Study of Gas Flame Acceleration & Deflagration to Detonation Transition

Aishwarya Kannan

[1] *Aishwarya Kannan, Mechanical Engineer, TuTr Hyperloop, National Centre for Combustion Research and Development, Indian Institute of Technology, Madras, Tamil Nadu*

Corresponding Author: Sridevi S, Student, Anna University – Madras Institute of Technology, Chennai, Tamil Nadu.

ABSTRACT: The acceleration of a flame and its detonation has applications in pulse detonation engines and a significant component to consider whilst regarding industrial safety. The present study is to understand the mechanism of a flame's acceleration, propagation and Deflagration-to-Detonation Transition (DDT) process. The Deflagration-to-Detonation Transition (DDT) is the process by which a subsonic wave progresses into a supersonic one. In this study, a 2-Dimensional axisymmetric tube is considered and the stoichiometric mixture of different hydrocarbon gaseous fuels such as Ethylene-Air mixture, Hydrogen-Air mixture, Methane-Air mixture are used with a pressure-based solver with absolute velocity formulation for performing computational analyses using the ANSYS-Fluent Computational Fluent Dynamics software package. The theoretical calculation pertained to the Chapman-Jouguet detonation theory. The computational work was carried out to calculate the run up distance from the region of ignition to the region of detonation and the DDT process was captured for the given time, from which the mechanism involved in the DDT process was inferred.

KEYWORDS: deflagration, detonation, ignition, Chapman-Jouget, CFD.

I. INTRODUCTION

Combustion, the phenomena, is used to heat air for rocket propulsion in Aerospace engineering. It is the process of oxidizing a fuel, typically an organic fuel such as natural gas or hydrocarbon fuel, at high temperature and pressure with an oxidizer such as air or oxygen in the presence of a catalyst. Aerospace engineers use Combustion because it can provide more power than other engines. It also can produce large amounts of heat and power. It is also used in fossil-fuel-run vehicles. It provides the heat needed for combustion reactions to release energy from the chemical bonds of hydrocarbons. Deflagration, is said to be, an explosion wherein, the speed of burning is lower than the speed of sound in the surroundings. The fire, in case of deflagration is characterised, by which, a flame travels rapidly, but at subsonic speed, through a gas. A detonation is more destructive than a deflagration, since higher pressure is generated during detonation.

Combustion

In the combustion, flames can propagate through a flammable fuel-air mixture as either deflagration or a detonation, depending on a complex interaction among factors such as the composition of the gas mixture, the ignition source and energy, the geometry of the surroundings. The chemical energy in reaction between fuel and oxidizer during Combustion is converted into heat and light. Combustion is a process, to transfer chemical energy to thermal energy, which is used for heating or propulsion. It is also a rocket engine that uses the exothermic chemical reaction between fuel and oxidizer to create thrust.

Deflagration

Deflagration is a combustion wave propagating through a gas at a speed lower than the local sound speed. The laminar flame velocity is one of the fundamental properties of the gas mixture. In practice flame acceleration phenomena in pipelines are usually characterized by a turbulent combustion front. It is a surface phenomenon. The products of deflagration go away from opposite to the direction of propagation of deflagration.

Detonation

Detonation is a type of combustion which involves, a supersonic exothermic front accelerating through a medium that eventually drives a shock front propagating directly in front of it. The rate at which detonation occurs, is higher than the sonic velocity in the medium. Detonation propagates through shock waves, supersonically with speeds in the range of 1 km/sec, and thereby, differ from deflagration which propagate with subsonic flame speeds in the range of 1 m/sec. Detonation takes place, in both conventional solid and liquid explosives, as well as in reactive gases. The velocity of propagation during detonation in solid and liquid explosives is much higher than that of propagation in gaseous ones, and hence this allows the wave system to be observed with greater detail. The direction in which the products of detonation travel lies in the same direction as that of the propagation of detonation

Fig 1.1 Rankine-Hugoniot curve

The solution of any steady state deflagration and detonation waves lies on the Hugoniot curve, which can be divided into several branches and regimes, corresponding to the different types of combustion waves (detonation or deflagration). In the figure 1.1 shows the region 1 is strong detonation, the gas velocity relative to the wave front is slowed down substantially from supersonic speed to subsonic. The region 2 represents a weak detonation as the gas velocity in relation to the wave front is slowed down substantially from supersonic speed to subsonic, though the burnt mixture still propagates with a velocity greater than that of speed. The region 3 is weak deflagration, gas velocity relative to the wave front is accelerated from a subsonic velocity to a higher subsonic velocity. The region 4 represents strong deflagration, as gas velocity relative to the wave front is accelerated from subsonic to supersonic substantially. The point A1 which is usually called the origin of the Hugoniot plot. From the graph: the curve is thus divided into five regions the two tangent points to the curve are called CJ Point (upper and lower). Regions of possible solutions are constructed by drawing tangents to the curve through the point A, and vertical and horizontal lines from A. It is implied, by the Rayleigh line expression in the 5th region, that u1 is imaginary. The 5th region is shown to be a physically impossible region. From the figure symbol p and ρ indicates pressure and density.

II. CHAPMAN JOUGET THEORY

The Chapman-Jouguet condition holds approximately in detonation waves in high explosives. It states that the detonation propagates at a velocity at which the reacting gases just reach sonic velocity (in the frame of the leading shock wave) as the reaction cases. As per Chapman-Jouguet theory, the detonation wave is comprised of a shock wave and a flame front. As the wavefront passes through the gas, the gas is compressed and the chemical reaction is completed at the rear ofthe wavefront. The detonation process is considered to be more efficient than the deflagration.

VCJ2 = 2(γ2 – 1) Q

Methane-Air Mixture :

$CH_4 + 2(O_2 + 3.76N_2) \rightarrow CO_2 + 2H_2O + 7.52N_2$

Heat of formation of Methane = -74.5 KJ/mol

Heat of formation of Oxygen = 0 KJ/mol

Heat of formation of Carbon dioxide = -393.5 KJ/mol

Heat of formation of Water = -285.8 KJ/mol

Heat formation in the reaction = - [(Heat formation in the Products) – (Heat formation in the reactants)]

= - [(-393.5 – 285.8) – (0 -74.5 + 0)]

= 604.8 KJ/mol

Heat of vaporization of Water = 40 KJ/mol

Heat in the reaction = 604.8 – 40

= 564.8 KJ/mol

Mass of the Reactants :

$CH_4 + 2(O_2 + 3.76N_2)$

[1(12) + 4(1)] + 2[2(16) + 3.76(28)] = [12 + 4] + 2[32 + 105.28]

= 290.56

We get the heat of 564.8 KJ for every 290.56 grams of Reactants.

Heat generated per kg.(Q) $= \frac{564.8}{290.56}$

= 1943.8325 KJ/kg

$V_{CJ}^2 = 2(\gamma^2 - 1)\, Q$

V_{CJ} = 1931.8795 m/s

Mean Molecular Mass :

$m = \frac{290.56}{10.52}$

$= 27.61977$

Specific Gas Constant :

$R = \frac{8.314}{27.61977}$

$= .30101624 * 10^3$

$= 301.01624$

Then $a_0 = \sqrt{\gamma * R * T}$

$= \sqrt{1.4 * 301.01624 * 298}$

= 354.3782 m/s

Then $M_{CJ} = \frac{1931.8795}{354.3782}$

$= 5.4514$

$\frac{P_{CJ}}{P_0} = \frac{1.4}{2.4} * 5.4514^2$

$= 17.3357$

Results from Theoretical Calculations :

Mixture	V_{CJ}	P_{CJ}	Velocity of products
Methane-Air	1931.8795 m/s	17.3357 atm	1064.4072 m/s

Table 3.1 Results from theoretical calculations

V_{CJ} Chapman Jouguet Velocity

P_{CJ} Chapman Jouguet pressure

III. VISUALISATION AND ANALYSIS OF DETONATION USING THE CFD SOFTWARE ANSYS

The most significant method of generating energy is combustion. The cost of energy will be significantly impacted by the increase in combustion efficiency. Due to decreasing costs and sufficient accuracy with minimal mistake, computational work is currently becoming more and more significant in addition to experimental testing. The computational testing employing Computational Fluid Dynamics (CFD) software will significantly reduce the amount of trial and error on experimental work, particularly for novel develop models.

Problem Definition

The schematic diagram of the computational domain and the computational mesh used for this study are shown in Figs. 4.2 and 4.3. A 2D axisymmetric tube introduces the stoichiometric mixture of methane-air at an inlet temperature of 300 K. The ensuing combustion involves several complex reactions. The several steps used to model this problem are described.

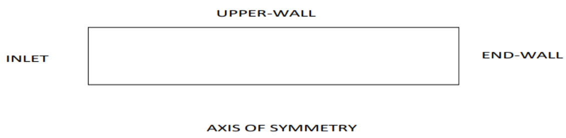


Fig 4.1 2D Axisymmetric Detonation Tube

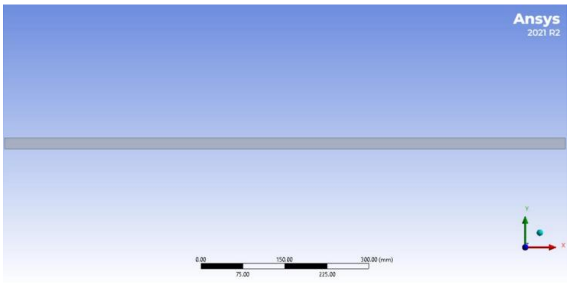


Fig 4.2 Computational domain

Solution Procedures

Although many simulations, where chemical species is involved, may require no special treatment during the solution process, however, situations do arise that, special simulation may be required for one or more of the solution techniques noted in this study, which is used to accelerate the convergence or improve the stability of more complex simulations. Solution procedures comprises of solution setup, models, theory of species transport and finite - rate chemistry, materials selection and boundary conditions applied, solution methods and patch setup.

General Setup

Solver	Pressure based
Velocity Formulation	Absolute
Time	Steady
2D Space	Planar

Models

The model setup done is as shown below.

Table 4.1 Model setup

S.NO	MODEL	SETTINGS
1	Energy	Enabled
2	Viscous	Laminar
3	Species transport	Enabled

ANSYS Fluent can be used to model the mixing and transport of chemical species by solving the conservation equations describing convection, diffusion, and reaction sources for each component species.

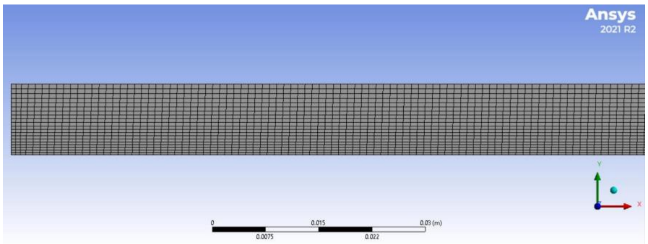


Fig 4.3 Computational mesh

Species Model Setup

Reactions	Volumetric
Chemistry Solver	Stiff Chemistry Solver
Inlet Diffusion	Enabled
Diffusion Energy Source	Enabled
Full Multicomponent Diffusion	Enabled
Thermal Diffusion	Enabled
Mixture Material	Methane-air
Turbulence-Chemistry Interaction	Finite-Rate/ No TCI

Material Selection and Boundary Conditions

The boundary conditions play a major role in this computational analysis. Hence, we did our part of experimenting with varied input conditions to arrive at one which we felt most apt for our analysis in order to obtain accurate results. The ANSYS Fluent defines six type of materials – fluids, solids, mixtures, combusting-particles, droplet-particles and inert-particles. Physical properties of fluids and solids which are associated with named materials. These materials are then assigned boundary conditions for zones.

MATERIAL PROPERTIES- FLUID (AIR)

Density	Ideal-gas
Viscosity	Sutherland Law

The boundary conditions at the inlet plane where specified as follows: Gauge pressure = 5000000 Pa, Initial pressure = 0 Pa, Initial temperature = 300 K with species mole fractions of hydrocarbon air mixture respectively. Methane- air – CH_4 = 0.0551 O_2 = 0.2203 CO_2 = 0.1514 H_2O = 0.1239

For solving the equation in the segregated manner, ANSYS FLUENT uses the phase coupled SIMPLEC (PC- SIMPLEC) algorithm for the pressure velocity coupling. PC- SIMPLEC algorithm is a tool which extends the SIMPLEC algorithm to multiphase flows. In this computational analysis SIMPLEC algorithm stands for semi-implicit method for pressure-linked equations consistent. It follows the same as the SIMPLEC algorithm, with the difference that the momentum equations are manipulated so the SIMPLEC velocity correction equations omit terms that are less significant than those in SIMPLEC. The SIMPLEC skewness correction supports ANSYS FLUENT, to obtain a solution on a highly skewed mesh in approximately the equivalent number of iterations, as required for a more orthogonal mesh.

Initialization & Patch Set-Up

Selecting the region is the initiation of detonation to occur. In the present study the initial spark was given by patching a high temperature of 2000 K into a region of the model that contained a sufficient premixed mixture for ignition to occur.

(i) NEW REGION
Adapt – Cell Register – New Region – Select with mouse – Save – Display

(ii) AXIS OF SYMMETRY
View – Views – Axis of symmetry – Apply

(iii) INITIALIZATION
Hybrid initialization has been used in order to get a better starting solution than the other alternative of standard initialization.

(iv) PATCH
Methane-air mixture has an ignition temperature of 1785.6374 K according to our calculations. Hence, the patched region has been assigned a temperature slightly higher than that, of 2000 K in order to facilitate immediate ignition in the region which has been patched.

Animation

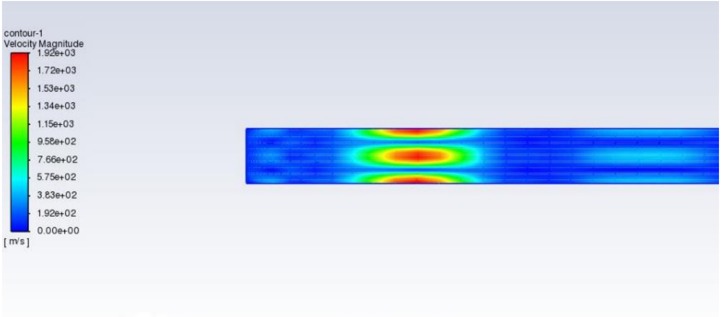
To visualize and analyze the flame propagation and detonation process, it is convenient to use an animation. It can be obtained by following the steps given below.

Calculation Activities – Solution Animation – In memory – Iteration – New object – Contours – Velocity – Select all regions – Save and Display

The calculation step is a process of iteration where the solution is continuously iterated over several steps until the solution converges.

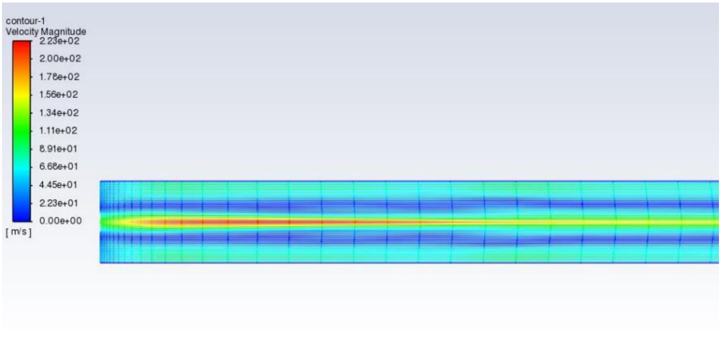
IV. RESULTS AND DISCUSSIONS

The analysis of the two-dimensional cross-section of the combustion pipe using ANSYS FLUENT provided us with the results as given below. It includes the scaled residuals graph obtained as well as the velocity contour in figures below.



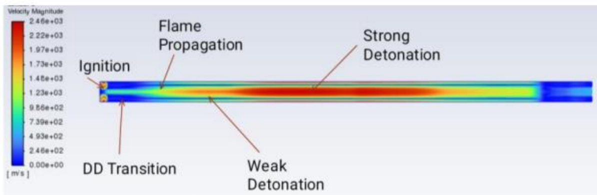
Velocity Contour depicting Flame Propagation

The figure above depicts the flame propagating soon after the ignition has occurred. The several regions correspond to the various velocities with which the flame propagates, according to the scale as mentioned.



Velocity Contour before Detonation

The figure above represents the propagation of flame and combustion process before the velocity shoots up and detonation occurs.

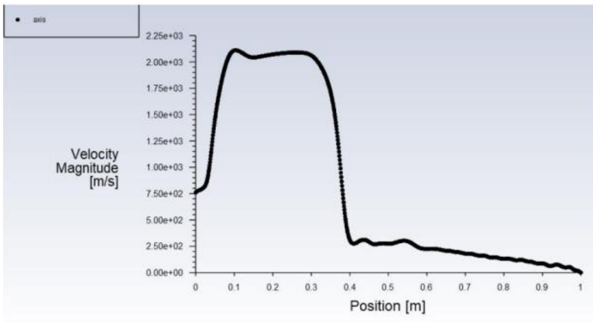


Regions of Detonation

The figure above depicts the different regions of the flame classified based on the velocity and detonation. The velocity plot as mentioned in the figure above helps study the velocity of flame propagation throughout the simulation experiment. From it, we can infer that the velocity shoots up and detonation occurs at about 0.08 m of the pipe length from the inlet.

It can be seen that there is a sudden increase in velocity at the point of ignition and after which a gradual decrease in velocity is observed.

It was noted that the detonation as observed in the simulations occurs at a velocity that is very close the theoretically calculated Chapman-Jouguet velocity. It was also observed that the introduction of obstacle or certain obstructions in the flow triggered the detonation process.



Velocity Plot

The velocity plot as mentioned in the figure above helps study the velocity of flame propagation through.08 m of the pipe length from the inlet.

in the flow triggered the detonation process

V. CONCLUSION

- The experiment confirmed that the theoretical Chapman-Jouguet velocity at which detonation occurs and the velocity obtained through simulation using ANSYS are very close to each other.
- Through the velocity plot, it was found that the run-up length is 0.08 m (from the inlet).

REFERENCES

[1]. Florian Ettner, Klaus G. Vollmer, Thomas Sattelmayer, "Numerical stimulation of the deflagration to detonation transition in inhomogeneous mixtures," published on 19 May 2014

[2]. “L. Petzold and W. Zhu, "Model reduction for chemical kinetics: An optimization approach," AIChE Journal, vol. 45, pp. 869-886, 1999.

[3]. S. H. Lam and D. A. Goussis, "CSP method for simplifying kinetics," International Journal of Chemical Kinetics, vol. 26, pp. 461-486, 1994.

[4]. N. Peters and F. A. Williams, "The asymptotic structure of stoichiometric methane-air flames," Combustion and Flame, vol. 68, pp. 185-207, 1987.