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Flame Quenching at Walls: A Source of Sound Generation

Abdulla Ghani¹ ·**Thierry Poinsot²**

Abstract This paper presents a numerical study of head on quenching (HOQ) (an extreme case of flame/wall interactions) as a source of sound generation, which in turn can trigger combustion instabilities and enhanced noise levels. High-fidelity numerical simulations are performed to investigate the impact of wall temperature, high chamber pressures and Lewis number of the fuel on the noise generation. It is demonstrated by theory and simulations that the underlying mechanism of sound generation is flame surface destruction (flame annihilation). Special emphasis is put on chemical modeling where simple and complex mechanisms were compared: it is shown that simple chemistry simulations overestimate the generated pressure peaks due to a too fast extinction of the heat release rate compared to the complex scheme. In contrast to the simple mechanism, the complex scheme accounts for minor and intermediate species production and destruction which slows down the extinction process and thus lead to a lower sound level. This effect has to be taken into account, especially in the context of Large Eddy Simulation (LES) of combustion instabilities and combustion noise where simple chemical descriptions are often employed.

Keywords Head on quenching · Noise generation · Chemistry modeling

1 Introduction

Modern combustion systems are not only underlying restrictions as low noise and pollutant emission but also compact combustion chamber design. High confinement ratios raise

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questions concerning interactions between flames and walls. Flame/wall interactions have already been investigated in many studies for heat transfer questions [1–5] but have not been yet considered as a source of direct combustion noise. The noise generation has a direct influence on the system stability since pressure fluctuations generate heat release modulations, which are known to trigger combustion instabilities [6, 7].

The most extreme case of flame/wall interaction is head on quenching (HOQ): the flame propagates at its laminar speed perpendicular to the wall and extinguishes at the wall. Most flame/wall interaction studies have investigated the distance of flame quenching, heat flux to the wall or the formation of hydrocarbons [8–10]. The generation of direct combustion noise due to HOQ has not been reported before although representing an important canonical test case. These transient combustion processes (flame ignition and extinction) need to be characterized in terms of sound generation as recently concluded by Ihme et al. [11]. Here, Direct Numerical Simulation (DNS) is used with the objective to identify flame quenching at walls as a source of noise. We will study HOQ for a wide range of relevant scenarios: various wall temperatures, combustion chamber pressures and fuel mixtures (represented by the Lewis number).

Chemistry modeling plays a significant role in the description of flame/wall interaction. Bruneaux et al. [8] showed that simple chemistry modeling using one reaction mechanism overestimates the wall heat fluxes during HOQ while a complex scheme with 52 reactions agreed better with experimental results. Westbrook et al. [10] investigated the formation of hydrocarbons employing detailed chemistry. In comparison to single-step chemistries, it was found that laminar flame speeds and flame thicknesses are not correctly reproduced by the simple schemes and lead to overestimated unburnt hydrocarbon contents. This study will highlight the effect of chemical kinetics modeling on the sound generation. For this, two chemistry mechanisms are utilized: a global scheme (called BFER) with 6 species and 2 reactions [12] which is here referred to as simple chemistry. These simple schemes are often employed in LES due to their low computational cost and the correct reproduction of laminar flame speeds and adiabatic flame temperatures over a wide range of equivalence ratios and pressures for gaseous [13, 14] and liquid fuels [15, 16]. The 'complex' scheme (called LU19) is an analytically reduced chemistry using 19 transported species and 11 species using Quasi Steady State approximation (QSSA) (Section 3). These mechanisms show significant differences in the generation of pressure fluctuations, something which has not been reported before. This study highlights the importance of correct chemistry modeling for future combustion instability and combustion noise studies. Besides, the flame/wall interactions are identified as a source of noise over a wide range of important applications.

The paper is organized as follows: modeling of sound generation by flame surface destruction is briefly recapitulated following the ideas of Talei et al. [17] (Section 2). Then, the numerical setup is presented in Section 3 followed by Section 4, validating the DNS against classical HOQ studies in terms of quenching distance and wall heat flux. The different scenarios of HOQ and the corresponding noise levels are presented in Section 5.

2 Modeling of Sound Generation by Premixed Flame Annihilation

The head on quenching process is characterized by flame quenching at the wall. Obviously, the perturbation of flame surface plays a significant role in the description of the sound gene ration [18–22]. Starting from the work of Lighthill [23] and its reformulation by Dowling (Chapter 13 in [24]), it was shown by Talei et al. [17] that far-field pressure fluctuations for one-dimensional, completely annihilated flames can be expressed by:

$$
p' = -\rho_u c_b \left(1 - \frac{T_u}{T_b} \right) s_L \tag{1}
$$

Interestingly, Eq. 1 depends only on the fresh gas density ρ_{μ} , the sound speed in the burnt gases c_b , the laminar flame speed s_L and the temperatures in the unburnt and burnt gases T_u and T_b , respectively. These variables can be easily obtained by one-dimensional solvers allowing a simple and fast determination of the pressure fluctuation. For Section 5, freely propagating, one-dimensional adiabatic flames were computed using CANTERA with the GRI-MECH 3.0 mechanism to feed Eq. 1.

3 Numerical Settings

The fully-compressible reacting multi-species Navier-Stokes equations are solved directly using the AVBP code. A two-step Taylor-Galerkin convection scheme provides fourth order accuracy in time and space Colin et al. [25] on structured meshes. It has excellent dispersion and dissipation properties and is characterized by its high spectral resolution. The outlet is treated as non-reflective using Navier-Stokes Characteristic Boundary Conditions (NSCBC) [26]. Top and bottom boundaries were set as symmetric so that the domain can be considered as 1D (Fig. 1). The wall temperature is varied in a range of temperatures from 300 to 900 K in 3 steps.

Chemistry for methane/air combustion is described by two different mechanisms: one is the analytical mechanism of [27] using 19 transported species and 11 QSSA species and 15 reactions (called complex chemistry LU19). QSSA allows a simplification of the chemical kinetic system by assuming that concentrations of intermediate species remain constant in time. As a result, the QSSA species concentrations are obtained by solving an algebraic equation instead of differential equations [28], reducing the number of transported species. The Prandtl number is constant ($Pr = 0.7$) whereas each species has its Schmidt number. This scheme has been validated against the GRI-MECH 3.0 mechanism using CANTERA in terms of flame speed, adiabatic flame temperature and major species (Fig. 2 right). The full GRI-MECH 3.0 scheme contains 53 species and 325 reactions and is referred to as the full chemistry. The simple mechanism (called BFER) is a globally reduced one, using 6 species and 2 reactions which do not capture the detailed physics of the complex chemistry [12]. Generally, simple chemistries are fitted to retrieve basic flame characteristics such as the laminar flame speed and the adiabatic flame temperature but fail in the correct reproduction

Fig. 1 Sketch of the one-dimensional domain

Fig. 2 Profiles of adiabatic flame temperature (divided by 100), flame speed, density and species mass fractions of a freely propagating stoichiometric flame. *Left*: Comparison between CANTERA with GRI-MECH 3.0 (lines) and DNS with simple chemistry BFER (symbols). *Right*: Comparison between CANTERA with GRI-MECH 3.0 (lines) and DNS with complex chemistry LU19 (symbols)

of radicals (Fig. 2 left). These mechanisms are preferred in the context of LES because of their low computational cost.

The one-dimensional domain is discretized with 6400 nodes in the axial direction $(L =$ 0.01 m) and 2 nodes in the transverse direction using cartesian elements. The mesh resolution has been chosen so that the generated pressure fluctuation is mesh independent. All simulations contain at least 40 points in the flame front. The far-field pressure fluctuations are recorded at $x/L = 0.9$ (probe P_{ff} in Fig. 1) for all cases.

Since HOQ is a transient process, the initialization has to be done carefully. First, the reacting flow is established in the 1D domain. Next, the steady flame is replaced 15 \times δ_f from the wall in a corrected velocity field: the laminar flame speed is subtracted to obtain a zero-velocity field in the fresh gas region. After a small transitional time, the flame propagates at its laminar flame speed s_L to the wall.

4 Validation of Laminar Head on Quenching

The accuracy of the DNS using the complex scheme LU19 is verified by comparison against DNS data from [9] for a laminar, one-dimensional methane-air flame burning at stoichiometry. As in the present study, [9] used two different wall temperatures T_w for HOQ (300) and 600 K). The authors of [9] have applied detailed chemical kinetics from [29] using 17 species and 52 reactions. First, the wall heat fluxes normalized by the flame power $q_f = \rho_u s_L c_p (T_b - T_u)$ are shown (Fig. 3 left). Time has been normalized by the flame time $t_f = \delta_f / s_L$. Good agreement is found for both wall temperatures. Next, the quenching distance is compared in terms of Peclet number $Pe = x/\delta_f$ that is the wall distance normalized by the thermal flame thickness for the undisturbed laminar flame. The definition of the thermal thickness is $\delta_f = \Delta T / max \left(\frac{\partial T}{\partial x} \right)$ $\frac{\partial T}{\partial x}$) [7]. The flame position is tracked by defining an iso-thermal contour of $T_{iso} = 1900$ K. The influence of the iso-thermal contour has been checked on the Peclet number Pe and only small deviations are found. Figure 3 right displays the Peclet numbers for the cases $T_w = 300$ K and $T_w = 600$ K which are reproducing the reference result with marginal differences as summarized in Table 1.

Fig. 3 *Left*: Normalized wall heat fluxes Φ_w . *Right*: Quenching distances expressed by Peclet numbers Pe

5 Laminar Head on Quenching: Direct Combustion Noise Generation

5.1 Wall temperature

In this section, the impact of equivalence ratio and wall temperature on the noise generation is examined. The time traces of pressure fluctuations for different equivalence ratios show that the highest sound levels are generated for stoichiometric flames (Fig. 4 left). At stoichiometric conditions, the smallest ratio of T_u/T_b and the highest laminar flame speed s_L is encountered (Eq. 1). The relation between pressure and heat release is evidenced by Fig. 4 right. The generated sound depends on the change of heat release rate, confirming theoretical and experimental observations [17, 19]. As already reported by Popp et al. [9], the heat release rate increases slightly in the presence of the wall before decreasing rapidly to zero. Figure 5 displays the effect of wall temperature on the generated sound. It is assumed, that fresh gases have the same temperature as the wall. For a flame burning at stoichiometry with incoming fresh gases at $T_u = 300$ K the sound generated is around 380 Pa. At stoichiometric conditions the highest pressure fluctuations are observed where laminar flame speed and adiabatic temperatures are also at maximum. Good agreement is found between DNS and the model of Eq. 1. Note that all pressure fluctuations are one-dimensional and propagate in the burnt gases at sound speed towards the outlet.

5.2 High pressure

Since realistic combustors operate at high pressures, it is interesting to see the effect of high pressure on the generation of noise. Pressure fluctuations are recorded for chamber

$T_w[K]$		Present study	Popp & Baum [9]
300	Φ_w	0.55	0.54
	Pe	0.78	0.70
600	Φ_w	0.63	0.68
	Pe	0.65	0.62

Table 1 Comparison of normalized wall heat flux Φ_w and Peclet number Pe of present simulations using the complex scheme LU19 with laminar HOQ DNS from [9]

Fig. 4 *Left*: Pressure fluctuation profiles for the different equivalent ratios ϕ recorded at probe P_{ff} . The wall temperature is $T_w = 300$ K for all equivalence ratios. *Right*: Evolution of pressure fluctuation, global heat release and the rate of change of the heat release for the stoichiometric flame using complex chemistry

pressures at 1, 5 and 10 bar (Fig. 6). As expected, the pressure fluctuations increase for higher pressures. The ratio of chamber pressure to pressure fluctuation during HOQ events is not linear: assuming linearity, pressure fluctuations for 10 bar would reach 3800 Pa. High pressures lead to lower pressure fluctuations which are correctly captured by the model of Eq. 1.

Global heat release rates \dot{Q}' during HOQ are plotted for 1, 5 and 10 bar in Fig. 7. Higher pressure generation levels are in correlation with the rate of change in the global heat release rate. For higher chamber pressures the gradient of \dot{Q}' becomes steeper and thus causes the higher noise level.

5.3 Lewis number

Fuel mixtures of CH_4/H_2 have become a possible path for future combustion since they are characterized by wider flammability limits, higher strain resistance and possibly lower CO concentrations [30]. Here, we will investigate its impact on HOQ noise generation. First,

Fig. 5 Effect of wall temperature on the generated sound. Pressure recorded at probe P_{ff} . Dashed lines depict the model in Eq. 1

Fig. 6 Effect of chamber pressure on the generated sound. *Dashed lines* depict the model in Eq. 1

following Dinkelacker et al. [31], an effective Lewis Le^* number can be determined by:

$$
\frac{1}{Le^*} = \frac{\chi_{CH_4}}{Le_{CH_4}} + \frac{\chi_{H_2}}{Le_{H_2}}
$$
 (2)

where χ_{CH_4} and χ_{H_2} denote the volumetric fractions of the fuel. Table 2 summarizes the effective Lewis numbers for the stoichiometric flame.

The sound generated for these mixtures is displayed in Fig. 8. The addition of H_2 does not affect the generated pressure fluctuations much. For mixtures up to 20% of H_2 addition, the fluctuations remain constant and increase for the stoichiometric case when 30% of H_2 is used, which is the highest Lewis number analyses here. The generated sound is correctly predicted by Eq. 1.

The quasi-constant sound level is confirmed by the temporal evolution of the global heat release. As already pointed out in the foregoing sections, the pressure levels depend on

Fig. 7 Effect of chamber pressure on the rate of change of the global heat release \dot{Q}'

Table 2 Effective Lewis numbers Le^* for different fuel mixtures of CH_4/H_2 following Eq. 2 of [31]

CH_4 content $[\%]$	100	90	80	
Le^* [-]	1.0345	1.2675	1.4934	1.7088

the rate of change of the heat release. Figure 9 indicates a similar rate of change of the global heat release resulting in similar pressure fluctuation levels. Note, that the effect of Lewis number on the production of sound due to flame-flame annihilation was examined by Jimenez et al. [32] for hydrogen/air flames. They concluded, that the Lewis number has an impact on the sound generation as shown here for the highest effective Lewis number $Le^* \approx$ 1.71. However, pure hydrogen/air flames behave differently to flames using hydrocarbon fuels and should be compared with caution.

5.4 Chemistry modeling

The effect of chemistry modeling is investigated in this section by first comparing the heat release profiles at $\phi = 1.0$ for three mechanisms: while GRI-MECH and LU19 chemistries agree very well in terms of shape and local values, the simple mechanism (BFER) overestimates the maximum local heat release by 25% for the stoichiometric case (Fig. 10 right). Additionally, reaction takes place later resulting in a marginal spatial shift. Nevertheless, all mechanisms agree well in laminar flame speed ($s_L = 0.379$ m/s for the complex mechanism and $s_L = 0.377$ m/s for the simple mechanism) since it is the integral of the heat release profile. Similar trends are observed for the lean case $\phi = 0.6$ but with a smaller error in the maximum local heat release (about 15%, not shown here).

Simulations are performed for a range of equivalent ratios and resulting pressure fluctuations are plotted for both chemistries (Fig. 11). In the leanest case ($\phi = 0.6$) the resulting pressure fluctuations are close to those predicted by the complex scheme. For the other cases, HOQ sound generation is overpredicted for the simple mechanism. Figure 10 right

Fig. 8 Effect of H² addition to the fuel mixture on the generated sound. *Dashed lines* depict the model in Eq. 1

Fig. 9 Effect of Lewis number on temporal evolution of the global heat release rate \dot{Q}'

Fig. 10 *Left*: Comparison of full, complex and simple chemistry for a one-dimensional, stoichiometric flame computed with CANTERA. *Right*: Evolution of pressure fluctuation and global heat release for the stoichiometric flame using simple chemistry

Fig. 11 Effect of chemistry modeling on the generated sound

Fig. 12 Comparison of normalized heat release profiles plotted before (*continuous lines*) and after (*dashed lines*) flame quenching. Profiles are normalized by maximum heat release from undisturbed flame obtained with full chemistry. *Left*: HOQ for complex chemistry. *Right*: HOQ for simple chemistry

displays the evolutions of pressure and global heat release for the stoichiometric case. Comparing to the results for the complex mechanism (Fig. 4 right), again a somehow linear behavior is observed between these quantities. The global heat release for the simple chemistry decreases rapidly in one flame time. The complex scheme indicated nearly three flame times until the heat release rate extinguishes. The maximum pressure fluctuation is around 450 Pa and is about 70 Pa higher than for the complex scheme. Interestingly, the rise of the global heat release in the vicinity of the wall is not captured by the simple chemistry. Since the wall heat fluxes between simple and complex schemes are very similar and the simple scheme reproduces the correct laminar flame speed, the difference on the generated sound can be explained by the local values of heat release. In particular, the 'pressure peak error' of about 15% can be mainly caused by the error in maximum heat release. Note that errors in the local heat release rate (in the order of 15%) for the flame at $\phi = 0.6$ leads to very similar pressure fluctuations for the simple and the complex chemistry (pressure peak error of about 2%). Figure 12 compares the heat release profiles at times before and after flame quenching (τ_q) for the complex (left) and simple (right) chemistry. The simple scheme features a complete extinction of the flame at $Pe = 0.67$ while the complex scheme indicates heat release rates still reaching 60% of the maximum value. These results are linked with

Fig. 13 Comparison of CO mass fraction profiles plotted before (*continuous lines*) and after (*dashed lines*) flame quenching. *Left*: HOQ for complex chemistry. *Right*: HOQ for simple chemistry

the profiles of the CO species (Fig. 13) where the simple mechanism (right) underpredicts the concentration compared to the complex scheme. The production of CO is an endothermic process and is described within the simple mechanism by the first of two reactions, not taking into account the production and destruction of minor and intermediate species. Due to this simplification, the heat release rates decrease faster in time and lead finally to higher pressure fluctuations.

6 Conclusion

The generation of pressure fluctuations has been investigated for laminar head on quenching. High-fidelity numerical simulations are performed over a range of equivalence ratios for various scenarios (wall temperature, Lewis number, chamber pressure) and exhibited high levels of direct combustion noise. It has also been shown that the theory developed by Talei et al. [17] for flame annihilation reproduces the numerical results and can easily be used for sound level estimations. This confirms that the mechanism of flame surface destruction is the leading mechanism for sound generation during HOQ. The sound level was found to depend on the rate of change of the global heat release rate. In a next step, chemistry modeling has been identified as a possible source of error in the generation of sound during HOQ: simple chemical kinetics feature higher pressure fluctuation amplitudes than complex schemes and theoretical results. While the error remains small for lean cases (about 2%), conditions near stoichiometry show pressure amplitude errors in the order of 15%. Since the chemical path of species production and destruction for the simple scheme is truncated, the temporal evolution (rate of change) of heat release rate is not correctly reproduced and can lead to erroneous pressure fluctuations.

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Compliance with Ethical Standards

Conflict of interests The authors declare that they have no conflict of interest.

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