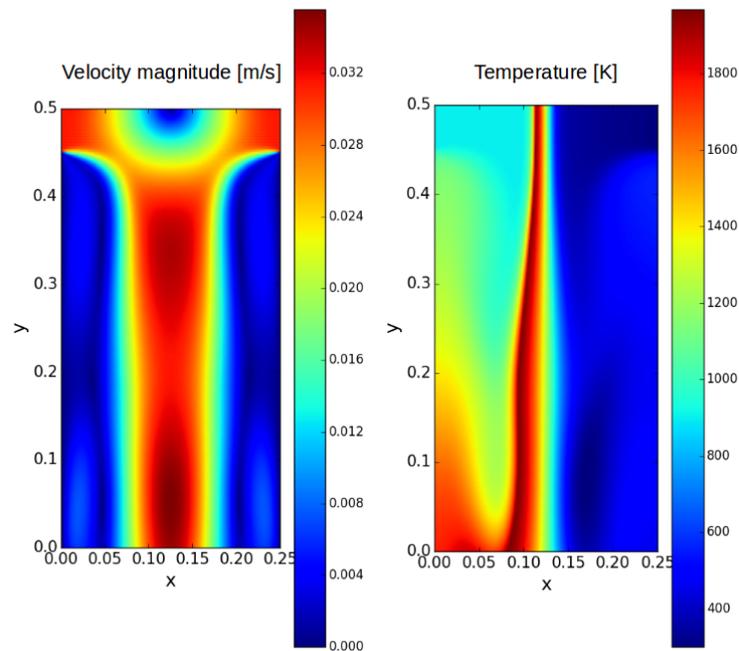


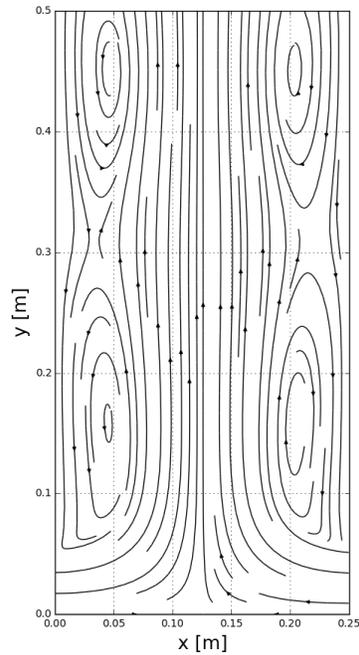
4.4 Reacting case (High Re number)

In this section, more discussions of the effect of high Reynolds number on the flame structure and flow field are made. In addition to the previous $Re=100$, here we introduce two more high Reynolds number conditions to the same problem. Except for the inlet speed, everything else remain unchanged for the initial and boundary conditions.

The most significant features from the higher Reynolds number conditions can be viewed from the more unstable and unsteady flow features. Multiple vortices can be found from the velocity magnitude and flow stream lines figures. As compared to the previous case, the flame gets thinner as Reynolds number increases. In addition, because of the flow unsteadiness the convergence rate never goes below the desired value of 0.01%. The repeatedly created vortices tend to make residual more fluctuated and hamper steadiness.

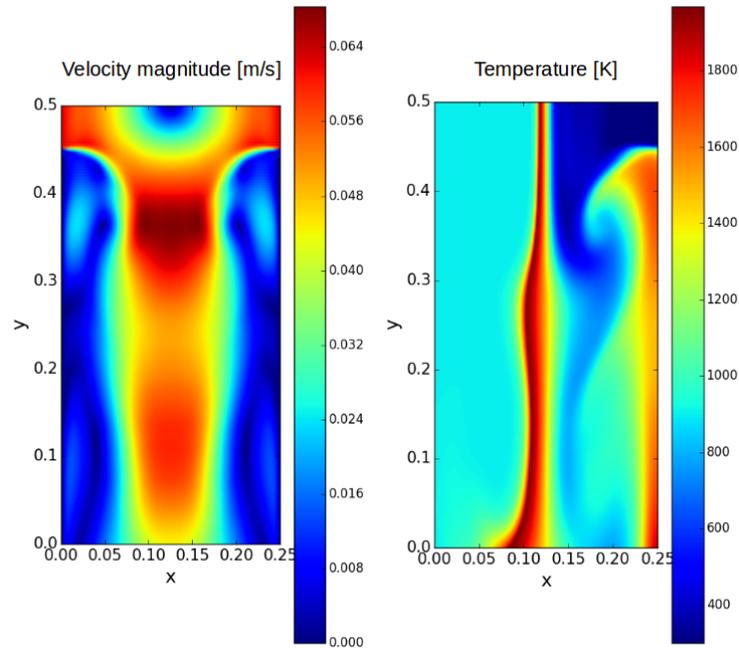
- Velocity magnitude and temperature contours, and flow streamlines ($Re=200$)

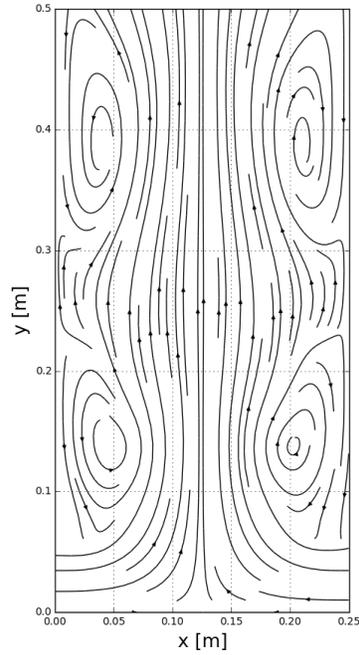




The higher Reynolds number conditions cannot be made with the current setup because the height of the domain is not sufficiently long to ensure the fully developed flow within the length. As found in the $Re=400$, the vortices seem to be more unstable and highly diluted. The flame thickness gets much thinner.

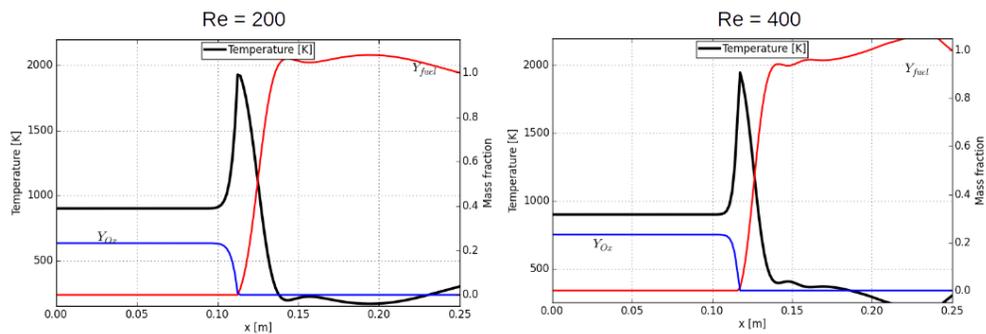
- **Velocity magnitude and temperature contours, and flow streamlines ($Re=400$)**





The flame structure qualitatively looks similar to the previous low Reynolds number case. Mostly interestingly, the flame reaction zone is formed within a shorter distance because of the higher momentum of two streams. Unfortunately, these two higher Reynolds number conditions make the maximum mixture fraction go over unity which is not acceptable theoretically. But in the numerical simulation, that can happen with some possible numerical instability. Because of the inherent oscillation feature of second order finite difference, the numerical instability seems to happen in the high velocity region which also possibly make stiff gradient in the flux computation.

- **Flame structure**



Conclusions

In this computer project, a simplified passive scalar transport equation is introduced and added to the numerical simulation solution method. Typical diffusion flame simulation requires to set more than 3 balance equations in addition to the continuity and momentum equations. By employing the passive scalar concept, we can reduce the number of equations very effectively and take an advantage of less computational effort. Addition of the new transport equation is very simple because it only needs to be added to the state vector and flux vectors. Brief observations from this computer project can be summarized as follows:

- Introduction of passive scalar concept demands less computational time and resources.
- The simplified assumption of the thermodynamic and chemical kinetics enables us to reduce the number of equation set.
- In this project, a counter flow diffusion flame is simulated and gives a good practice for the diffusion flame exploration.
- The mixture fraction goes from 0 to 1 (from pure oxidizer to pure fuel) and the stoichiometric condition is made at lean mixture fraction position.
- Increasing Reynolds of inlet stream makes the flame thickness thinner and flow features unstable.