Assessing the Impacts of Viscosity and Radiative Transfer in Internal Detonation Scenarios Involving Hydrogen-Air Mixtures

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Abstract

Predictions from a hydro code are compared against those obtained from a computational fluid dynamics (CFD) framework to numerically assess the effects of: viscous and radiative losses associated with a propagating pressure wave, the point source ignition approximation, and their subsequent impact on the over-pressure characteristics during internal detonation scenarios involving hydrogen-air mixtures. The hydro code employed: TNT equivalencies to represent the heat of hydrogen combustion and solved the inviscid (Euler) equations in conjunction with the JWL equation of state for momentum transport. The CFD simulations resolved the detonation wave employing: the SRK equation of state, Large Eddy Simulations and employed spectrally-averaged mean absorption coefficients for the radiative properties. Detonation wave propagation in air (non-reacting) as well as in premixed hydrogen-air mixtures (reacting) were studied employing a 21-step detailed chemistry mechanism. The adequacy of our modeling procedure was first established by obtaining reasonable agreement between our predictions from the two modeling frameworks with reported measurements from a small- scale explosion study. The same CFD modeling methodology was subsequently extended to larger scales. The heats of reaction resulted in acceleration and strengthening of the wave front in both lean and rich hydrogen-air mixtures investigated in this study, with trends agreeing with predictions from flame speed theory. However, viscous losses resulted in a noticeable weakening of the detonation wave during its propagation. Including the effects of radiative transfer had no impact on the wave propagation due to the relative magnitudes of the radiative source and chemical heat release terms.

Index terms— hydrogen detonation; hydro code; detailed chemistry; radiative heat transfer; CFD.

1 Assessing the Impacts of Viscosity and Radiative Transfer in Internal Detonation Scenarios Involving Hydrogen-Air Mixtures

Lucky Nteke Mulenga ? & Gautham Krishnamoorthy ? Abstract-Predictions from a hydro code are compared against those obtained from a computational fluid dynamics (CFD) framework to numericall yassess the effects of: viscous and radiative losses associated with a propagating pressure wave, the point source ignition approximation, and their subsequent impact on the over-pressure characteristics during internal detonation scenarios involving hydrogen-air mixtures. The hydro code employed: TNT equivalencies to represent the heat of hydrogen combustion and solved the inviscid (Euler) equations in conjunction with the JWL equation of state for momentum transport. The CFD simulations resolved the detonation wave employing: the SRK equation of state, Large Eddy Simulations and employed spectrally-averaged mean absorption coefficients for the radiative properties. Detonation wave propagation in air (non-reacting) as well as in premixed hydrogen-air mixtures(reacting) were studied employing a 21step detailed chemistry mechanism.

The adequacy of our modeling procedure was first established by obtaining reasonable greement between our predictions from the two modeling frameworks wither ported measurements from a small-scale explosion study. The same CFD modeling methodology was subsequently extended to larger scales. The heats of reaction resulted in acceleration and strengthening of the wave front in both lean and rich hydrogen-air mixtures investigated in this study, with trends agreeing with predictions from flame speed theory. However, viscous losses resulted in a noticeable weakening of the detonation wave during its propagation. Including the effects of radiative transfer had no impact on the wave propagation due to the relative magnitudes of the radiative source and chemical heat release terms. Introduction he response of structures to dynamic pressure loading during an accidental detonation scenario is a critical component of industrial hazard assessment. In order to carry out this assessment accurately, fidelities in: the magnitude and duration of the overpressures, as well as the positive and negative impulses resulting from the detonation wave are desired. During the accidental detonation of an explosive mixture in a realistic scenario, the nature of interactions between the blast waves and structures in an irregular geometry is quite complex. This makes it difficult to use or extend analytical expressions for pressure profiles that have been established for simple enclosures to other geometric configurations [1].

Further, compositional non-homogeneities resulting from the convective and diffusive forces within the enclosure and after-burn effects can further strengthen a propagating detonation wave due to chemical heat release. This can reduce the applicability of established analytical expressions and scaling laws even further. Therefore, computational fluid dynamics (CFD) codes that can resolve these complex geometric and multi-physics characteristics adequately are often utilized to simulate such scenarios. Among these are: 1. Hydrocodes (such as ANSYS AUTODYN [2]): That employs TNT equivalencies for detonation initiation and solves inviscid (Euler) equations with a real gas equation of state to quickly resolve the propagation of a detonation wave. Heats of reactions and radiative losses are ignored in this framework.

2. Multiphysics CFD codes (such as ANSYS FLUENT [3]): That have the ability to include the effects of turbulence, gas-phase reactions and radiative losses in the detonation wave albeit at an increased computational cost relative to the hydro codes. While both computational frameworks have been employed in isolation to simulate different detonation scenarios, comparing and validating their predictions against measurements from the same detonation experiment can provide insights into the importance of different models that are ignored in hydro code simulations. Therefore, the primary goal of this manuscript is to assess the effects of after-burn chemistry, viscous and radiative losses during the propagation of a detonation wave to enable users to select appropriate modeling options and CFD frameworks for carrying out their study. The adequacy of our modeling methodology is demonstrated in this study by studying hydrogen-air systems due to the abundance of experimental measurements, well-established chemistry mechanisms and availability of radiative property models for water vapor. However, it will be clear that the same methodology can be extended to study after-burn and radiative transfer resulting from the decomposition products of condensed-phase explosives where these effects may be more pronounced.

2 a) The Importance of Detailed Chemistry and Viscous

Effects Recent studies that have employed large cell sizes in conjunction with the Large Eddy Simulation (LES) methodology to model hydrogen explosions in domain sizes of practical interest have provided encouraging signs that such calculations are computationally feasible within a reasonable time frame [4,5]. These two studies by Zbikowski et al. [4,5] employed the progress variable formulation to simulate the propagation of the reaction front in premixed hydrogen-air mixtures. The chemical kinetics in this methodology was incorporated through the specification of a detonation velocity that goes into the source term of the progress variable equation. However, due to the dependence of the detonation velocity on the mixture equivalence ratios, extending the progress variable framework to simulate detonation in non-homogeneous mixtures is not straightforward. Nevertheless, simulation of deflagration (flame propagation) in nonhomogeneous hydrogen-air mixtures using the progress variable combustion model has recently been demonstrated [6].

In spite of the lower computational cost and stability associated with the progress variable approach, a recent study reported by Feldgun et al. [7] concluded that in order to account for the residual blast pressures in confined explosions accurately, the effects of after burn chemistry needs to be taken into account. Further, the heat capacity ratio (which changes as a result of after burn chemistry) was seen to have a stronger effect on the gas pressure predictions than the internal energy of explosion. Liberman et al. [8] showed that predictions of temperature-gradient induction lengths that are thought to play a vital role in triggering detonations in deflagration-to-detonation (DDT) scenarios are sensitive to the chemistry models employed in the simulations. Minimal induction length predictions when employing detailed chemistry models along with accurate kinetictransport models were found to be 2-3 orders of magnitude greater than those predicted employing single -step global chemistry models. Therefore, these two studies [7,8] highlight the importance of employing detailed chemistry models during simulations of detonation scenarios whenever computationally feasible.

3 b) The Importance of Radiative Transfer

The importance of including the effects of radiative transfer in the context of dust explosions in hydrogen-oxygen mixtures was examined by Liberman et al [9,10]. By considering the gas mixture to be transparent and the

dispersed phase to be radiatively participating, radiative transfer was found to cause heating of the particles ahead of the flame followed by re-emission of this radiation. This radiative preheating of the mixture ahead of the flame either increased the flame velocity or triggered detonation through the Zeldovich gradient mechanism [11]. Therefore, the studies by Liberman et al [9,10] highlight the importance of including the effects of radiative transfer in the detonation wave simulations.

While hydro codes do not include the effects of viscosity, detailed chemistry and radiative transfer, they have yielded reasonable agreement with experimental measurements of detonating hydrogen-air mixtures in small scale geometries where after-burn chemistry was not important [12]. This was accomplished by representing the heat of combustion of the hydrogen-air explosive mixtures in terms of TNT equivalencies and initiating the detonation over a point source. However, in larger geometries, viscous and radiative losses may become more important with increase in the wave propagation time. Further, if the wave propagates in a premixed hydrogen-air mixture, the heat of reaction can result in acceleration and strengthening of the wave and exacerbate the effects of radiative transfer, resulting in phenomena that cannot be taken into account easily in hydro codes. Therefore, in this study we examine hydrogen-air mixtures to: 1. Assess the validity of the approximations inherent in hydro-codes when simulating a spherical detonation wave resulting from the detonation of a gaseous charge. These approximations include: assumptions of a point source, assumptions of a perfectly spherical wave, absence of turbulence, presence of

4 C

confinements and the assumption of an energy efficiency of one where all of the chemical energy released goes towards the propagation of the pressure wave. 2. To assess the impacts of viscous and radiative losses during the propagation of a pressure wave resulting from the detonation of hydrogen-air mixtures at larger scales. 3. Investigate the effects of heat of reaction towards strengthening or weakening a detonation wave as it propagates through a premixed hydrogen-air mixture.

In contrast to the dust explosion study by Liberman et al [9,10], we consider a radiatively participating gas phase (air or water vapor). Since the shock layer was determined to be optically thin (kL « 1), where k is the absorption coefficient (in m -1) and L the path length (in m), a spectrally averaged Planck mean absorption coefficient for the radiative properties of water vapor [13] and air [14] were computed for the scenarios and employed in conjunction with an optically thin radiation modeling approximation. As per this approximation, the temperature and pressure dependent absorption coefficients were computed as: K air = 3.7516 x 10 -6 ? (P) 1.31 ? exp (5.18 x 10 -4 T -7.13 x 10 -9 T 2)

(1)K H2O (g) = 5.4 x 10 7 ? (T) -2.35 ? P H2O**(2)**

These were then employed to compute the radiative source term (divergence of the radiative flux q) in the energy equation at each spatial location as:) (4 4 4 ? ? = ? ? T T K q ? (3)

where ? is the Stefan-Boltzmann constant, K the absorption coefficient, T and T ? are the local and surrounding temperatures respectively. Equations 1 through 3 were implemented as a User-Defined Function in ANSYS FLUENT. The optically thin radiation approximation has previously been used in estimating radiation from air in hypersonic shock layers [15] as well as from radiatively participating combustion products in mildly radiating combustion flames [16].The adequacy of our modeling procedures are first establishedby comparing our numerical predictions using both computational frameworks against reported measurements from a small-scale explosion study [17].

The modeling methodology was then extended to other scenarios encompassing changes to the domain size and premixed hydrogen-air mixtures.

5 II.

6 Methods

Our hydro code prediction methodology for the small scale (Case 1) explosion study followed closely the procedure adopted by Zyskowski et al [12] and is summarized in brief. The containment is a parallelepiped wooden box of length, width and height 500, 400 and 300 mm respectively with twelve pressure sensors located at various points on the containment surface (Figure 1a). During the experiments, detonation was initiated by igniting an explosive gaseous hydrogenoxygen mixture at stoichiometric conditions within a hemispherical soap bubble of radius 30 mm. Since ANSYS AUTODYN cannot simulate the energy released during hydrogen-oxygen detonations directly, the energy released during the combustion process was represented through an equivalent amount of TNT detonation and patched over a radius of 30 mm. The initial phases of the blast wave propagation were simulated in 1D (radial direction only) assuming spherical symmetry in the shock wave development. The subsequent phases (after 0.1 ms of elapsed time) of the blast waves were carried out in 3D through a mapping of the 1D solution into a 3D domain. By utilizing the thermodynamic properties in the ANSYS AUTODYN library, air was modeled employing the ideal gas equation of state (Eq.4) whereas the Jones-Wilkins-Lee (JWL) equation of state was employed to model TNT (Eq. 5):?? = (?? ? 1) ? ?? ? ?? (4) ?? = ?? 1 * ?1 ? ð ??”ð ??” ?? 1 ?? ? * ?? ??? 1 ?? + ?? 2 * ?1 ? ð ??”ð ??” ?? 2 ?? ? * ?? ??? 2 ?? + ð ??”ð ??”?? ??**(5)**

In Eqs (4) and (5) p, ? and ? represent the pressure, density and specific heat ratios respectively. ?? is the internal energy, ?? 1 , ?? 2 , ?? 1 , ?? 2 are constants, ð ??"ð ??" is report of the specific heat and??the specific volume.

In the CFD simulations using ANSYS FLUENT, a 3D representation of the parallelepiped geometry of the small-scale geometry (Case 1) was created and a hemispherical bubble of 30 mm was patched with the thermodynamic state associated with the combustion products resulting from combustion of a stoichiometric hydrogen-oxygen mixture in a constant volume reactor. In Case 2, the domain was enlarged 10 times in each direction and a hemispherical bubble of radius 300 mm was patched with TNT. In order to run the detonation scenarios successfully, we had to create a spherical indentation of radius 30mm (for Case 1) and 300mm (for Case 2) as shown in Figure 1b. The domain was meshed with 63,300 quadrilateral elements resulting in nearly the same sizes as those employed in the AUTODYN simulations. In order to initiate the detonation, 3 computational cells normal to the hemispherical surface were patched with a temperature of 3473 K (as shown in Figure 1b) corresponding to the adiabatic flame temperature of stoichiometric hydrogen-oxygen mixtures. Next, based on the volume of the detonation kernel and the patched temperature, the ideal gas equation of state was employed to compute the pressure within the detonation volume.

Table 1 summarizes the initial conditions within the detonation kernel in the two computational frameworks when simulating detonation of a stoichiometric hydrogen-oxygen mixture. The propagation of the detonation wave in air (non-reacting) as well as lean and rich premixed hydrogen-air mixtures were also simulated employing ANSYS FLUENT. It was ensured that the critical radius and critical energy for detonation initiation was greater than the values reported in Liu et al [18]. The simulations were allowed to run for 2ms (for Case 1) or 20ms(for Case 2) and pressure profiles were recorded at the gauges placed throughout the geometry. The various modeling options employed in the two computational frameworks are summarized in Table **??**.The Pressure-Based Coupled solver where the momentum and pressure-based continuity equations are solved together was employed in ANSYS FLUENT for the Pressure-Velocity coupling across all scenarios. It is worth noting that for these spherical detonation scenarios, the mesh resolution (~1 cm for Case 1 and ~10 cm for Case 2) have previously been deemed be adequate when employed in conjunction with the LES model [20,21]. The minimum size of the control volume employed by Molkov et al. [20] in their study was 40 cm whereas Tomizuka et al. [21] deemed cell sizes less than 20 cm to be adequate for simulating hydrogen-air explosion in a large domain.

7 III.

8 Results And Discussion

9 a) Small-Scale Study (Detonation wave propagation in air)

The transient pressure predictions at the different gauges in the small scale (1 X) explosion study (Case 1) are shown in Figure 2. A reasonably good agreement between the two modeling frameworks as well as the experiment is observed, indicating the adequacy of our modeling procedures. As seen in Figure 1a, Gauge 12 is located closest to the onset of detonation and therefore experiences the pressure pulse the fastest. Gauge 1 on the other hand is located the farthest and this is reflected in the pressure pulse arrival time. Since Case 1 corresponds to the detonation of a shock wave arising from high-pressure water vapor (the combustion product of a stoichiometric hydrogenoxygen mixture) through air, there is no after-burn chemistry involved in this scenario. Further, the temperature increase across the shock wave was modest (~30 K) that accounting for the effects of radiative transfer in air by computing absorption coefficients and radiative source terms through Eqs. 1 and 3 had no impact on the results.

10 b) Large-Scale Study 10x (Detonation wave propagation in air)

Next, the propagation time of the pressure wave before it encountered the containment surface was increased ten-fold by making the domain ten times larger. The contours of gauge pressure, velocity and viscosity ratios (turbulent viscosity/molecular viscosity) after 3 ms in the large scale explosion study are shown in Figure 3. As seen in Figure 3c, the turbulent sub-grid viscosity computed using the Smagorinsky LES model [3] is four orders of magnitude greater than the molecular viscosity. It was envisioned that the increase in viscosity in conjunction with the increase in propagation time would slow down the propagation of primary and secondary shocks. To ascertain this, Case 2 was also simulated using both the ANSYS AUTODYN and ANSYS FLUENT frameworks. The transient pressure predictions at the different gauges comparing the LES calculations (ANSYS FLUENT) against the in viscid Euler calculations (ANSYS AUTODYN) are shown in Figure **??**.

The magnitudes of the first peak of the reflected over-pressures at the different gauges are similar to those observed in the small-scale study (cf. Figure 2) albeit the shock wave arrival time has increased by a factor of ten due to the enlarged domain. This confirms the adherences to Hopkinson's similitude since the reduced distance of the pressure sensor (R/E 1/3) is the same in both cases, where R is the distance from the explosion center and E the energy released during the reaction. There are discernable differences between the results from the two modeling frameworks with the pressure wave from the inviscid AUTODYN calculations travelling faster than the

LES calculations using ANSYS FLUENT. Again, the effects of radiative transfer did not have any bearing on the predictions (LES calculations without radiative transfer were identical to those with radiative transfer and not shown in Figure **??** for brevity).

The temperature increase across the shock wave was found to be only 30 K and this is reflected in the radiative source term magnitude of about 1 W/m 3 . Our previous study of radiative transfer across shock waves in air during atmospheric re-entry [15] showed that the radiative source terms need to have magnitudes of 4,000 to 10,000 W/m 3 to have an impact on the density and velocity profiles.

11 c) Pressure wave propagation in lean and rich hydrogen-air mixtures

The propagation of the detonation wave in fuellean and fuel-rich premixed hydrogen air mixtures within the domain was simulated next. The domain compositions corresponding to these two scenarios are shown in Table 1. The chemistry was accounted for employing a 21-step detailed chemistry mechanism for hydrogen-air combustion [19]. The equivalence ratios/compositions for the fuel-lean and fuel-rich conditions were intentionally chosen based on the large Global Journal of Researches in Engineering ( ) Volume XVII Issue III Version I 14 Year 2017 C differences in the laminar burning velocities observed in closed vessel gas explosion experiments by Dahoe [22].The peak flame speeds were observed at the fuelrich composition of 40 mol % H 2 whereas the flame speed at the fuel lean composition of 20 mol% H 2 were lower by a factor of nearly three. Eq. (2) was employed to compute the radiative properties of water vapor. Eq. (2) in fact represents a curve-fit to the Planck mean absorption coefficients computed from line-by-line data reported in Rivière and Soufiani [13]. The goodness of this fit is shown in Figure **??**. The contours of Planck mean absorption coefficient in m -1 and the radiative source term after 0.5 ms in the large scale explosion study at fuel-rich and fuel-lean domain conditions are shown in Figure 6. While the magnitudes of the absorption coefficient are identical in both scenarios, the radiative source term magnitude in the fuel-rich condition is nearly twice that under fuel-lean conditions. Further, the wave propagation is faster under fuel-rich conditions and about 5 times faster than the nonreacting case (comparing the positions of the shock wave in Figures 3 and 6).

Figure **??** shows contours of gauge pressure, velocity and reaction source terms after 0.5 ms in the fuel-lean and fuel-rich condition scenarios. Although the gauge pressures are identical, the velocities are 20% lower in the fuel-lean condition which qualitatively correlates with the observations of Dahoe [22] for hydrogen-air deflagration scenarios. The differences in the detonation velocities are more evident when looking at the transient pressure profiles at two of the gauges shown in Figure **??**. While the over-pressures are identical in both cases, the detonation velocity is clearly higher during fuel-rich conditions.

In order to discern the effects of viscosity during the propagation of the reacting detonation wave, an additional set of calculations were carried out employing the inviscid option in ANSYS FLUENT. The transient pressure predictions at the different gauges are shown in Figure **??**. It is worth noting that in Gauge 12 which is closer to the center of explosion (cf. Figure 1b), the arrival times and intensity of the pressure wave are unaffected by viscosity. However, by the time the detonation wave reaches Gauge 1, a distinct weakening of the pressure wave is noticeable in both fuel-lean and fuel-rich scenarios.

Figure 10 shows the impact of including radiative transfer effects on the detonation wave propagation. In spite of the higher magnitude of the radiative source term resulting from the higher temperatures of the reacting shock front seen in Figures (6c and 6d), including the effects of radiative transfer had no bearing on the shock wave propagation characteristics (i.e., magnitudes and arrival times). This is due to the fact that the magnitude of the reaction source term to the energy equation (Figures **??** (e, f)) were three orders of magnitude greater than the corresponding magnitudes of the radiative source term (Figures 6 (c, d)), therefore minimizing the impact of radiation on the wave propagation characteristics.

12 IV.

13 Conclusions

In lieu of the growing recent evidence advocating the importance of detailed chemistry models, viscous effects and radiative transfer in detonation scenarios, the primary goal of this manuscript was to assess these effects to enable users to select appropriate modeling options and CFD frameworks (hydro-codes versus complex multi-physics codes) for their study. Hydrogen-air mixtures were investigated in this study due to the availability of experimental measurements, well-established chemistry mechanisms and radiative property models for the combustion products at high temperatures and pressures.

Predictions from a hydro code were compared against combustion simulations employing CFD techniques. The hydro-code solved the inviscid Euler equations with the JWL equation of state. Detonation was initiated using established TNT equivalencies for a stoichiometric hydrogen-oxygen mixture. The CFD simulations rigorously resolved the detonation wave employing: the SRK equation of state for densities, Large Eddy Simulations for turbulence and spectrally averaged Planck mean absorption coefficients. In addition, a 21-step detailed chemistry model was employed in scenarios where the detonation wave was allowed to propagate through lean and rich premixed hydrogen-air mixtures. In the CFD simulations, detonation was initiated by patching the adiabatic

flame temperature in a spherical volume of gas at the center of the domain and employing the ideal gas equation of state to determine the pressure in the patched region at constant volume reactor conditions. Further, a temperature and pressure dependent Planck mean absorption coefficient for the radiative properties of water vapor and air were implemented in the CFD code as add-on functions and employed in conjunction with an optically thin approximation. As a result of comparing the predictions from these two modeling frameworks across the investigated scenarios encompassing variations in: domain size and reacting/non-reacting scenarios, the following conclusions can be drawn:

1. Predictions from the two modeling frameworks against reported measurements from a small-scale (Case 1) explosion study were in reasonable agreement, thereby establishing the adequacies of our modeling methodologies. This alleviates concerns regarding the effects of the approximations inherent in hydro codes when the explosion of a gaseous charge is simulated by converting it to TNT equivalencies when after-burn effects are not deemed important. These include: assumptions of a point source, assumptions of a perfectly spherical wave, absence of turbulence, presence of confinements and the assumption of an energy efficiency of one where all of the chemical energy released goes towards the propagation of the pressure wave. 2. When the same methodology was extended to larger scales (Case 2), the over-pressure predictions compared well in adherence to Hopkinsons Scaling Law. While there was a ten-fold increase in the wave propagation times to reach the enclosure surface in the larger domain, the over pressure characteristics were unaffected by the effects of radiative transfer in both Case 1 and Case 2 since the temperature increase across the shock was modest (~30 K) when the wave was propagating in air. 3. When the detonation wave was allowed to propagate in rich (40 mol% hydrogen) and lean (20 mol% hydrogen) premixed hydrogen-air mixtures, the resulting heat of reaction resulted in a significant acceleration and strengthening of the wave front.

Although the magnitudes of the over-pressures were similar in both lean and rich mixtures, the detonation wave propagation was faster in the rich mixture. These trends agree qualitatively with measurements from closed vessel gas explosion experiments.

Further, comparing inviscid calculations with those employing a turbulence model showed viscous losses to result in a noticeable weakening of the detonation wave during its propagation. 4. The magnitude of the radiative source was three orders of magnitude lower than that of the chemical heat release source term. Therefore, including the effects of radiative transfer had very little bearing on the over-pressure amplitudes and arrival times in the reacting flow scenarios. While the current study was limited to hydrogen-air mixtures, the proposed methodology can now be extended to study the effects of after-burn and radiative transfer during the detonation of condensed phase explosives where their impacts may be more significant. [1] [2] [3]

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[2] © 2017 Global Journals Inc. (US) Assessing the Impacts of Viscosity and Radiative Transfer in Internal Detonation Scenarios Involving Hydrogen-Air Mixtures

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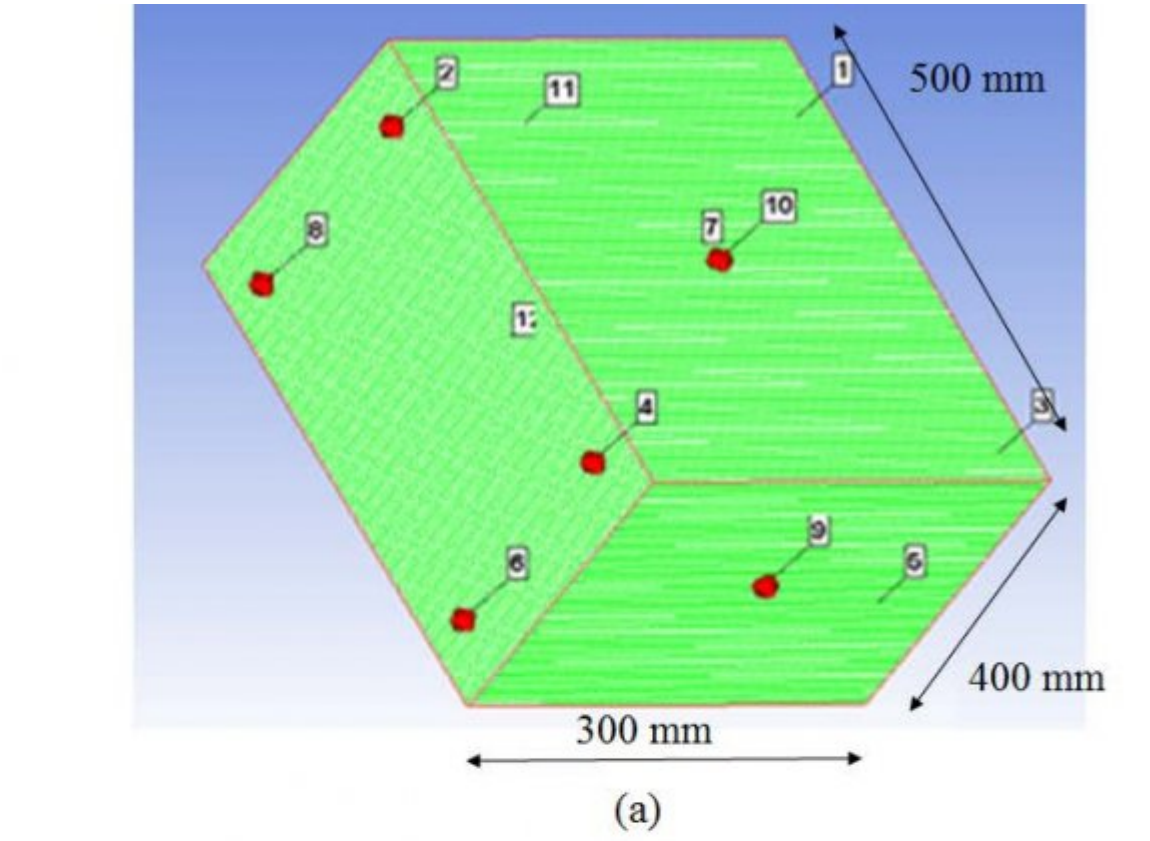

Figure 1:

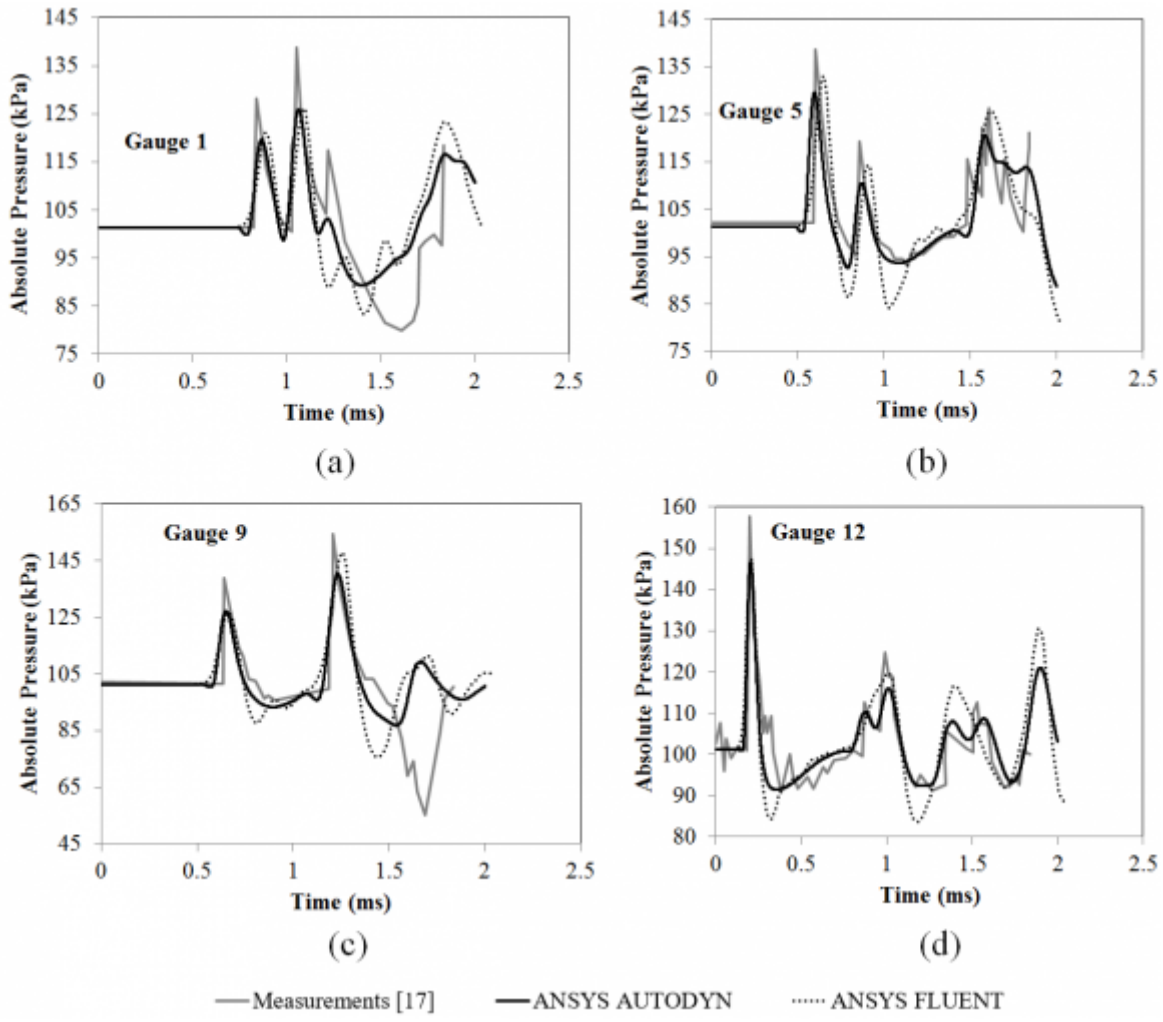

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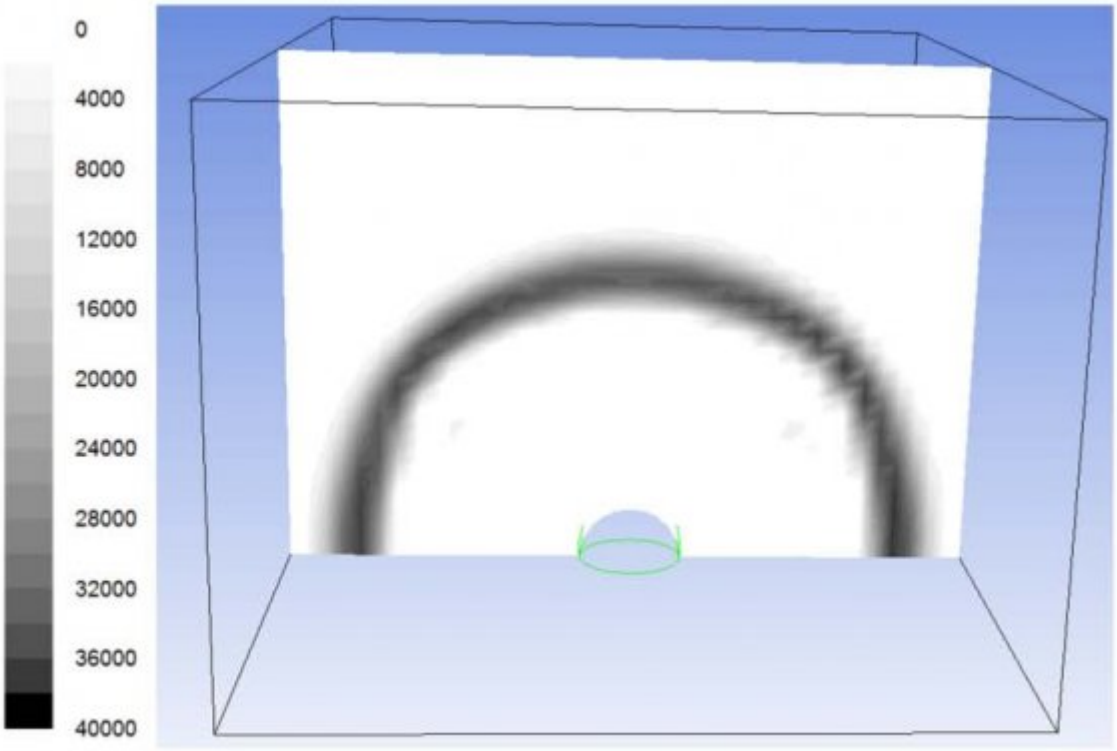
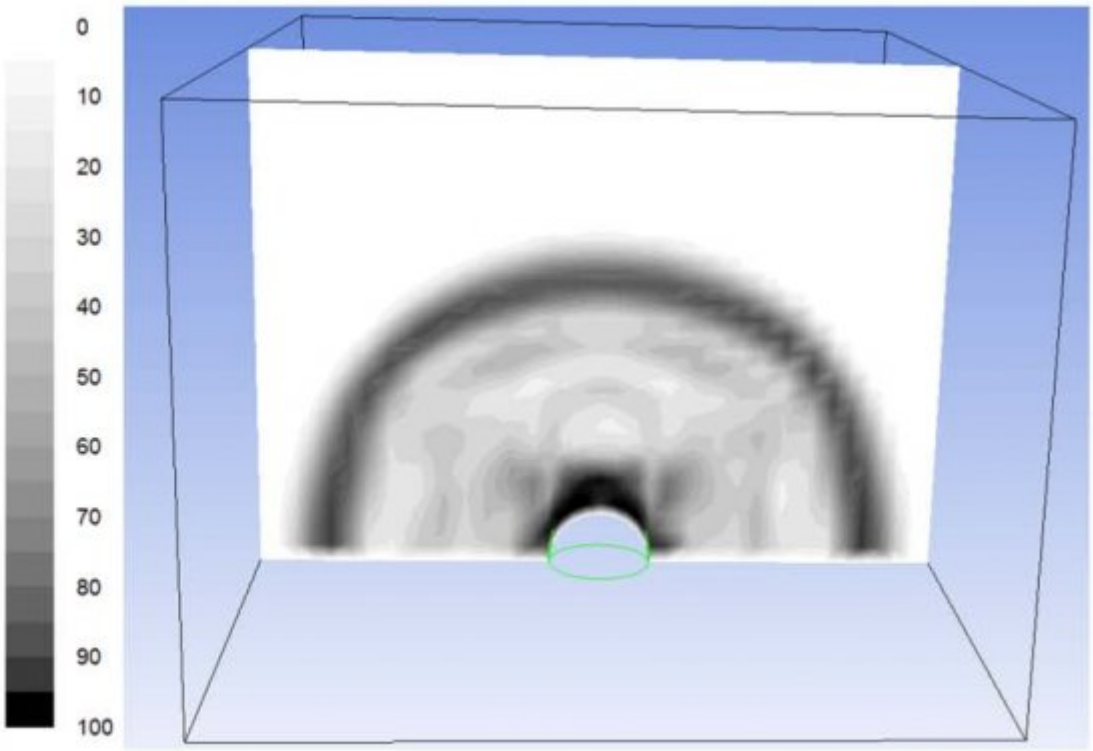
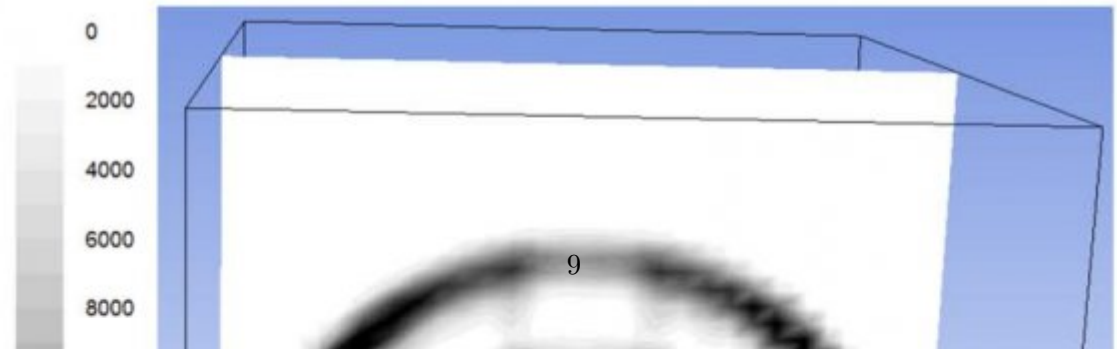
Figure 2: CFigure 1 :



(a) Gauge pressure (Pascal)



(b) Velocity (m/s)



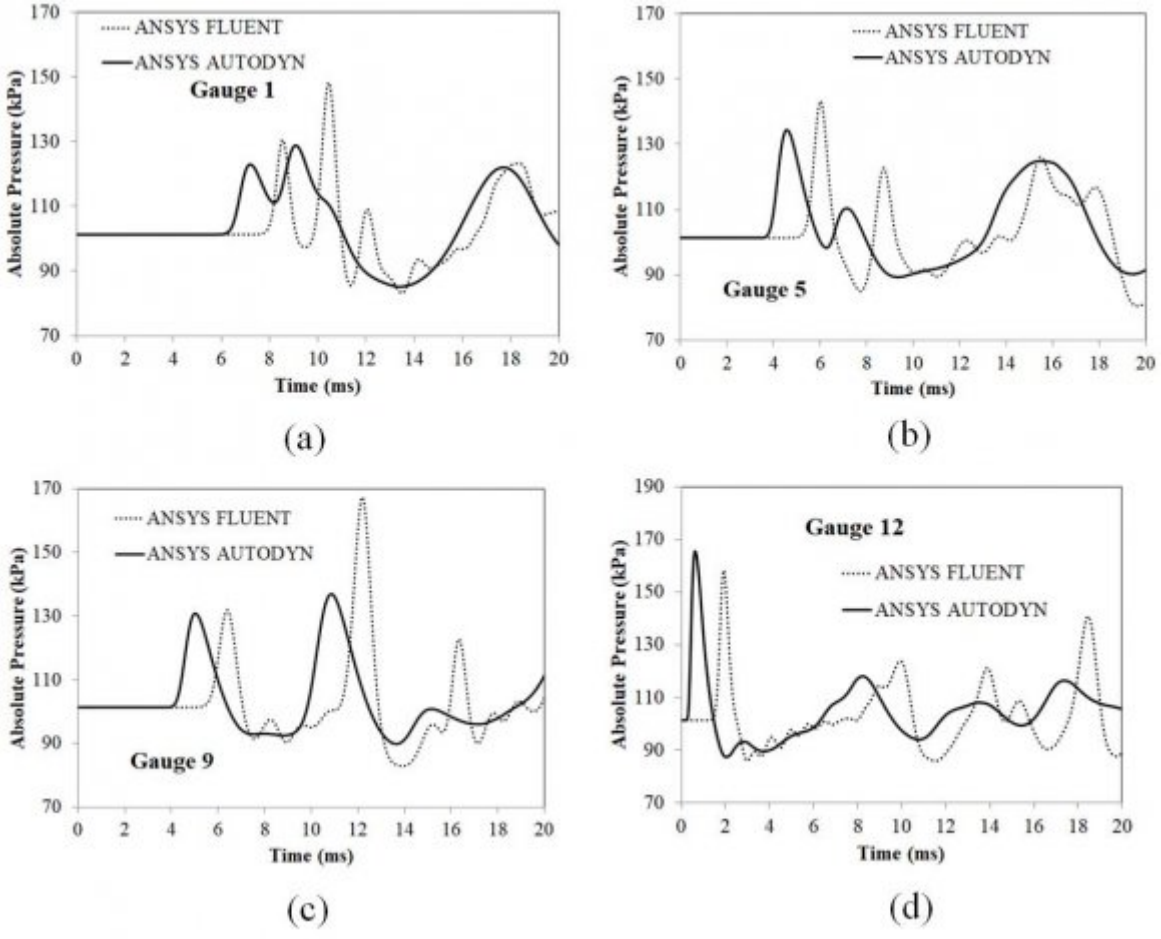


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Figure 4: Figure 3 :

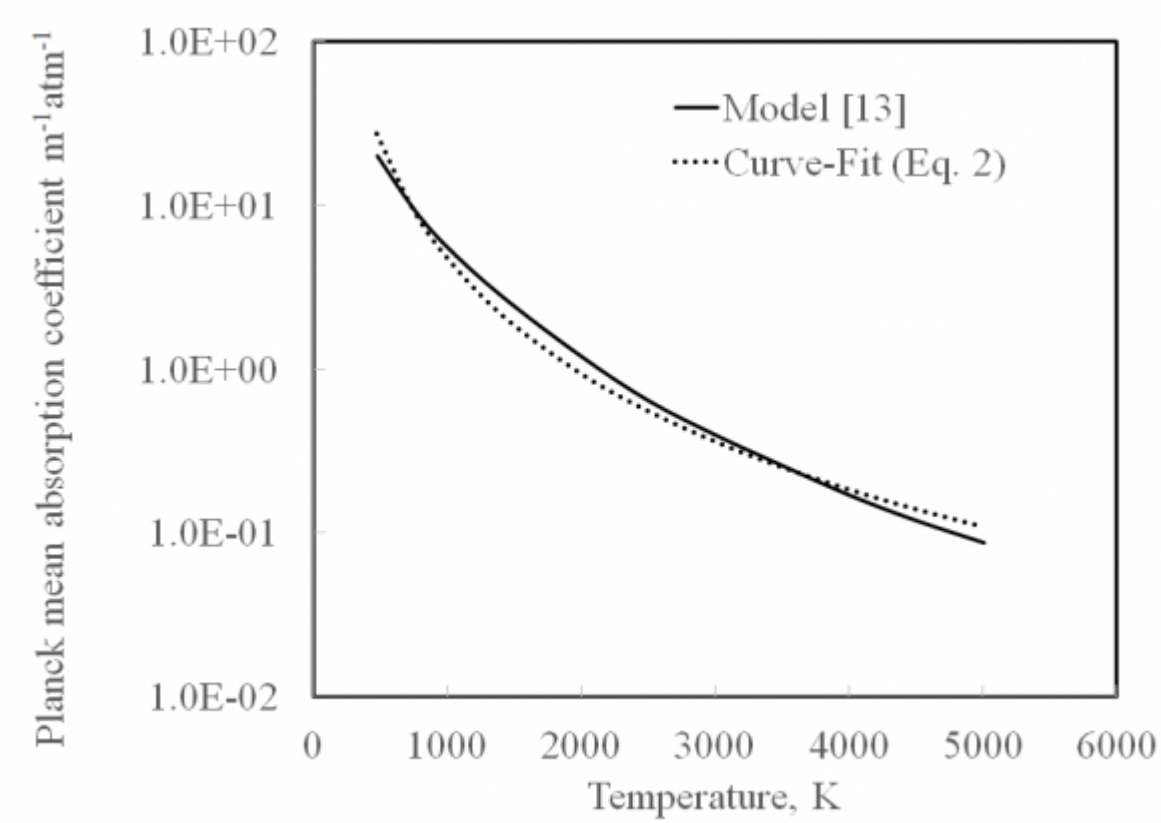

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Figure 5: Figure 4 : 2017 CFigure 5 :

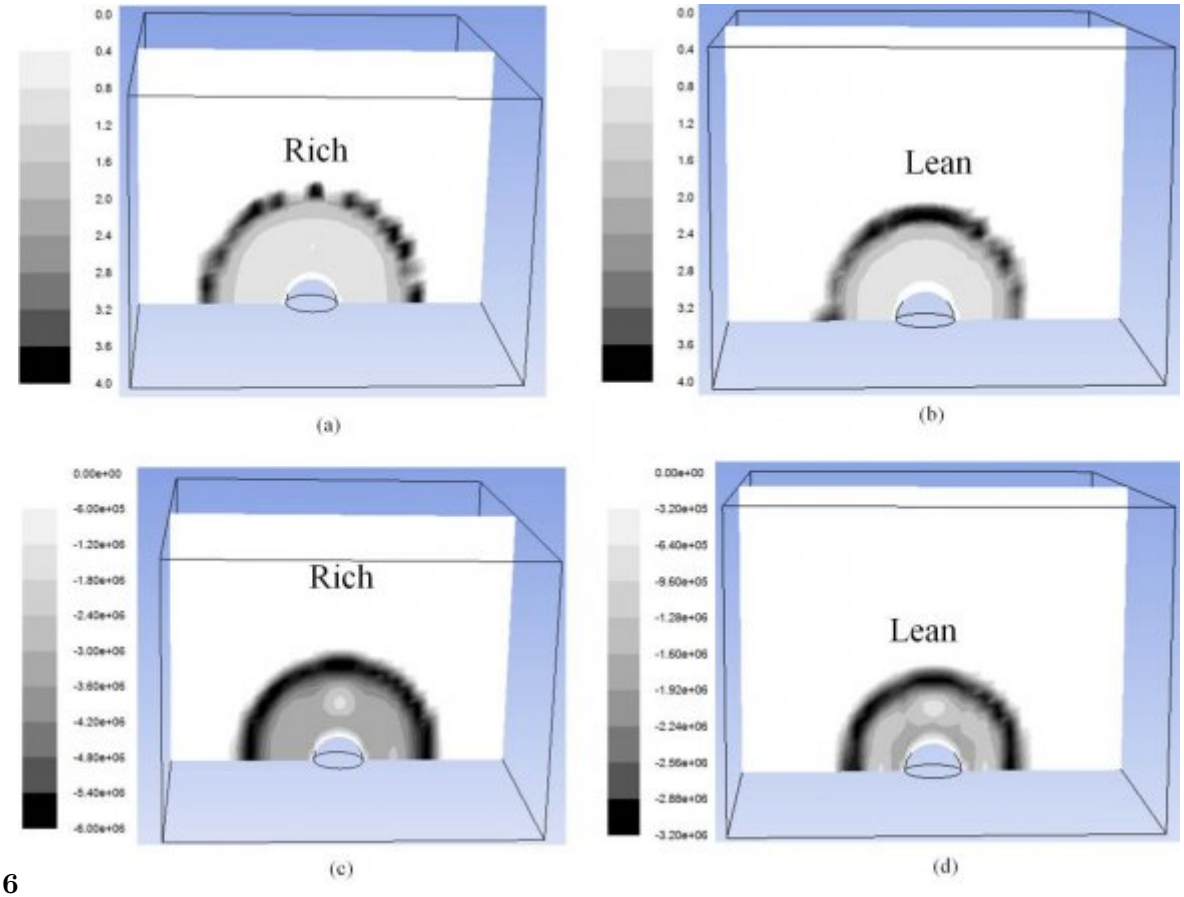

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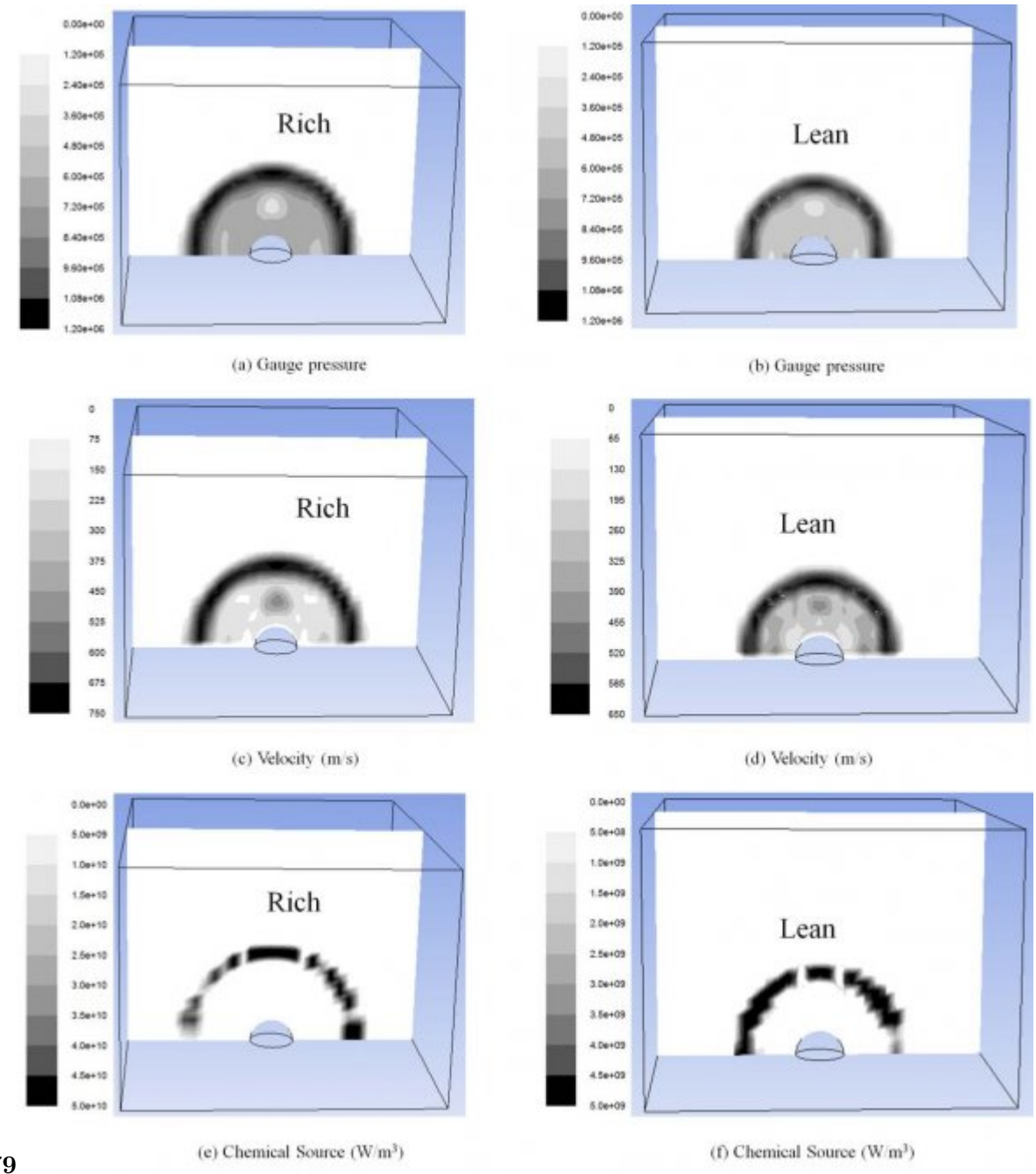
Figure 6: Figure 6 :



(a) Gauge pressure (b) Gauge pressure

(c) Velocity (m/s) (d) Velocity (m/s)

(e) Chemical Source (W/m^3) (f) Chemical Source (W/m^3)

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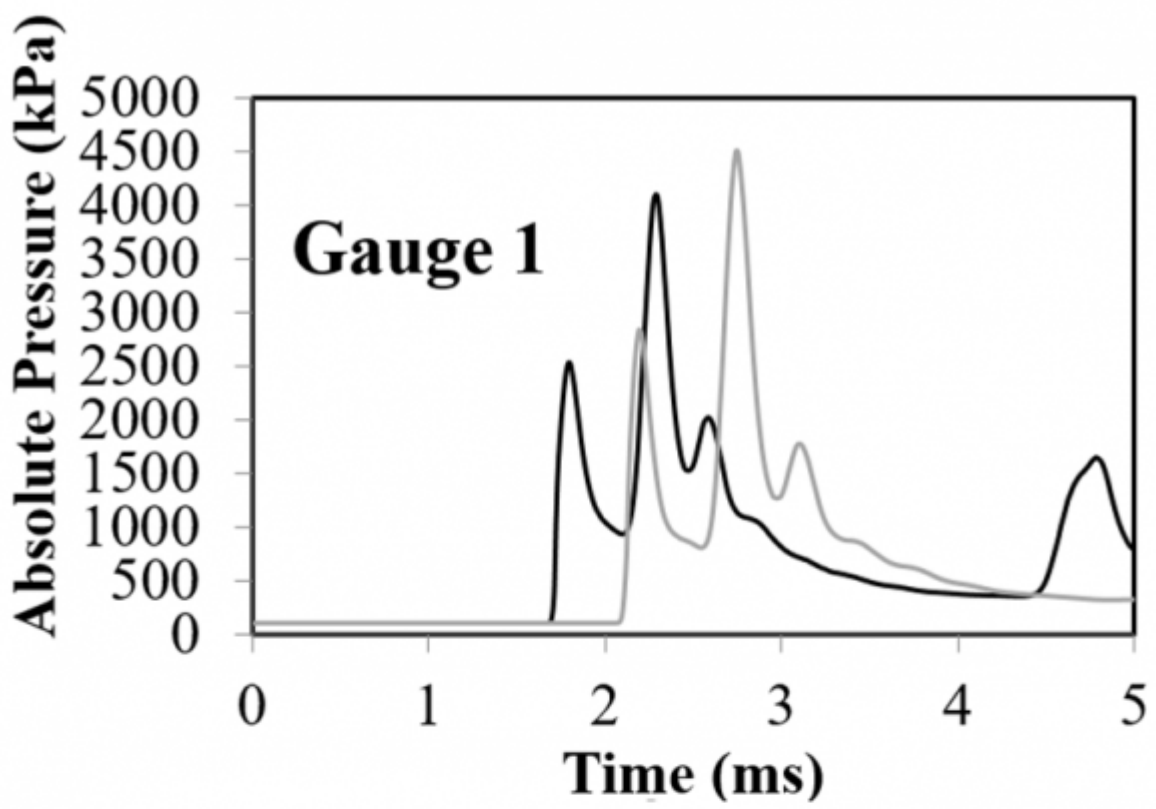
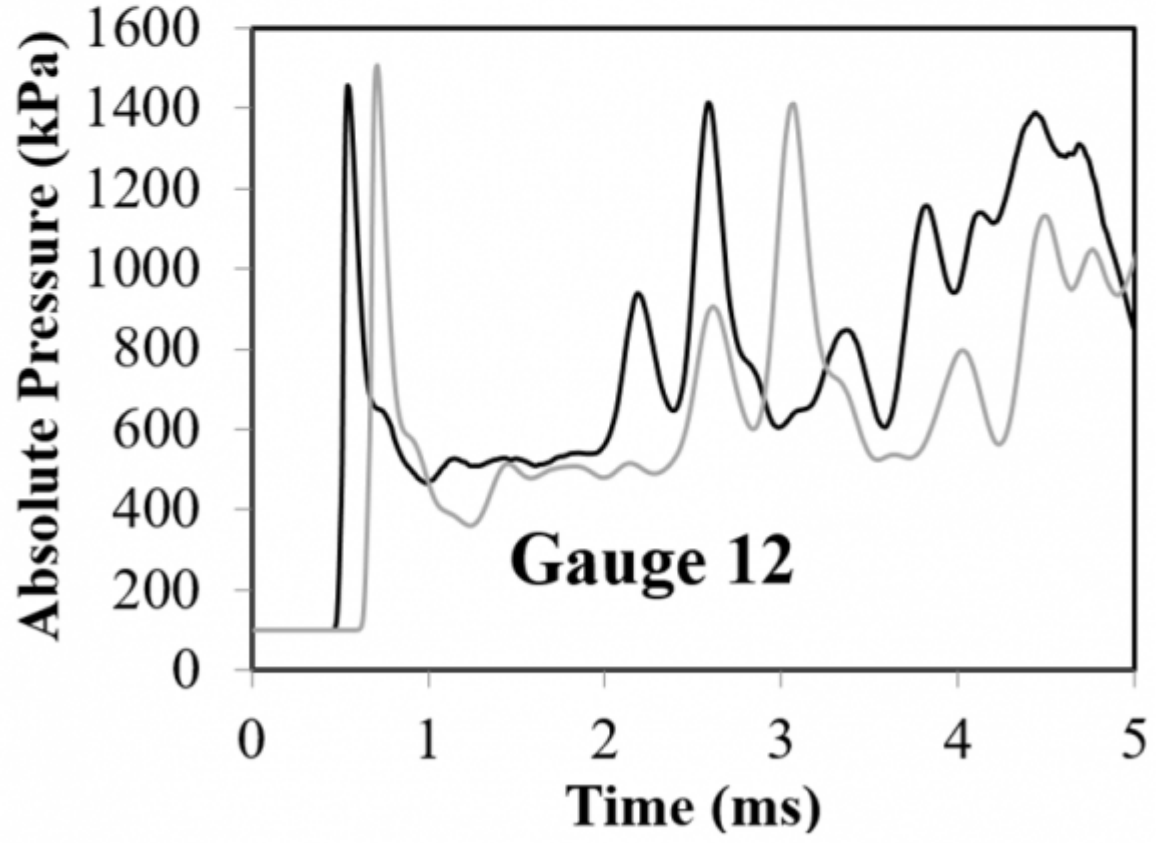
Figure 7: Figure 7 : 2017 CFigure 8 :Year 2017 CFigure 9 :


Absolute Pressure (kPa)
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
Gauge 1
0
1
2
3
4
5
Time (ms)

(a)


Absolute Pressure (kPa)
1600
1400
1200
1000
800
600
400
200
0
Gauge 12
0
1
2
3
4
5
Time (ms)

(b)

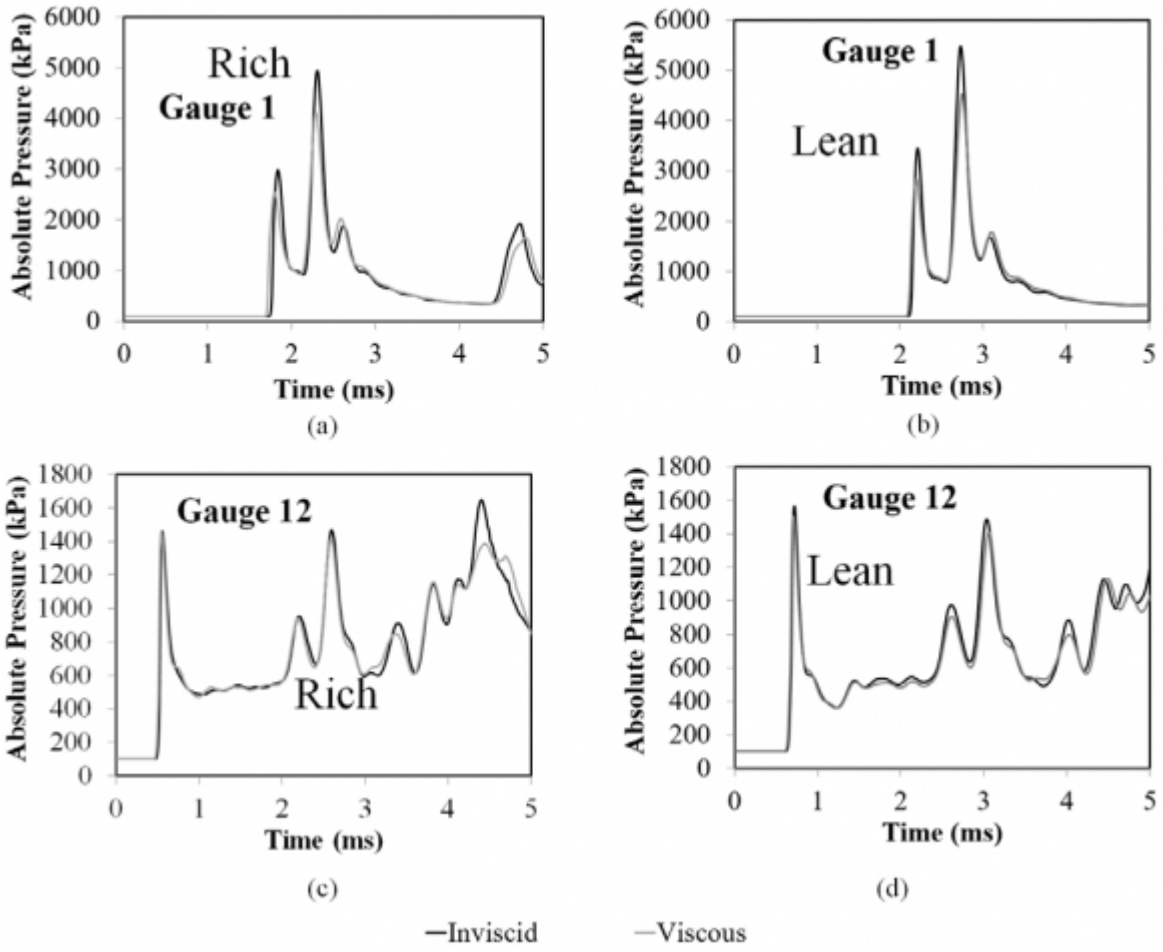

Absolute Pressure (kPa)
Rich
Gauge 1
Time (ms)
(a)
Gauge 1
Lean
Time (ms)
(b)
Gauge 12
Rich
Time (ms)
(c)
Gauge 12
Lean
Time (ms)
(d)
—Inviscid
—Viscous

Figure 9:

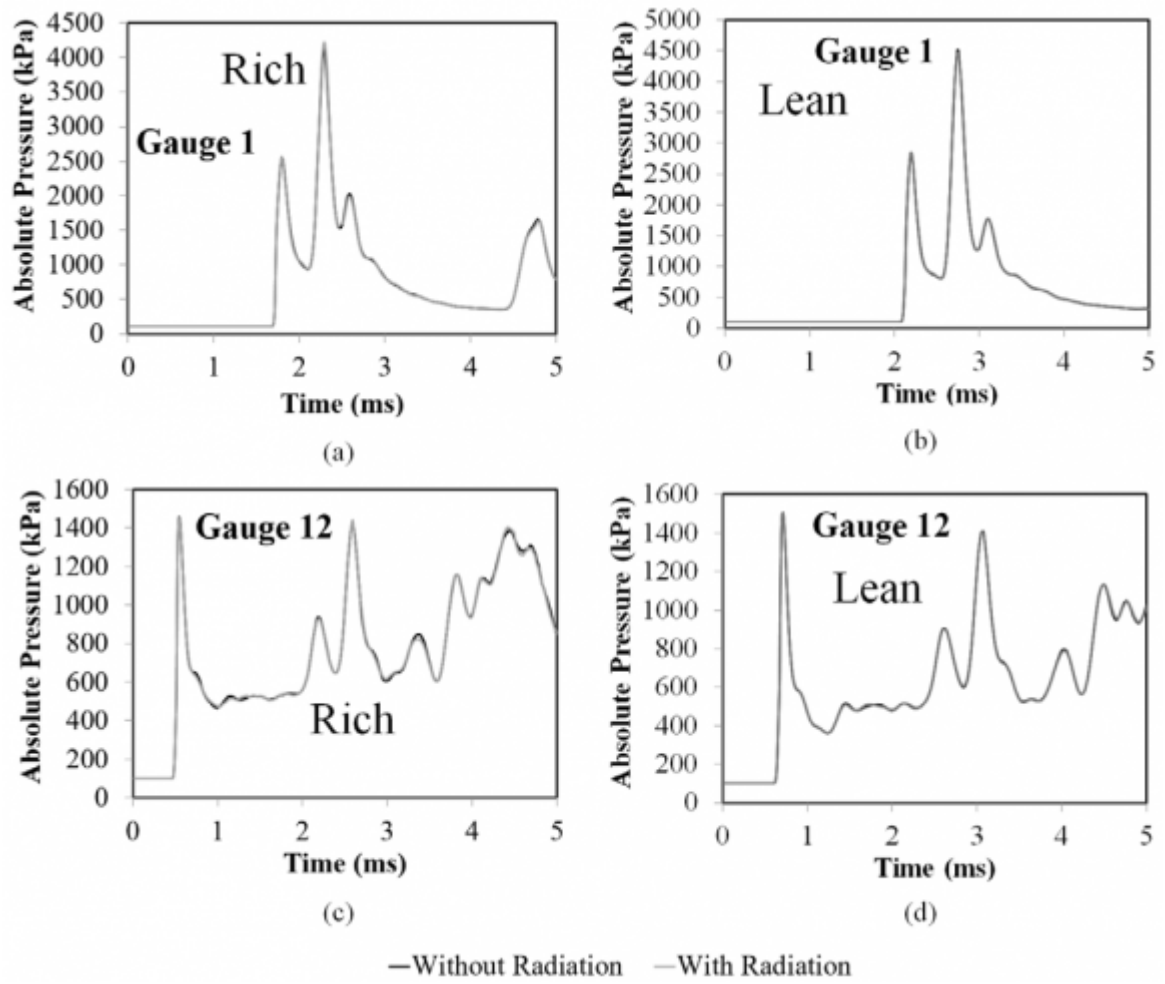


Figure 10:

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[Note: of the Effects of Radiative Transfer, Turbulence Radiation Interactions, and Finite Rate Chemistry in]

Figure 11: Table 1 :

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.2 Conflict of Interest

The author(s) declares no conflict of interest.

[Ya et al. ()] , . B Ya , V B Zeldovich , G M Librovich , G I Makhviladze , Sivashinsky . *Astronautica Acta* 1970. 15 p. 313.

[Fluent ()] '0: Theory guide'. Ansys Fluent . *ANSYS. Inc* 2011. p. 14.

[O'connaire et al. ()] 'A Comprehensive Modeling Study of Hydrogen Oxidation'. M O'connaire , H J Curran , J M Simmie , W J Pitz , C K Westbrook . UCRL-JC-152569. *Int. J. Chem. Kinet* 2004. 36 p. .

[Tomizuka et al. ()] 'A study of numerical hazard prediction method of gas explosion'. T Tomizuka , K Kuwana , T Mogi , R Dabashi , M Koshi . *International Journal of Hydrogen Energy* 2013. 38 p. .

[Renard et al. ()] 'Benchmark experiments for the validation of numerical codes'. J Renard , C Desrosier , I Sochet . *16th international symposium military aspects of blast and shock*, (Oxford) 2000. p. .

[Krishnamoorthy and Clarke ()] 'Computationally Efficient Assessments References Références Referencias the Mach 20 Reentry F Flight Vehicle'. Gautham Krishnamoorthy , Lauren Elizabeth Clarke . *Journal of Computational Engineering* 2016.

[Liberman et al. ()] 'Effect of thermal radiation heat transfer on flame acceleration and transition to detonation in particle-cloud hydrogen flames'. M A Liberman , M F Ivanov , A D Kiverin . *Journal of Loss Prevention in the Process Industries*, 2015. 38 p. .

[Hazard of chemical rockets and propellants handbook, General safety engineering design criteria, I, National Technical Informati 'Hazard of chemical rockets and propellants handbook, General safety engineering design criteria, I, National Technical Information Service'. *JANNAF* 1972. p. .

[Scala and Sampson ()] *Heat Transfer in Hypersonic Flow with Radiation and Chemical Reactions*, S M Scala , D H Sampson . 1963. General Electric Co., Phidelphia. (PA Missile and Space Division)

[Molkov et al. ()] 'Hydrogen-air deflagrations in open atmosphere: large eddy simulation analysis of experimental data'. V V Molkov , D V Makarov , H Schneider . *International Journal of Hydrogen Energy* 2007. 32 (13) p. .

[Dahoe ()] *Laminar burning velocities of hydrogen-air mixtures from closed vessel gas explosions*, A E Dahoe . 2005. 18 p. . (Journal of Loss Prevention in the Process Industries)

[Zbikowski et al. ()] 'LES model of large scale hydrogenair planar detonations: Verification by the ZND theory'. Mateusz Zbikowski , Dmitriy Makarov , Vladimir Molkov . *international journal of hydrogen energy* 2008. 33 (18) p. .

[Barlow et al. ()] 'Nitric oxide formation in dilute hydrogen jet flames: isolation of the effects of radiation and turbulence-chemistry submodels'. R S Barlow , N S A Smith , J-Y. Chen , R W Bilger . *Combustion and Flame* 1999. 117 (1) p. .

[Zbikowski et al. ()] 'Numerical simulations of large-scale detonation tests in the RUT facility by the LES model'. Mateusz Zbikowski , Dmitriy Makarov , Vladimir Molkov . *Journal of hazardous materials* 2010. 181 (1) p. .

[Liberman et al. ()] 'On detonation initiation by a temperature gradient for a detailed chemical reaction models'. M A Liberman , A D Kiverin , M Ivanov . *Physics Letters A* 2011. 375 p. .

[Feldgun et al. ()] 'Prediction of the quasi-static pressure in confined and partially confined explosions and its application to blast response simulation of flexible structures'. V R Feldgun , Y S Karinski , I Edri , D Z Yankelevsky . *International Journal of Impact Engineering* 2016. 90 p. .

[Liberman et al. ()] 'Radiation heat transfer in particle-laden gaseous flame: Flame acceleration and triggering detonation'. M A Liberman , M F Ivanov , A D Kiverin . *Acta Astronautica* 2015. 115 p. .

[Zyskowski et al. ()] 'Study of the explosion process in a small scale experiment-structural loading'. A Zyskowski , I Sochet , G Mavrot , P Bailly , J Renard . *Journal of Loss Prevention* 2004. 17 p. .

[Liu et al. ()] 'Study on the critical parameters of spherical detonation direct initiation in hydrogen/oxygen mixtures'. Qingming Liu , Yunming Zhang , Shuzhuan Li . *International Journal of Hydrogen Energy* 2015. 40 p. .

[Sathiah et al. ()] 'The role of CFD combustion modeling in hydrogen safety management-IV: Validation based on non-homogeneous hydrogen-air experiments'. Pratap Sathiah , Ed Komen , Dirk Roekaerts . *Nuclear Engineering and Design* 2015.

[Autodyn ()] *Theory manual revision 4.3. Century Dynamics*, Ansys Autodyn . 2005. Concord, CA.

[Rivière and Soufiani ()] 'Updated band model parameters for H2O, CO2, CH4 and CO radiation at high temperature'. Philippe Rivière , Anouar Soufiani . *International Journal of Heat and Mass Transfer* 2012. 55 (13) p. .