A Preliminary Heat Transfer Analysis of Pulse Detonation Engines

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ABSTRACT

Detonation engines offer higher theoretical thermal efficiencies as compared to their deflagration-based counterparts. Simultaneous pressure gain during heat addition through the detonation wave provides the superiority to the Zeldovich-von Neumann-Döring (ZND) cycle which is used to define the thermodynamic process of detonation engines. Combustion temperatures can rise as high as 3000 K across the detonation wave. The continuous exposure to such elevated temperature may risk the integrity of the structural components of the engines. Consequently, heat management of the detonation engines highlights an important parameter on the construction of a demonstrator. In order to be able to design an appropriate cooling system, both for pulse detonation and rotating detonation engines (PDE & RDE), an accurate estimation of the heat load stands as an essential prerequisite. Hence, a preliminary numerical study of the heat transfer on a pulse detonation engine model was conducted to quantify the heat load. Conservation equations for deflagration-to-detonation transition (DDT) in detonation engines were solved through open source fluid dynamics solver OpenFOAM equipped with ddtFoam module. Reactive flow field of premixed mixtures (Hydrogen-air) was modeled with a URANS second-order approximate Riemann solver equipped with Weller combustion model, and Arrhenius equations of O'Connaire reaction scheme for Hydrogen-air detonation. Multiple boundary conditions were tested to achieve the most appropriate model. Natural convection over the lateral combustor peripheries found to be the most realistic boundary condition for the problem. In order to observe cooling process better, PDE tubes in different length were also simulated. Finally, the transient heat transfer phenomenon across the pulse detonation tube is documented for various conditions investigated.

KEYWORDS: *detonation engine, heat transfer, pulse detonation, OpenFOAM, combustion*

NOMENCLATURE

Latin
c – Reaction progress variable
D – Diffusion coefficient
f_b – Body force
G – Flame quenching factor
h – Enthalpy
k – Thermal conductivity
p – Pressure
q – Heat flux
R – Specific gas constant
s – Flame speed
T – Temperature
t – Time
V – Velocity
Greek
ξ – Flame wrinkling factor
λ – Heat transfer coefficient
ρ – Density
σ – Deviatoric component of total stress tensor
τ – Dimensionless auto-ignition delay time
ω – Source term
Subscripts
c – For reaction progress variable
ign - Ignition
L – Laminar
T – Turbulent
t – Total
U – Unburnt
w – Wall

τ – For dimensionless auto-ignition delay time
∞ - Ambient

1 INTRODUCTION

Detonation engines are one of the most attractive propulsion systems in the 21th century due to their higher theoretical thermal efficiency and specific impulse compared to deflagration engines. Based on their frequencies, these systems are classified into two main categories; pulse (PDE) and rotating detonation engines (RDE). Differing from periodically ignited PDEs, RDEs work with much higher frequencies thanks to continuously rotating detonation shock or shocks.
The main principle behind the detonation engines is Zeldovich-von Neumann-Döring (ZND) process, which assumes that the detonation shock is frozen and fluid flows through the shock with an immediate escalation of pressure and temperature [1]. The relevant model is illustrated on Fig. 1 [2]. Throughout detonation, flame speed is constant and named as Chapman-Jouget (CJ) speed. This is known as Chapman-Jouget principle, basis of detonation theory.

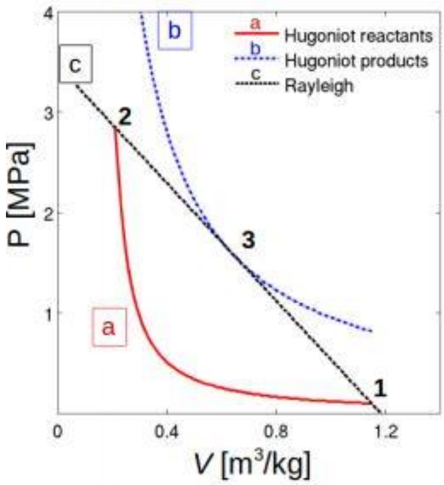

Figure 1: Pressure specific volume diagram of ZND cycle [2].

Since the middle of the last century, analyses on detonation engines have been being performed either experimentally or numerically and gained speed throughout 21st century. Earlier measurements of thrust, hydrogen (fuel) flow, air flow and temperature for intermittent detonation shocks was made by Nicholls, Wilkinson and Morrison [3]. Experiments on ZND cycle proved that detonation engines are 6-7% more efficient than traditional combustors [4]. Paxson et al. performed experiments and numerical simulations for determination of heat transfer from PDE and compared the results [5]. Apart from hydrogen-air mixture, numerical simulations for PDE filled with octane-air mixture and comparisons with experimental results were performed to compute heat fluxes from PDE [6]. Also, experiments on heat losses from RDEs performed under unsteady heating shows maximum heat losses occurs from the mixing region and number of detonation shocks affects heat transfer [7]. Frolov et al. developed a numerical tool which simulates operation process of RDEs to determine design parameters for combustion chamber and isolators [8]. Numerical analyses on heat loss from detonation engines performed by open-source and packaged softwares [9, 10].
For accident free flights and launches, design and optimization of detonation engines should be carefully studied and perfected. Structural failures are particularly due to thermal expansion and material erosion. This enhances importance of heat transfer studies on detonation engines. Hence, analysis of heat loss on detonation engines is primarily aimed for this project. In parallel to this purpose, pulse detonation engine (PDE) was solved under adiabatic, isothermal and Neumann type boundary conditions. Also, solutions of various fixed temperature gradients were compared to investigate engine performances under different ambient temperatures. For the simulations, ddtFoam module, prepared by Florian Ettner [11], of the open source CFD toolbox OpenFOAM since it is the most accurate solver for detonation simulations, as presented in Section 2.2.

2 METHODOLOGY

2.1 Numerical Tool

Throughout deflagration, DDT, and detonation; mass, momentum and energy are conserved and perfect gas law is used as the equation of state. These are shown in Eqs. 1-4.

$$\partial\rho/_{\partial t} + \nabla \cdot (\rho\vec{V}) = 0 \quad (1)$$

$$D(\rho\vec{V})/_{Dt} + \vec{V} \cdot \nabla(\rho\vec{V}) = -\nabla p + \nabla \cdot \vec{\sigma} + \vec{f_b} \quad (2)$$

$$D(\rho h_t)/_{Dt} = D(\rho\vec{V})/_{Dt} - \nabla \cdot \vec{q} + \vec{\sigma}:\nabla\vec{V} \quad (3)$$

$$p = \rho RT \quad (4)$$

For heat transfer from detonation engines with a constant heat flux, conduction in the hydrogen-air mixture and natural convection around the engine were equalized, as shown in Eq. 5, to determine the temperature gradient.

$$-k(\partial T/_{\partial y}) = \lambda(T_w - T_\infty) \quad (5)$$

Heat flux over the boundaries is calculated by previously determined temperature gradient and average thermal conductivity of existing gases that components of are determined by cubic polynomials of temperature.

In order to analyze PDEs is ddtFoam, an add-on OpenFOAM solver developed by Florian Ettner is used [11]. ddtFoam is capable to solve both deflagration and detonation successively thanks to inclusion of two computationally independent but physically supplementary solvers named pddtFoam and ddtFoam. pddtFoam is the pressure-based solver for deflagration process and driven by PISO algorithm. It is required for initialization of detonation and computation until DDT starts since deflagration is followed by detonation in real life. Then, the solver is switched to density-based ddtFoam, consisting of a second order approximate Riemann solver [11]. Unsteady Reynolds Averaged Navier-Stokes (URANS) equations are solved by k-ω Shear Stress Transport (k-ω SST) model for turbulence [11].

Weller's combustion model [12] is adopted as the deflagration model. It is based on the placement of reaction progress variable (c), indicating instantaneous state of combustion, in convection-diffusion equation, presented in Eq. 6, and its solution. Note that, ω_c is the source term of Eq. 6, and s_T and s_L are turbulent and laminar flame speeds, respectively.

$$\partial(\rho c)/_{\partial t} + \nabla\rho c \cdot \vec{V} = -\nabla \cdot \rho D \nabla c + \omega_c \quad (6)$$

$$\omega_c = s_T(\nabla c)\rho_u G \quad (7)$$

$$s_T = \xi s_L \quad (8)$$

For detonation model of hydrogen-air mixture, Arrhenius equation of O'Conaire reaction scheme [13], reaction progress variable and dimensionless auto-ignition delay time (τ) (Eq. 9) are used. c and τ are included to convection-diffusion equation separately, as presented in Eqs. 6 and 10.

$$\tau = t/t_{ign} \quad (9)$$

$$\partial(\rho\tau)/_{\partial t} + \nabla\rho\tau \cdot \vec{V} = -\nabla \cdot \rho D \nabla \tau + \omega_\tau \quad (10)$$

Deflagration and detonation may be also modeled as a single hybrid model with a turbulent source term ($\omega_{c,turb}$) from Weller's combustion model [12] and an ignition source term ($\omega_{c,ign}$) from the detonation model. This model is expressed in Eq. 11.

$$\partial(\rho c)/_{\partial t} + \nabla\rho c \cdot \vec{V} = -\nabla \cdot \rho D \nabla c + \omega_{c,T} + \omega_{c,ign} \quad (11)$$

2.2 Validation and Verification of the Numerical Solver

DdtFoam was initially tested on a shock tube case to verify its aerodynamic shock capture capability. In accordance with this purpose, ddtFoam results were compared with Ettner's simulations [11] and results of sonicFoam and an analytical shock tube model [14].
After aerodynamic verification with shock tube [15], the solver was validated by a comparison of a PDE case and Ettner's experimental and numerical results. This comparison was made for a premixed hydrogen-air mixture with 25% molar fraction of hydrogen in a tube having 5.4 m length and 6 cm diameter and 7 ribs with a blockage ratio of 30%. The computational mesh for the case, shown on Fig. 2, has cubic cells with a spatial discretization of 2 mm, as used by Ettner [11]. According to the results illustrated on Fig. 3, deflagration and detonation processes are simulated by the solver verified and validated against the experimental results in the literature.

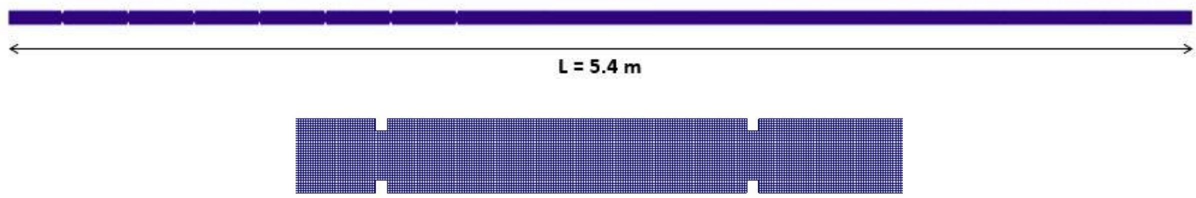

Figure 2: Computational domain of PDE (top) and detailed zoom of the mesh (bottom)

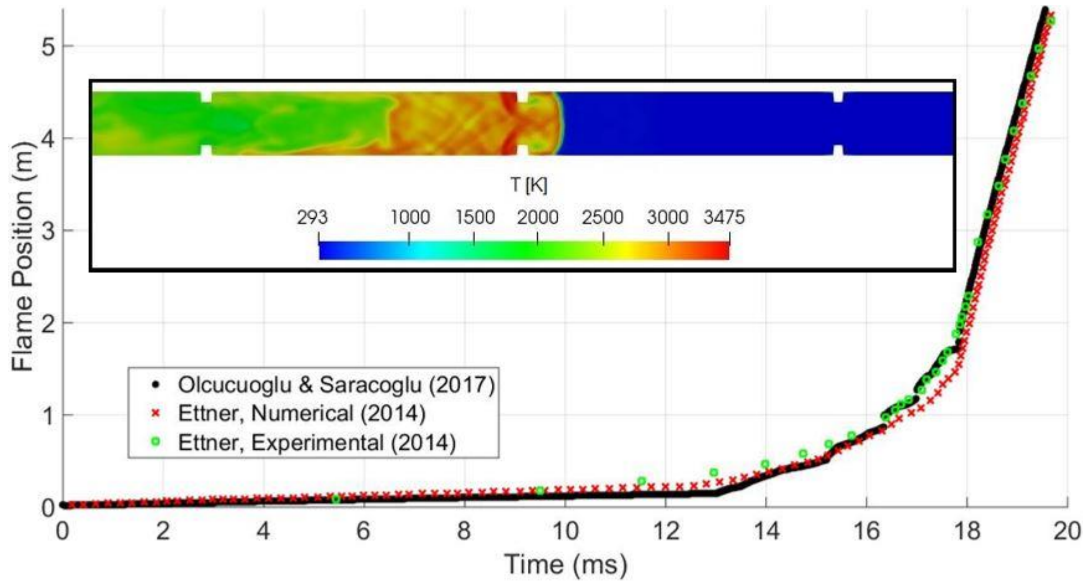

Figure 3: Flame propagation results compared to Ettner's numerical and experimental findings [11]

3 RESULTS

Premixed hydrogen-air mixture with 25% molar fraction of hydrogen in a tube having a length of 5.4 m and a diameter of 6 cm was initially simulated under adiabatic conditions. Then, isothermal and iso-heat flux (Neumann type boundary condition) scenarios were also investigated. The geometry modeled for PDE is similar to Figure 2, but it has 9 obstacles instead of 7. Again, the mesh has cubic cells with 2 mm spatial discretization. An initial ignition was modeled to trigger detonation as a semicircle with 2mm diameter and 2204.7 K temperature (Fig. 4).

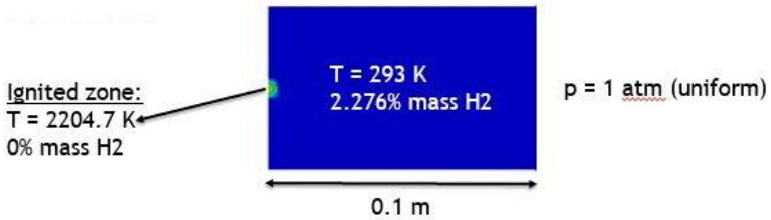

Figure 4: Initial conditions for premixed PDE simulations.

Comparison of the transient flame position data belonging to adiabatic, isothermal warm wall (at 1000 K) and iso-heat flux cases are presented on Fig. 5. According to the results, deflagration propagates similarly for all cases. Having approximately same CJ speeds (1966 m/s for adiabatic and 1976 m/s for isothermal), the only difference between adiabatic and isothermal cases shapes during deflagration-to-detonation transition (DDT) stage. Nevertheless, the case with constant temperature gradient has slightly better performance than others since DDT occurs faster despite having similar deflagration and DDT stages with the adiabatic case. CJ speed for this case is 1973 m/s. Note that, although the case with constant heat flux has a lower CJ speed, the flame reaches at the end the earliest due to faster DDT process.

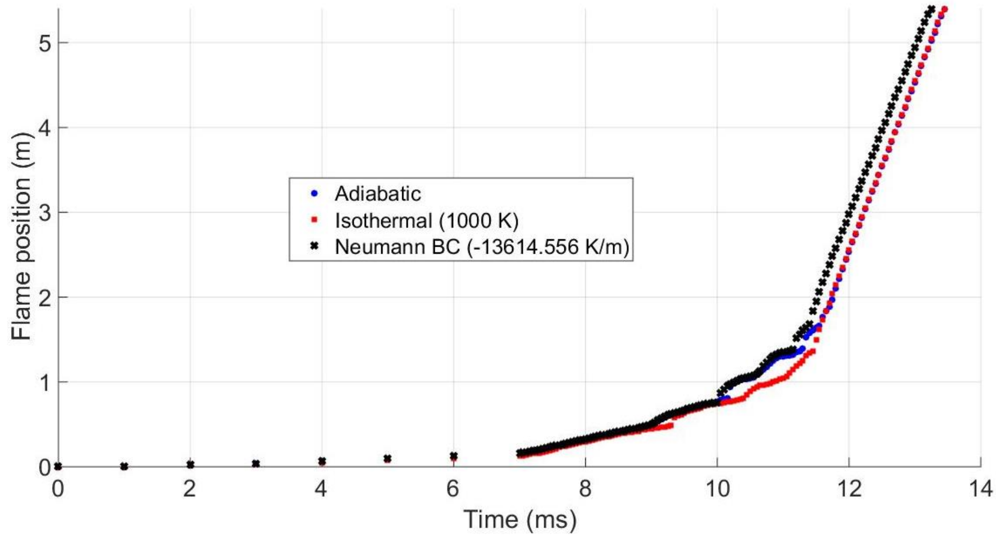

Figure 5: Flame propagations for homogeneous hydrogen-air mixture under adiabatic, isothermal and Neumann type boundary conditions

For the case with Neumann type boundary condition, assuming natural convection outside of PDE was assumed. A heat transfer coefficient was determined for the ambient temperature of 293 K (20^{0}C) and a wall temperature of 2800 K (average temperature of the mixture on the boundary field behind the shock). Besides, thermal conductivity of the mixture was estimated for the mentioned conditions. As a result, conduction in the burnt gas and natural convection outside of the engine were equalized and a constant temperature gradient was estimated as -13614.556 K/m [15-17]. Heat flux and temperature distributions along top and bottom walls are shown on Fig. 6. Almost all of heat losses occurred behind the detonation shock due to suddenly increased temperature behind the shock.

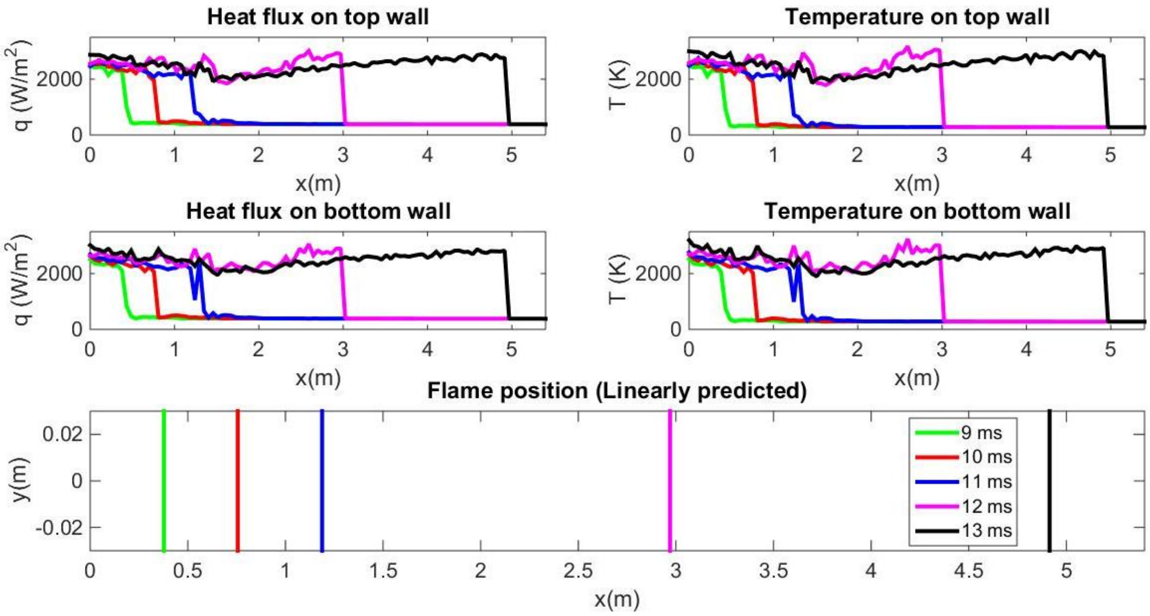

Figure 6: Heat flux and temperature variations along the tube for simulations with constant temperature gradient of -13614.556 K/m with predictions of flame positions

The effects of environment and mixture homogeneity were investigated with Neumann type boundary conditions because the differences appeared more distinctly for this condition. Changes in environmental conditions and homogeneity of the mixture affect the performance of PDE. To investigate effects of the surroundings, simulations with different temperature gradients were performed to analyze effects of variances in the ambient. New gradients were determined through adding 25% of the initial estimate to and subtracting 25% of the initial estimate from the first gradient. Results of the case with higher temperature gradient are shown on Fig. 7 while the case with lower temperature gradient is illustrated on Fig. 8. As seen, heat flux and temperature did not fluctuate during detonation of homogeneous mixtures. According to Figs. 6, 7 and 8; if heat loss increases, the flame reaches at the end of PDE. Therefore, PDE has a better performance for conditions with strong cooling (Fig. 8).

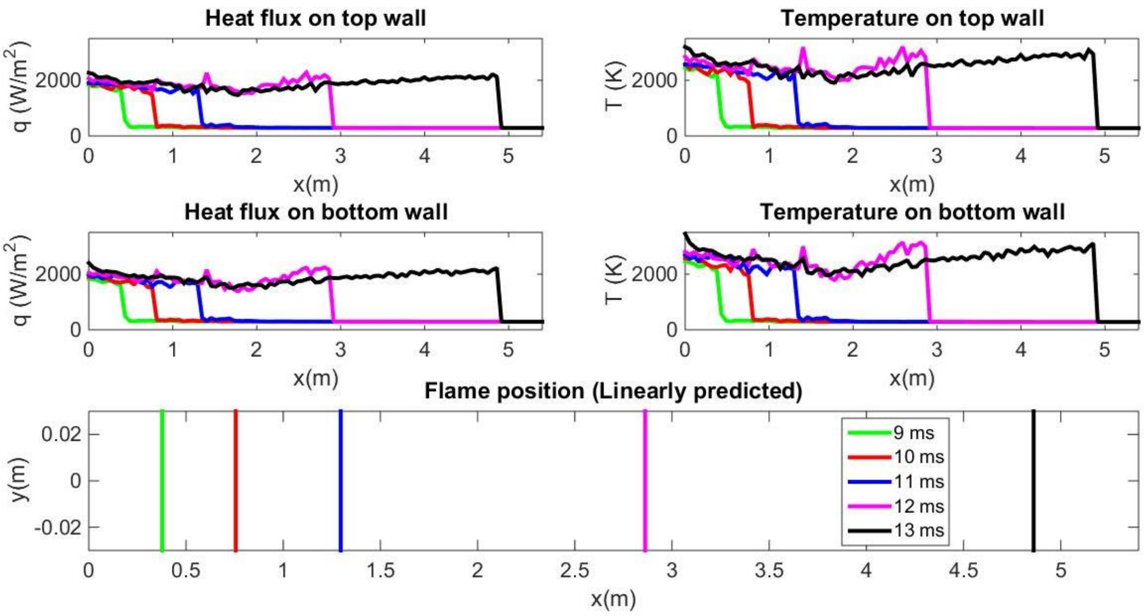

Figure 7: Heat flux and temperature variations along the tube for simulations with 25% lower temperature gradient (-10210.917 K/m) and predictions of flame positions

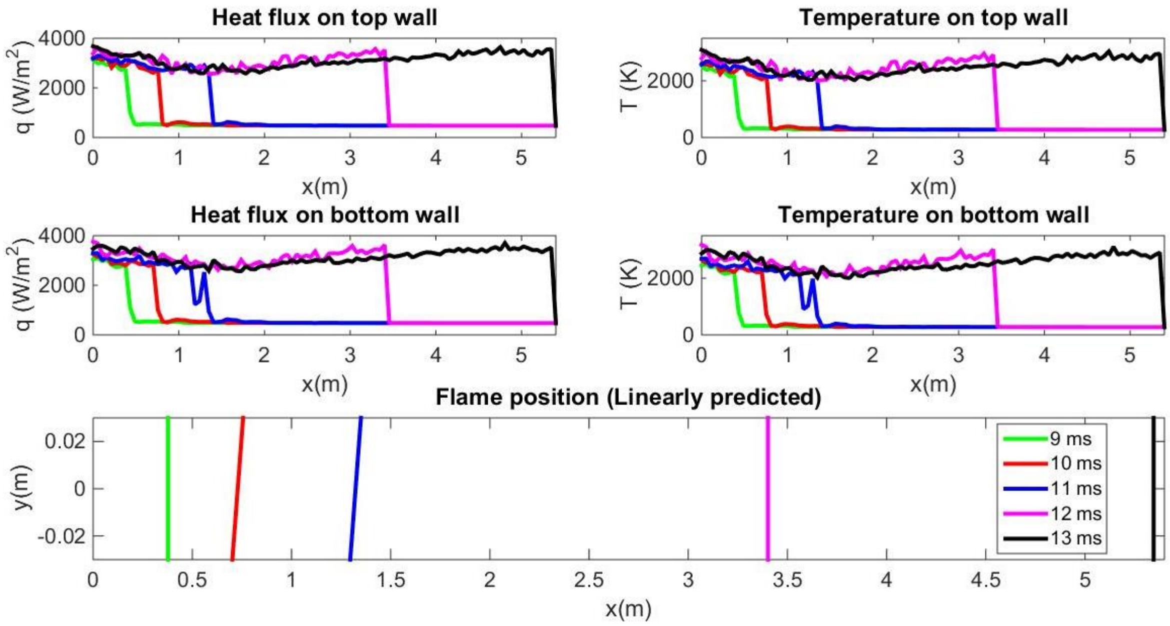

Figure 8: Heat flux and temperature variations along the tube for simulations with 25% higher temperature gradient (-17018.195 K/m) and predictions of flame positions

Fuel-air mixture homogeneity is another key factor for the engine performance. Varied hydrogen concentrations in differed horizontal layers of PDE affects propagation of detonation. To investigate the effect of homogeneity, PDE filled with stratified mixture of hydrogen and air (with the same amount of hydrogen in total) was also solved and its results are illustrated on Fig. 9. Note that, the case is modelled with higher hydrogen concentration on upper layers and -13614.556 K/m temperature gradient on both top and bottom walls of the detonation tube to model the heat loss. For stratified case, the flame reaches at the exit at 12.5 ms while it reaches 13.25 ms for the premixed case. The most distinct difference between premixed and stratified cases is fluctuations on temperature and heat transfer. As seen on Figs. 6 and 9, inhomogeneity causes bigger oscillations and faster propagation. Also, heat loss and temperature are different on top and bottom walls because of different hydrogen concentrations on varied heights. The effect of inhomogeneity may also be seen by comparing flame position graphs on Figs. 6 and 9. The reason for more inclined flame front for stratified case is varied fuel concentrations along the tube; however, the shock becomes vertical during detonation.

The characterization of the wall cooling of PDE cycle under different tube constructions was tested for a longer PDE tube consuming premixed hydrogen-air mixture (with the same composition for the PDE documented in Fig. 6) under Neumann type boundary condition for temperature gradient. For this simulation, the length of the tube was doubled (10.8 m) with the same diameter and obstacle configuration. Since tube diameter has not changed, Nusselt number and consequently temperature gradient remained the same (-13614.556 K/m). The results are processed to acquire the wall heat transfer rate and temperature for both top and bottom wall as well as the flame position (Fig. 10). The results depicted in Fig. 6 and Fig. 10 shows that the duration of the single PDE cycle, regardless of the time passing for detonation wave to travel to the other end of the tube, is not enough for the PDE to cool down to the temperatures below 1800 K under natural convection. Morevoer, the location of the lowest temperature also does not depend on the tube length since the lowest temperature is observed approximately 2 m away from the ignition wall. The lowest temperature location remains constant, around the 6th notch, while the detonation shock is propagating. Furthermore, the lowest temperature is 60.69% of the gas temperature observed on the detonation shock in 5.4 m tube while it is 63.05% for 10.8 m tube. Since the temperature on detonation shock is constant due to Chapman-Jouget condition, the temperature profile along PDE is not significantly affected from the length of the tube.

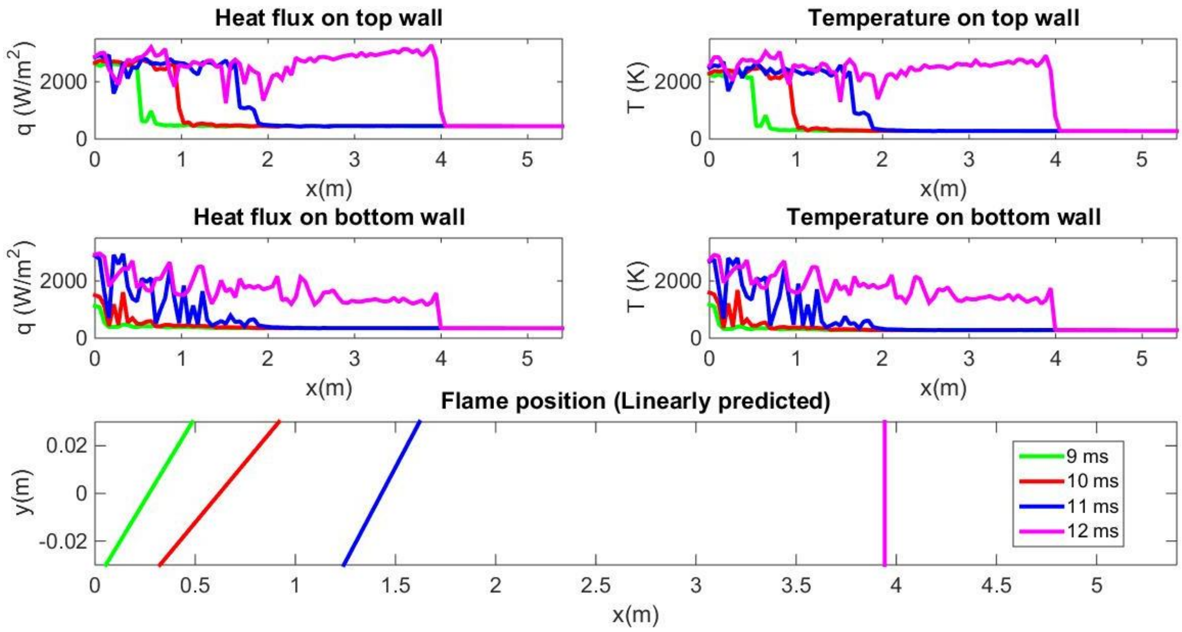

Figure 9: Heat flux and temperature variations along the tube for simulations of stratified hydrogen-air mixture with constant temperature gradient of -13614.556 K/m with predictions of flame positions

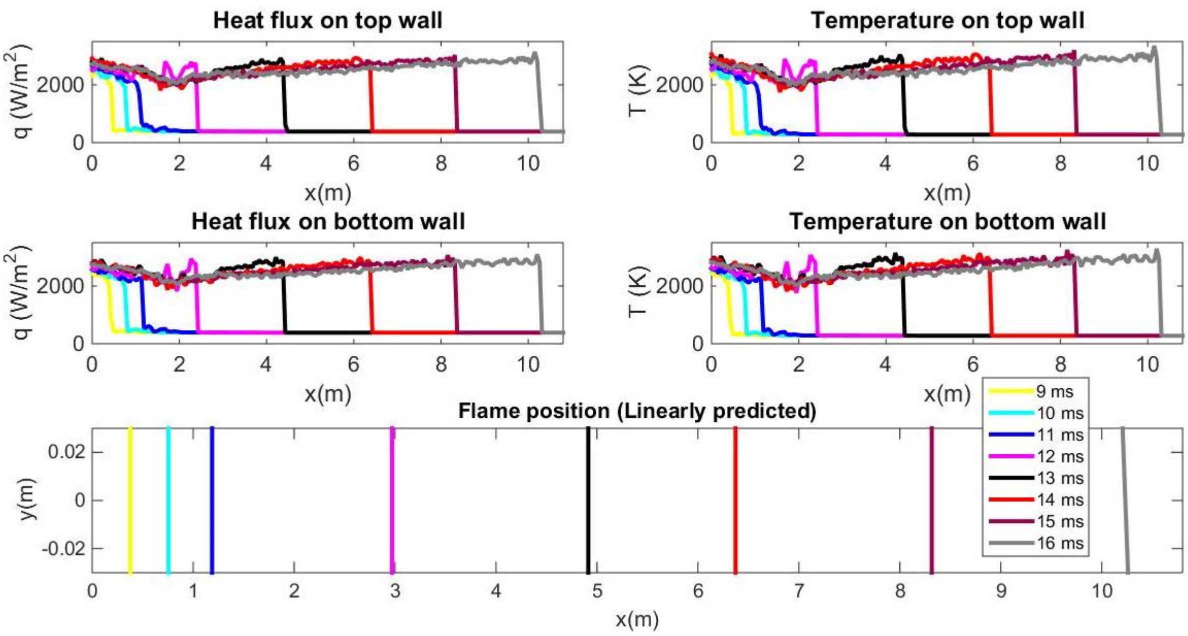

Figure 10: Heat flux and temperature variations along the tube having a length of 10.8 m for premixed simulations with constant temperature gradient of -13614.556 K/m with predictions of flame positions

4 CONCLUSIONS

As the temperatures behind the detonation shock enhances above 3000 K, the generated heat should be rejected through an appropriate cooling system to keep structural integrity of pulse and rotating detonation engines. Hence, heat transfer analyses on detonation engines gained importance. Owing to the deficiency of such analyses in the literature, the current study was pursued. In parallel to this purpose, an open source reactive flow solver for detonation is used for this study to estimate performances of pulse detonation engines under varied heat transfer conditions. To ensure the capability of the solver, it is validated and verified previous numerical and experimental studies on detonation in the literature. Subsequently, pulse detonation engine filled with homogeneous hydrogen-air mixture was simulated under adiabatic, isothermal and natural convection conditions. For natural convection, a constant temperature gradient was estimated by assuming above-mentioned conditions. Also, natural convection analyses were performed with various temperature gradient and an inhomogeneous fuel-air mixture. Consequently, flame propagates faster under Neumann type boundary condition than others. Increase in heat loss and stratification of the mixture accelerates flame propagation; however, the length of the tube does not affect this phenomena. Besides, a PDE period is inadequate for cooling of the engine walls even if a longer tube is used. However, these inferences stand as preliminary estimations for heat transfer analyses of detonation engines. For more accurate results, conjugate heat transfer may be considered for the analyses through more advanced numerical tools under development by the authors.

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