Effects of Turbulence and Temperature Fluctuations on Syngas Auto-ignition

Pinaki Pal[1,*], Hong G. Im[2], Margaret S. Wooldridge[1, 3], Andrew B. Mansfield[1]

[1]*Department of Mechanical Engineering, University of Michigan, Ann Arbor, MI 48109, USA*
[2]*Clean Combustion Research Center, King Abdullah University of Science and Technology, Thuwal 23955-6900, Saudi Arabia*
[3]*Department of Aerospace Engineering, University of Michigan, Ann Arbor, MI 48109, USA*

Abstract

A theoretical scaling analysis has been conducted to identify non-dimensional criteria to distinguish between weak and strong auto-ignition regimes for a compositionally homogeneous reactant mixture, in the presence of turbulent velocity and temperature fluctuations. Based on the analysis, a turbulent ignition regime diagram was proposed that provides guidance on expected ignition behavior based on the thermo-chemical properties of the mixture and the flow/scalar field conditions. The diagram extends the Zeldovich's original theory by combining turbulent flow and scalar characteristics in terms of the characteristic Damköhler and Reynolds numbers of the system, thereby providing comprehensive understanding of the physical and chemical mechanisms controlling ignition characteristics. In this study, two-dimensional direct numerical simulations (DNS) are conducted for a lean syngas/air mixture at parametric conditions located at different regions on the regime diagram. Analysis of the simulation results is carried out in order to provide validation of the regime diagram.

Introduction

In view of limited oil and gas reserves and growing environmental concerns, there is a growing interest in the combustion of syngas derived from various conventional and alternative fuel sources for stationary power generation [1]. Syngas offers considerable opportunity for clean use of coal with potential for near-zero pollutant emissions, including greenhouse gases, when combined with carbon capture and sequestration methods. Due to the high flame temperatures and NO_x emissions associated with high hydrogen content fuels like syngas, a common combustion strategy is to operate in the lean premixed mode [2]. However, combustion of lean syngas mixtures faces challenges such as flame instability, blowout and flashback, and autoignition [3]. In particular, as for the autoignition characteristics of syngas mixtures at typical gas turbine operating conditions (20 bar and above), a compilation of recent experimental and computational studies reported in Petersen et al. [4], showed significant discrepancies between measurements and predictions based on homogeneous adiabatic calculations with detailed chemistry, especially at low temperature (< 1000 K) conditions.

Subsequently, a number of studies were carried out to identify the main cause of such discrepancies. Experimental studies using rapid compression facilities (RCF) indicated that the discrepancies might be attributed to the non-uniform temperature and mixture fields arising from wall heat loss and flow vortex generation [5, 6]. A recent study by Mansfield and Wooldridge [7] conducted imaging experiments of syngas autoignition within an RCF, and reported an early phase front propagation, called the "weak" ignition regime, at high-pressure low-temperature conditions. They also confirmed that the ignition delay in such conditions was significantly shorter, by several orders of magnitude, than the corresponding homogeneous ignition delay prediction. They further provided a pressure-temperature diagram to distinguish the weak versus strong ignition regimes. Moreover, several criteria to identify the transition between weak and strong ignition regimes were evaluated, including the criterion originally developed by Zeldovich [8]. The modified formula proposed by Sankaran et al. [9] which is based on the ignition delay time sensitivity, ($d\tau_{ig}/dT$), was found to reproduce the experimentally observed trends very well. Ihme [10] and Wu and Ihme [11] used simple one- and two-dimensional models to demonstrate that the presence of turbulent fluctuations could lead to significant ignition advancement. These recent series of findings have led to a consensus in the community that scalar non-uniformities are the likeliest causes of the discrepancies between zero-dimensional modeling and the homogeneous autoignition delay time data [12].

The importance of the ignition delay time sensitivity has also been recognized in earlier studies of shock tubes [13, 14, 15], where the $d\tau_{ig}/dT$ iso-lines clearly distinguish the "weak" and "strong" ignition behavior, which has led to the well-known Zeldovich's theory and criteria [8]. The issue of premature ignition by local hot spots has also been revisited in recent shock tube experiments [16, 17].

Considering the established significance of thermal and compositional non-uniformities on auto-ignition characteristics, the main objective of the present work is to extend the understanding to develop rational criteria to predict the conditions associated with the different auto-ignition regimes for general turbulent mixing conditions. To this end, the diagrams shown in the experimental studies [7, 13], which focused on a regime criterion solely based on chemical characteristics of the ignition sensitivity, are not sufficient; such a criterion lacks other potentially important information about the level of scalar fluctuations which can trigger front initiation and propagation. To elaborate further, the

* Corresponding author: pinaki@umich.edu

Zeldovich criterion [8], which was further refined and demonstrated by Sankaran et al. [9], defines the non-dimensional number, *Sa*, as

$$\mathrm{Sa} = \beta \frac{S_L}{S_{sp}} = \beta S_L \left| \frac{d\tau_{ig}}{dT} \nabla T \right|, \quad \beta = 0.5 \tag{1}$$

where S_L is the laminar flame speed, $S_{sp} = [(d\tau_{ig}/dT).\ \nabla T]^{-1}$ is the spontaneous ignition front propagation velocity, and τ_{ig} is the ignition delay time for the homogeneous mixture at the average or bulk temperature. The factor $\beta < 1$ reflects the fact that sufficiently rapid spontaneous front propagation is needed in order to ensure strong ignition. Equation (1) is referred to as the Zeldovich-Sankaran criterion in the remainder of the text. The ignition regime criterion predicts weak ignition if $Sa > 1$, as the deflagration front dominates the ignition behavior, and strong ignition if $Sa < 1$, in which case the spontaneous ignition process dominates [18]. Therefore, it is evident that the ignition regimes are determined by the ignition delay sensitivity ($d\tau_{ig}/dT$) and the temperature distribution (∇T), which is determined by the scalar field distribution. In RCF and shock tube auto-ignition studies of syngas, thermal gradients on the order of 5 K/mm are expected [7]. However, systematic studies of the effects of flow and scalar field fluctuations are needed to expand the predictive regime diagram to realistic combustion devices where much larger temperature gradients can be expected.

Recently, in the work by Im et al. [19], theoretical scaling analysis was used to extend the regime criterion in terms of non-dimensional parameters that are commonly used in characterizing turbulent combustion systems such as Damkohler number and Reynolds number. In the following, the development of the regime diagram is briefly described first. The relevant physical quantities are identified and simplifying assumptions are introduced. Subsequent derivations of relevant scaling relations then lead to the ignition regime criterion with turbulent combustion parameters. Finally, 2D DNS are performed at parametric conditions located at different regions on the regime diagram. The corresponding auto-ignition characteristics are analyzed to assess the validity of the regime diagram.

Problem Definition and Assumptions

Figure 1 shows a schematic of the problem under consideration, and important characteristic quantities. The length scales include the chamber length, *L*, the integral length scale, *l*, the Taylor microscale, λ, and the laminar flame thickness, δ_f. In general, *l* is considered a fraction of *L*, and λ/l scales with the turbulent Reynolds number as will be discussed later. The laminar flame speed, S_L, and the root-mean-square (RMS) turbulent velocity fluctuation at the integral scale, *u'*, are important velocity scales that will be compared to the other relevant velocities to be determined later. For the scaling analysis, the following simplified assumptions are made:

1. Weak ignition is primarily caused by front propagation originating from small scale local temperature fluctuations, such as local hot spots and the effects of large scale bulk temperature gradients, such as gradients caused by wall heat losses, are not considered. This is based on the experimental observations that early stage ignition kernels are often generated in the interior of the combustor, not necessarily near the wall region.
2. The mixture composition is homogeneous and only the temperature fluctuations are considered. The scales of initial temperature and velocity fluctuations are comparable and correlated.
3. The Prandtl number of the mixture is unity, so that combined with assumption 2, the dissipation of temperature fluctuations is mainly driven by turbulent flows. This implies that the time and length scales for turbulent velocity and scalar fields are the same (i.e. the Batchelor scale is identical to the Kolmogorov scale).

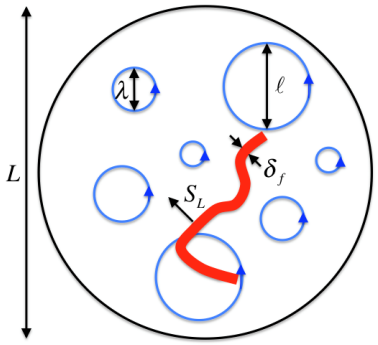

Figure 1: A schematic of combustion chamber with various physical length scales.

To characterize the turbulent velocity and scalar fields, key non-dimensional parameters are introduced. Following the framework of Liñán and Williams [20], a rational way to characterize turbulent combustion systems is to use the turbulent Reynolds number, which represents the intensity of turbulence, and the characteristic turbulent Damköhler number, which represents the intensity of chemical reaction. For the integral scale eddy whose velocity, length, and time scales are characterized by *u'*, *l*, and $\tau_l = l/u'$, respectively, the turbulent Reynolds number is defined as:

$$\mathrm{Re}_l = \frac{u'l}{\nu} \tag{2}$$

where υ is the kinematic viscosity of the bulk mixture gas. As for the measure of the chemical intensity, two ignition Damköhler numbers are defined as:

$$\mathrm{Da}_l = \frac{\tau_l}{\tau_{ig}} \tag{3}$$

which is referred to as the *integral* Damköhler number, and

$$\mathrm{Da}_\lambda = \frac{\tau_{\lambda_T}}{\tau_{ig,10\%}} \tag{4}$$

which is referred to as the *mixing* Damköhler number, In Equations (3) and (4), τ_{ig} is the ignition delay time for the homogeneous reactant mixture at the bulk temperature, and $\tau_{ig,10\%}$ is the lowest 10% ignition delay of the initial mixture, representing the shortest ignition time scale of the initial mixture. $\tau_{ig,10\%}$ is defined as the homogeneous ignition delay at temperature T_{min} + 0.9(T_{max}-T_{min}), where T_{min} and T_{max} are the minimum and maximum initial temperatures in the domain. τ_{λ_T} is the mixing time scale associated with the Taylor microscale for the temperature field, λ_T, which is determined in terms of the RMS temperature fluctuation, T', and the mean temperature dissipation rate, $2\alpha\widetilde{|\nabla T|^2}$, and is written as

$$\tau_{\lambda_T} = \frac{T'^2}{\alpha\widetilde{|\nabla T|^2}},\ \lambda_T^2 = \frac{T'^2}{\widetilde{|\nabla T|^2}} \tag{5}$$

in analogy with those of the Taylor microscale for turbulent velocities

$$\tau_\lambda = \frac{u'^2}{\nu\widetilde{|\partial u_j/\partial x_j|^2}},\ \lambda^2 = \frac{u'^2}{\widetilde{|\partial u_j/\partial x_j|^2}} \tag{6}$$

Based on assumption 3, it follows that the mixing time and length scales for temperature are interchangeable with those for turbulent velocities, such that

$$\tau_{\lambda_T} = \tau_\lambda,\ \lambda_T = \lambda \tag{7}$$

The Scaling Analysis

The main objective of the scaling analysis is to derive an expression for the Zeldovich-Sankaran criterion in terms of the characteristic Reynolds and Damköhler numbers. From the theory of homogeneous turbulence [21], the scaling relation yields:

$$\frac{\lambda}{l} = \mathrm{Re}_l^{-1/2},\ \frac{\tau_\lambda}{\tau_l} = \frac{\lambda/u'_\lambda}{l/u'} = \frac{\lambda}{l}\frac{u'_\lambda}{u'} = \left(\frac{\lambda}{l}\right)^{2/3} = \mathrm{Re}_l^{-1/3} \tag{8}$$

It follows that

$$\mathrm{Da}_\lambda = \frac{\tau_{\lambda_T}}{\tau_{\mathrm{ig},10\%}} = \frac{\tau_\lambda}{\tau_{\mathrm{ig},10\%}} = \mathrm{Da}_l\,\mathrm{Re}_l^{-1/3}\frac{\tau_{ig}}{\tau_{ig,10\%}} \tag{9}$$

The significance of Da_λ is that it is the ratio of the characteristic temperature dissipation time to the characteristic ignition delay time at the bulk mean temperature. Therefore, if, $Da_\lambda < 1$, the temperature fluctuations are dissipated before ignition occurs, thus it is unlikely to exhibit the weak ignition behavior triggered by reaction front propagation.

Next, the Zeldovich-Sankaran criterion, Eq. (1), is extended to turbulent conditions. To this end, it is assumed that the occurrence of the hot-spot-induced pre-ignition is proportional to the statistical mean temperature gradient, such that

$$\mathrm{Sa} \approx \beta S_L\left|\frac{d\tau_{ig}}{dT}\right|\widetilde{|\nabla T|} \tag{10}$$

where it is estimated that

$$\widetilde{|\nabla T|} \approx \frac{T'}{\lambda_T} \approx \frac{T'}{\lambda} = \frac{T'}{l\,\mathrm{Re}_l^{-1/2}} \tag{11}$$

Therefore, Equation (10) is written as

$$\mathrm{Sa} \approx \beta S_L\left|\frac{d\tau_{ig}}{dT}\right|\frac{T'}{l}\mathrm{Re}_l^{1/2} = \beta\left(\frac{S_L}{\delta_f}\right)\left(\frac{\delta_f}{l}\right)T'\left|\frac{d\tau_{ig}}{dT}\right|\mathrm{Re}_l^{1/2} \tag{12}$$

which includes the length scale ratio, δ_f/l where δ_f is the characteristic flame thickness. Following Liñán and Williams [20],

$$\frac{\delta_f}{l} = \mathrm{Re}_l^{-1/2}\,\mathrm{Da}_{l,f}^{-1/2} = \mathrm{Re}_l^{-1/2}\left(\frac{\tau_l}{\tau_f}\right)^{-1/2} = \mathrm{Re}_l^{-1/2}\,\mathrm{Da}_l^{-1/2}\left(\frac{\tau_{ig}}{\tau_f}\right)^{-1/2} \tag{13}$$

Combining Equations (12) and (13), the turbulent ignition regime criterion can be written as:

$$\mathrm{Sa} = K\mathrm{Da}_l^{-1/2},\ K = \beta\left(\frac{T'}{(\tau_f\tau_{ig})^{1/2}}\right)\left|\frac{d\tau_{ig}}{dT}\right| \tag{14}$$

where K is referred to as the normalized thermal ignition sensitivity. In comparison with the laminar version in Eq. (1), $S_L|\nabla T|$ has now been expressed as $\left(T'/\tau^*\right)\mathrm{Da}_l^{-1/2}$ through the dimensional scaling, with a *reduced* time scale, $\tau^* = (\tau_f\,\tau_{ig})^{1/2}$. The final ignition regime criterion becomes:

$$\begin{cases}\mathrm{Da}_l < K^2: \text{ weak ignition}\\ \mathrm{Da}_l > K^2: \text{ strong ignition}\end{cases} \tag{15}$$

As discussed with Eq. (9), an additional condition of $Da_\lambda > 1$ needs to be satisfied to ensure weak ignition, since otherwise the temperature fluctuations are likely to dissipate away before the front forms. Finally, $Da_l < 1$ would ensure an even stronger mixing scenario, since eddies at all scales would have time scales shorter than the ignition delay time, such that all temperature fluctuations would be dissipated and only strong ignition would be expected.

The Regime Diagram

Compiling the above scaling analysis leads to the regime diagram as shown in Fig. 2 [19]. The auto-ignition processes in nearly homogeneous mixtures with turbulent fluctuations are characterized in the *Da-Re* space, to represent the relative chemical and turbulence intensities determined by the chemistry, thermodynamics and turbulent transport in the gas mixture. It is shown that the primary factor to determine the ignition regime is Da_l, while Re_l modifies the conditions further.

First, for a given Re_l, the Zeldovich-Sankaran criterion indicates that the weak/mixed ignition regime is possible for $1 < Da_l < K^2$. If, $Da_l > K^2$ then the reactant mixture is either too reactive (small τ_{ig}) or the mixture ignition characteristics are not sensitive to the temperature fluctuations (small $d\tau_{ig}/dT$), such that the entire mixture ignites almost at the same time despite some level of temperature fluctuations. This is referred to as the *reaction-dominant* strong ignition regime. On the other hand, if $Da_\lambda < 1$, then the turbulent mixing is rapid (small τ_l) such that the temperature fluctuations are dissipated before the local ignition takes place. In contrast to the $Da_l > K^2$ case, this is referred to as the *mixing-dominant* strong ignition regime. The K parameter includes the ignition delay sensitivity, which is more than just a time scale characterization, and depends strongly on the auto-ignition chemistry of the specific fuel.

Between the limits $1 < Da_l < K^2$, weak ignition is possible; however, the mixing Damköhler number, Da_λ, provides an additional criterion for this region of the regime diagram. Considering that the dynamics of turbulent mixing and dissipation is commonly characterized by the Taylor scale, λ, a proper criterion to determine the mixing-dominant strong ignition would be the ratio of the Taylor mixing time, τ_λ, to the ignition time, τ_{ig}. Therefore, the $Da_\lambda = 1$ condition serves as a more refined criterion within the limits of $1 < Da_l < K^2$ to further identify the boundary between the weak and strong ignition regimes. Considering Eq. (9), this line appears on the regime diagram with a slope of 1/3, indicating that the occurrence of weak ignition phenomena will become less likely as the turbulent Reynolds number of the mixture increases. Still, the conditions between $Da_\lambda < 1$ and $Da_l > K^2$ are a "grey" zone, in that some mixed mode ignition in which a mild level of front propagation followed by a strong ignition may occur. This is denoted as the *mixing-dominant mixed/strong* ignition regime.

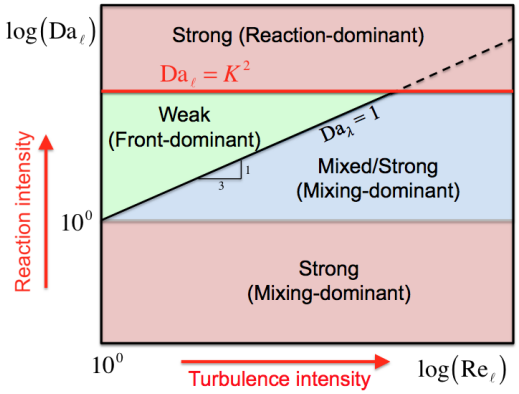

Figure 2: Regime diagram for strong and weak ignition for nearly homogeneous reactant mixture with temperature fluctuations and turbulence [19].

The regime diagram serves as a qualitative guidance to the expected ignition behavior. The appropriate autoignition regime can be identified given the knowledge of the thermo-chemical properties of the mixture (e.g. pressure, temperature, reaction chemistry, etc.), and the characteristic turbulent flow parameters (e.g. Reynolds number, turbulence/scalar fluctuation intensity, etc.). If the initial condition of the mixture falls into the weak ignition or mixed/strong ignition regimes, then large discrepancies in the ignition delay prediction against the measured data (especially when the measured state conditions are bulk or averaged values) can be expected and must be treated carefully.

Validation: 2D DNS of Syngas Auto-ignition

Two-dimensional DNS of auto-ignition of a turbulent syngas-air mixture in a closed volume in the presence of initially homogeneous composition and inhomogeneous temperature fields are performed to validate the regime diagram. For the present study, the DNS code named S3D [22, 23] is used to solve the full compressible Navier-Stokes, species continuity and total energy equations for a reactive gas mixture using a fourth-order explicit Runge-Kutta method [24] for time integration and an eighth-order central differencing scheme for spatial discretization with a tenth-order filter to remove any spurious high-frequency fluctuations in the solution [25]. A detailed syngas/air chemical kinetic mechanism with 12 species and 33 chemical reactions [26] is employed. The mechanism was linked with CHEMKIN and TRANSPORT libraries [27, 28] for computing reaction rates and thermodynamic and mixture-averaged transport properties. Periodic boundary conditions were imposed in all directions to represent the constant volume ignition process.

The initial conditions include a mean temperature of 1100 K, mean syngas/air equivalence ratio of 0.5 (H_2: CO = 0.7:1), diluted with twice the amount of N_2 present in air and a uniform pressure of 20 atm, yielding a homogeneous ignition delay time (τ_{ig}) of 2 ms, laminar flame thickness of 16 μm, and laminar flame speed (S_L) of 67.7 cm/s. The initial mean flow velocities are set to zero. Turbulent velocity fluctuations are superimposed on the stationary mean velocity field based on an isotropic kinetic energy spectrum function [29]. A random temperature field, similar to a turbulent kinetic energy spectrum, is also superimposed on the mean temperature field. The temperature field is uncorrelated with the turbulent velocity field.

The computational domain is a square box of 6.4 × 6.4 mm^2, which is discretized with 640 grid points, resulting in a grid resolution of 10 μm. For the parametric conditions considered herein, the most energetic turbulent length scale, l, is set at 2.5 mm. However, the RMS velocity fluctuation (u') is varied, yielding different integral time scales. A constant RMS temperature fluctuation of 20 K is prescribed. This leads to $K^2 = 4.5$ and $\tau_{ig,10\%} = 0.746$ ms. For the temperature field also, the most energetic length scale is set to 2.5 mm. Figure 3 shows the initial temperature field which is same for all three cases. Details of the parametric cases and the corresponding regime diagram parameters are listed in Table 1. Based on the discussion in the previous section, it is expected that case A and case C will show strong ignition and case B will exhibit weak ignition characteristics.

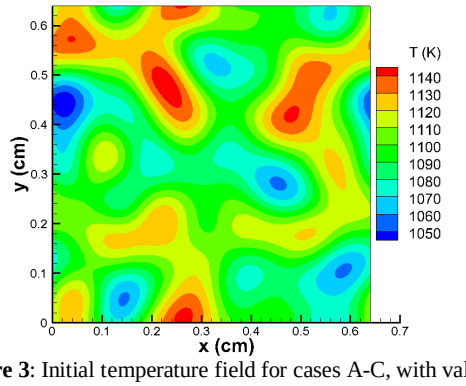

Figure 3: Initial temperature field for cases A-C, with values ranging from 1043 K (blue) to 1147 K (red).

Table 1. Physical and regime diagram parameters of the DNS cases

Case	l (mm)	u' (m/s)	τ_l (ms)	Da_l	Re_l	Da_λ
A	2.5	0.2	12.5	6.08	68.5	4.1
B	2.5	1.25	2.0	1.00	428	0.4
C	2.5	5	0.5	0.25	1712	0.06

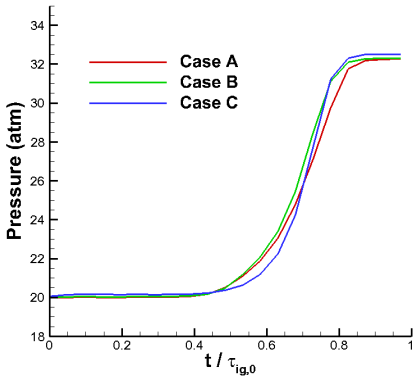

Figure 4: Pressure traces for cases A-C.

Figure 4 shows the evolution of pressure with time normalized to the ignition delay time for the homogeneous mixture for the three parametric cases. It is evident that the pressure rise occurs slightly earlier for case B, which can be attributed to the compression heating of end gas by the propagating ignition fronts. This suggests that weak ignition is encountered in case B and the strong ignition regime is prevalent in cases A and C. This observation agrees with the apriori prediction from the regime diagram and provides some validation for the theory. More detailed analysis of the simulation results to characterize the auto-ignition behavior using the computational singular perturbation (CSP) [30] methodology is currently underway.

Conclusions

A regime diagram to predict weak and strong ignition regimes for a compositionally homogeneous reactant mixture with turbulence and temperature fluctuations is reviewed [19]. The diagram provides guidance on expected ignition behavior based on the thermo-chemical properties of the mixture and the flow/scalar field conditions. The analysis is an extension of the previous studies [8, 9] and incorporates the turbulent flow and scalar characteristics in terms of the characteristic Damköhler and Reynolds numbers of the system. The theoretical framework provides a more unified and comprehensive understanding of the physical and chemical mechanisms controlling ignition characteristics compared to the existing experimental maps, which are solely based on the ignition delay sensitivity.

It is recognized that the Zeldovich-Sankaran criterion includes the ignition delay sensitivity, ($d\tau_{ig}/dT$), as a critical factor. Therefore, the traditional regime characterization based on the Damköhler and Reynolds numbers (such as those for turbulent premixed combustion regimes), based on time scales only, is not sufficient to describe the transition between weak and strong ignition phenomena, and the introduction to the sensitivity parameter, K, is necessary. The regime diagram further shows how turbulence characteristics would affect the Zeldovich-Sankaran criterion based on the Kolmogorov theory of homogeneous isotropic turbulence.

The Zeldovich-Sankaran criterion indicates there is a region where mixtures with high-K values or high thermal sensitivity are more susceptible to weak ignition. 2D DNS studies of syngas-air auto-ignition are performed at different parametric conditions belonging to different regions on the regime diagram. Preliminary analysis of the pressure time histories provide an indication of the effects of turbulence and temperature distributions compared with homogeneous conditions.

Acknowledgments

The authors acknowledge the financial support of U.S. DOE via NETL award number DE-FE0007465 and King Abdullah University of Science and Technology. The authors thank Dr. Paul G. Arias of KAUST for the contributions in the development of simulations.

References

[1] F.L. Dryer, M.S. Wooldridge, E.L. Peterson, V.G. McDonell, H.G. Im, US DOE UTSR meeting (2014).
[2] G.A. Richards, M.M. McMillian, R.S. Gemmen, W.A. Rogers, S.R. Cully, Prog. Energy Combust. 27(2) (2000) 141–169.
[3] T. Lieuwen, V. McDonell, D. Santavicca, T. SattelMayer, Combust. Sci. Technol. 180(6) (2008) 1169–1192.
[4] E.L. Petersen, D.M. Kalitan, A.B. Barrett, S.C. Reehal, J.D. Mertens, D.J. Beerer, R.L. Hack, V.G. McDonell , Combust. Flame 149 (2007) 244–247.
[5] G. Mittal, C.J. Sung, R.A. Yetter, Int. J. Chem. Kinet. 38 (2006) 516-529.
[6] S.M. Walton, X. He, B.T. Zigler, M.S. Wooldridge, Proc. Combust. Inst. 31 (2007) 3147–3154.
[7] A.B. Mansfield, M.S. Wooldridge, M.S. 2014. Combust. Flame 161 (9) (2014) 2242-2251.
[8] Y.B. Zeldovich, Combust. Flame 39 (1980) 211–214.
[9] R. Sankaran, H.G. Im, E.R. Hawkes, J.H. Chen, Proc. Combust. Inst. 30 (2005) 875–882.
[10] M. Ihme, Combust. Flame 159 (2012) 1592-1604.
[11] H. Wu, M. Ihme, Combust. Flame 161 (2014) 2317-2326.
[12] US DOE, Hydrogen from Coal Program - Research, Development and Demonstration Plan (2009).

[13] J.W. Meyer, A.K. Oppenheim, Proc. Combust. Inst. 13 (1971) 1153–1164.
[14] E.S. Oran, T.R. Young, J.P. Boris, A. Cohen, Combust. Flame 48 (1982) 135-148.
[15] E.S. Oran, J.P. Borris, Combust. Flame 48 (1982) 149-161.
[16] Y. Uygun, S. Ishihara, H. Olivier, Combust. Flame 161 (2014) 2519-2530.
[17] T. Javed, E. Es-sebbar, M. Jaasim, J. Badra, H.G. Im, A. Farooq, 7th European Combustion Meeting, Budapest, Hungary, March 30 – April 2 (2015).
[18] P. Pal, A.B. Mansfield, M.S. Wooldridge, H.G. Im, 12th Int. Conf. Combust. and Energy Util. (2014).
[19] H.G. Im, P. Pal, M.S. Wooldridge, A.B. Mansfield, Combust. Sci. Technol. (under review).
[20] A. Linan, F.A. Williams, Oxford University Press (1993).
[21] H. Tennekes, J.L. Lumley, MIT press (1972), Cambridge, MA.
[22] J.H. Chen, A. Choudhary, B. de Supinski, M. DeVries, E.R. Hawkes, S. Klasky, W.K. Liao, K.L. Ma, J. Mellor-Crummey, N. Podhorszki, R. Sankaran, S. Shende, C.S. Yoo, Comput. Sci. Disc. 2 (2009) 015001.
[23] J.H. Chen, Proc. Combust. Inst. 33 (2011) 99-123.
[24] C.A. Kennedy, M.H. Carpenter, Appl. Numer. Math. 14 (1994) 397-433.
[25] C.A. Kennedy, M.H. Carpenter, R.M. Lewis, Appl. Numer. Math. 35 (2000) 117-219.
[26] J. Li, Z. Zhao, A. Kazakov, M. Chaos, F.L. Dryer, J.J. Scire, Int. J. Chem. Kinet. 39 (2007) 109–136.
[27] R.J. Kee, F.M. Rupley, E. Meeks, J.A. Miller, CHEMKIN-III: a fortran chemical kinetic package for the analysis of gas-phase chemical and plasma kinetics, Tech. Rep. SAND96-8216, Sandia National Laboratories, 1996.
[28] R.J. Kee, G. Dixon-Lewis, J. Warnatz, M.E. Coltrin, J.A. Miller, a fortran computer code package for the evaluation of gas-phase multicomponent transport properties, Tech. Rep. SAND86-8246, Sandia National Laboratories, 1986.
[29] T. Passot, A. Pouquet, J. Fluid. Mech. 118 (1987) 441-466.
[30] S. Gupta, H.G. Im, M. Valorani, Proc. Combust. Inst. 34 (2013) 1125–1133.