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MODELING OF FLAMELESS COMBUSTION OF HYDROGEN IN COMBUSTOR OF A GAS TURBINE

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ABSTRACT: Flameless combustion has attracted significant interest in recent years due to its high thermal efficiency, low pollutant emissions and homogenised temperature in the combustion chamber. Moreover, it is convenient to replace common combustion systems by flameless combustion at relatively low cost. It is thus predicted that flameless combustion will be used widely in the future. In this paper flameless combustion is modelled by use of a network of ideal reactors such as perfectly stirred and plug flow reactors. A flameless combustion chamber for a gas turbine is modelled by this approach. The proposed combustion chamber can be generalised for any given gas turbine. The fuel that is utilized is assumed to be hydrogen. High adiabatic flame temperature and carbon-free pollutant emissions are some of hydrogen advantages. It is shown that flameless combustion suppresses thermal NO_x formation. Moreover, the effects of main parameters on flameless combustion are investigated.

Keywords: Flameless combustion, hydrogen, network of reactors, plug flow reactor, perfectly stirred reactor.

NOMENCLATURE

c_p	Specific heat (kJ/kg.K)	P	Perimeter (m)
h	Enthalpy (kJ/kg)	$\dot{Q}$	Heat rate (kW)
$\dot{m}$	Mass flow rate (kg/s)	R_u	Universal gas constant (kJ/mol.K)
t_R	Residence time (s)	T	Temperature (K)
v_x	Velocity (m/s)	V	Volume (m^3)
A	Cross sectional area (m^2)	Y	Mass fraction
MW	Molar mass (kg/mol)	ρ	Mass density (kg/m^3)
N	Number of species	ω_i	Production rate ($mol/m^3.s$)

INTORDUCTION

Flameless Combustion: Reducing pollutant emissions in combustion products has been one of the most important issues investigated in combustion community. One major pollutant is considered to be nitric oxides. Many methods have been presented to reduce NO_x emissions, namely, exhaust gas recirculation (EGR), air staging and the use of low NO_x emission burners. Using some of these methods will reduce concentration of oxygen at high-temperature regions. Combustion efficiency is another essential parameter in combustion processes. An appropriate method for raising efficiency is the preheating of inlet air with combustion products. However, these methods cause a high temperature in combustion chamber and therefore may lead to an enormous increase in NO_x emissions.
However, more recently many works have been performed to improve combustion efficiency by preheating the inlet air, and at the same time controlling NOx emissions. One such method combines EGR with inlet air preheating. This technique is known as flameless combustion. The combustion air is preheated and then injected to the combustion chamber, where it is mixed with the re-circulated portion of the combustion products. Therefore, the oxygen concentration will reduce in the vicinity of the reaction zone. This technique also lowers the peak temperature in the combustion chamber and leads to a more uniform temperature distribution. A lower peak temperature will relax the material requirements for the combustion chamber enclosure. In other words, it will not be necessary to select the material of the combustion chamber enclosure with high temperature residence.
The benefits of flameless combustion can be summarized as follows:
1- High thermal efficiency
2- Low fuel consumption
3- Low pollutant emission
4- Smooth temperature in combustion chamber
5- Low noise [*e.g.,* Wunning 1997]

Hydrogen Fuel: Fossil fuels that are used notably today cause high pollutant emissions. These pollutants include CO, NO_x, greenhouse gases and unburned hydrocarbons. On the other hand, the sources of these fuels are restricted and will be finished in the future. Therefore, these fuels should be replaced with suitable alternative energy sources. The energy carrier of the future should possess certain characteristics that include being free of carbon and nitrogen elements. Hydrogen is an appropriate option for this purpose with a special molecular structure that is free from both carbon and nitrogen leading to lower pollutant emission compared to fossil fuels. The only pollutant formed in hydrogen combustion in air is NO_x.
Although hydrogen is a suitable alternative to fossils fuels, it is not found in the nature as a pure substance in abundant quantities. Rather, some chemical components such as water or hydrocarbons include hydrogen in their molecules. Hydrogen can be used as an energy carrier in the future, when produced from renewable sources of energy. Today, enormous amounts of hydrogen are produced in petrochemical industry from natural gas by steam reforming technique. However, hydrogen production from fossil fuels leads to carbon emissions. Therefore, hydrogen should be produced from other methods such as electrolysis of water. The required electrical power should not be provided by power plants running on fossil fuels. This energy can come from the wind power, solar energy or other renewables. For instance a part of

the electrical power produced from solar energy is used to electrolyze water. The main product of hydrogen combustion is water; therefore water will be recycled in these processes.

Previous Studies: In recent years a variety of approaches have been suggested to increase combustion efficiency and reduce pollutant emissions. For instance, flameless combustion method was suggested by Wunning [1997]. In their work the theory of flameless combustion was formulated and practical methods of its measurement were introduced. Most investigations on flameless combustion have been experimental. It has been illustrated that in order to achieve flameless combustion the inlet air should be preheated up to self ignition temperature of the air-fuel mixture. Flameless combustion of fossil and non-fossil fuels have been investigated. For instance, Yu [2010] investigated flameless combustion of hydrogen-methane fuel mixtures and their pollution emissions. In this work, the combustion chamber was modelled using a network of ideal reactors consisting of three ideal reactors (PSR). Mancini [2007] calculated the efficiency of flameless combustion of natural gas using a turbulent flow model. Furthermore, to provide the background detailed chemistry the flow jet was subdivided into a network of perfectly stirred reactors (PSR). Swithenbank et al. [1973] modelled flame combustion in a gas turbine combustor with a network of ideal reactors such as PSR and PFR. It was illustrated that by increasing the hydrogen percentage in the fuel, CO production will decrease considerably but NO production will be unaffected. Generally, NO production in flameless combustion is small. Colorado [2010] investigated flameless combustion of bio-fuels. Adachi [2007] studied flameless combustion of biomass fuel and methane, and considered effect of inlet air preheating on combustion efficiency and NO_x production. The effect of different amounts of CO_2 and O_2 in atmosphere on the rate of burning in flameless combustion is examined by Heil [2010]. Schaffel [2009] analysed a laboratory combustion chamber using a variety of fuels and calculated the corresponding pollutant emissions.
Compared to experimental works, few numerical investigations have been conducted on flameless combustion. Most of such studies have used computational fluid dynamics (CFD) methods for the modelling. For instance, the combustion efficiency of a particular combustion chamber was calculated numerically by Tabacco [2002]. The effect of turbulence on flameless combustors was studied numerically by Galletti [2009].
Flameless combustion in the combustion chamber of gas turbines has been the subject of other investigations. Duwig [2008] studied the combustion chamber of a gas turbine using large eddy simulation method. The effect of various arrangements of air and fuel inlet nozzles on combustion chamber of a gas turbine was investigated numerically and experimentally by Arghode and Gupta [2011].
In the present work, flameless combustion of hydrogen in the combustion chamber of a gas turbine is studied and the effects of flue gas recirculation, inlet air preheat temperature, operating pressure and fuel equivalence ratio are investigated. NO_x emissions and combustor exhaust gas temperature are also examined and discussed.

THEORY

Perfectly Stirred Reactor (PSR): A relatively uniform temperature distribution forms in a combustor with flameless combustion. This characteristic of flameless combustion can be used

to model the combustor with ideal reactors. One such ideal reactor is a "perfectly stirred reactor" (PSR). One feature of PSR model reactor is the homogenised temperature and species mass fractions.

Conservation equation of species mass fraction in PSR reactor is given as:

$$\dot{\omega}_i MW_i V + \dot{m}(Y_{i,in} - Y_{i,out}) = 0 \tag{1}$$

The energy equation for PSR is:

$$\dot{Q} = \dot{m}\left(\sum_{i=1}^{N} Y_{i,out} h_i(T) - \sum_{i=1}^{N} Y_{i,in} h_i(T_{in})\right) \tag{2}$$

Plug Flow Reactor (PFR): For plug flow reactors a one-dimensional flow condition is assumed. The governing equations of a PFR are given in Eqs. (3)-(6).

$$\frac{d\rho}{dx} = \frac{\left(1 - \frac{R_u}{c_p MW_{mix}}\right)\rho^2 v_x^2\left(\frac{1}{A}\frac{dA}{dx}\right) + \frac{\rho R_u}{v_x c_p MW_{mix}}\sum_{i=1}^{N} MW_i \dot{\omega}_i\left(h_i - \frac{MW_{mix}}{MW_i} c_p T\right)}{\mathrm{P}\left(1 + \frac{v_x^2}{c_p T}\right) - \rho v_x^2} \tag{3}$$

$$\frac{dT}{dx} = \frac{v_x^2}{\rho c_p}\frac{d\rho}{dx} + \frac{v_x^2}{c_p}\left(\frac{1}{A}\frac{dA}{dx}\right) - \frac{1}{v_x \rho c_p}\sum_{i=1}^{N} h_i \dot{\omega}_i MW_i \tag{4}$$

$$\frac{dY_i}{dx} = \frac{\dot{\omega}_i MW_i}{\rho v_x} \tag{5}$$

$$\frac{dt_R}{dx} = \frac{1}{v_x} \tag{6}$$

Network of Ideal Reactors: To simulate flameless combustion process in a combustor of gas turbine, a network of PSR and PFR is used. A typical gas turbine reactor network is shown in Fig. 1. Generally, a gas turbine reactor network consists of a flame/ignition zone, a recirculation zone, and a post-flame zone [*e.g.*, Swithenbank et al. 1973]. However, depending on how the fuel and oxidizer are delivered and the complexity of the flow field, additional reactors and inlets might be required to represent the combustor properly. The reactor network shown in Fig. 1 has two reactor network clusters. The first cluster represents the region around the flame in the combustor and the second cluster uses a single PFR for the post-flame region between the flame and turbine inlet. The first PSR is set as the mixing zone because the fuel stream is partially premixed.

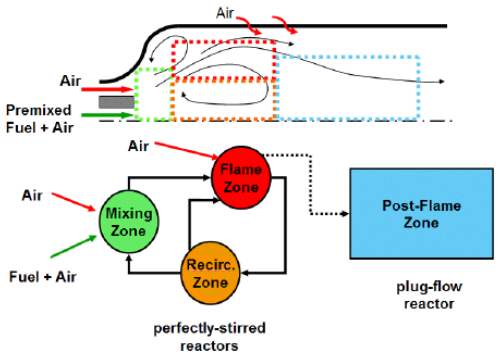

Fig. 1. Schematics of a combustor model for a gas turbine [*e.g.*, Swithenbank et al. 1973; Kee et al. 2003].

A flame zone PSR is connected to the mixing zone directly. This is followed by a recirculation zone for back mixing of hot combusted gas. There should be a recycling flow to model exhaust gas recirculation (EGR). Thus, another flow path is added to the combustor as shown in Fig. 2. General characteristics of each zone are taken from the work of Swithenbank et al. [1973].

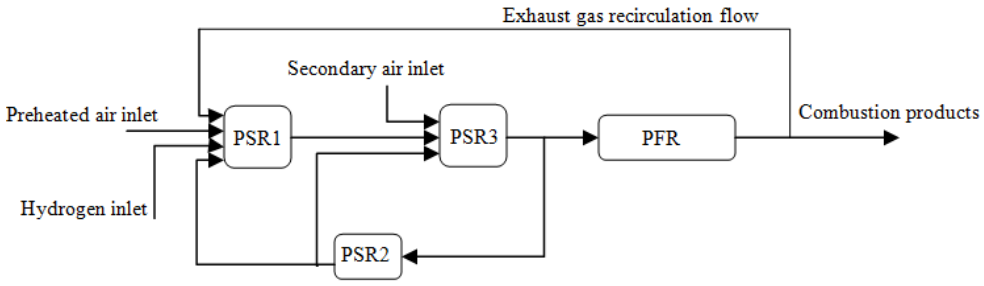

Fig. 2. Proposed model for the combustor of a gas turbine

Chemical Reactions Kinetics: The kinetics used for hydrogen combustion involves 23 reactions and 11 species. The rate equations are cast in the Arrhenius form, as follows.

$$k(T) = AT^{b} \exp\left(-\frac{E_A}{R_u T}\right) \tag{7}$$

In this equation A and b are constants and E_A is the activation energy. The reactions along with the corresponding coefficients are given in Table 1.

Table 1. Hydrogen combustion mechanism [Turns 2006]

No.	Reaction	A	b	E_A
1	H+O2+M ↔ HO2+M	3.61E+17	-0.72	0
2	H+H+M ↔ H2+M	1.00E+18	-1	0
3	H+H+H2 ↔ H2+H2	9.20E+16	-0.6	0

4	H+H+H2O ↔ H2+H2O	6.00E+19	-1.25	0
5	H+OH+M ↔ H2O+M	1.60E+22	-2	0
6	H+O+M ↔ OH+M	6.20E+16	-0.6	0
7	O+O+M ↔ O2+M	1.89E+13	0	-1788
8	H2O2+M ↔ OH+OH+M	1.30E+17	0	45500
9	H2+O2 ↔ OH+OH	1.70E+13	0	47780
10	OH+H2 ↔ H2O+H	1.17E+09	1.3	3626
11	O+OH ↔ O2+H	3.61E+14	-0.5	0
12	O+H2 ↔ OH+H	5.06E+04	2.67	6290
13	OH+HO2 ↔ H2O+O2	7.50E+12	0	0
14	H+HO2 ↔ OH+OH	1.40E+14	0	1073
15	O+HO2 ↔ O2+OH	1.40E+13	0	1073
16	OH+OH ↔ O+H2O	6.00E+08	1.3	0
17	H+HO2 ↔ H2+O2	1.25E+13	0	0
18	HO2+HO2 ↔ H2O2+O2	2.00E+12	0	0
19	H2O2+H ↔ HO2+H2	1.60E+12	0	3800
20	H2O2+OH ↔ H2O+HO2	1.00E+13	0	1800
21	O+N2 ↔ NO+N	1.40E+14	0	75800
22	N+O2 ↔ NO+O	6.40E+09	1	6280
23	OH+N ↔ NO+H	4.00E+13	0	0

Governing Equations and Solution Method: The governing equations for a PSR are given in Eqs. (1)-(2) and those for PFR are specified in Eqs. (3)-(6). To solve the set of nonlinear algebraic equations for a PSR a Newton-Raphson method is implemented. The algorithm solves the system of algebraic equations by first applying a damped modified Newton algorithm to the set of nonlinear algebraic equations represented by Eqs. (1)-(2). However, in the event that the Newton algorithm fails to converge during the iteration, the solution estimate will automatically be conditioned by integration of the time-dependent version of the equations over a fixed number of time steps. This time-stepping procedure provides a new starting estimate for the Newton algorithm that is closer to the steady-state solution, increasing the likelihood of convergence for the Newton method. After time-stepping, the algorithm tries again for convergence and, if this fails, it takes additional time steps on the transient solution to further improve the initial iterate. Ultimately, the Newton iteration converges on the steady-state solution.

On the other hand, the set of governing equations for a PFR are of ordinary differential equation type. However, this is a set of stiff equations since the equations' coefficients vary several orders of magnitude in their values. To solve this set of equations, a stiff solver based on the Runge-Kutta algorithm is implemented.

The governing equations for each reactor are solved with the information from the solution of previously solved reactors used as input to the other reactors when required. To obtain a solution for a network of reactors, this procedure is started from an initial guess, which is "corrected" during the following iterations until a converged set of solutions is obtained.

RESULTS AND DISCUSTION

The main parameters are set for the model shown in Fig. 2 such that flameless combustion is achieved in the combustor. For this purpose, the inlet air temperature is approximately set to the self ignition temperature of hydrogen fuel. Furthermore, the percentage of EGR is set to 50%, meaning that half of the exhaust gas is recycled back to the combustion chamber. The values of the main parameters for the base case are listed in Table 2. In the next step of the study, effects of the variation of each contributing parameter on flameless combustion characteristics are investigated.

Effect of Operating Pressure: Our simulation results show that the combustion chamber temperature changes rapidly with the operating pressure at low pressures but it does not vary at pressures higher than a certain value. This is because the reaction mechanism used in this study is not sensitive to pressures higher than about 3 atm. On the other hand, NO emission shows an increasing trend with the pressure, although with a decreasing slope as the pressure is increased. Fig. 3 represents the variations of exhaust gas temperature and NO emission with the operating pressure.

Table 2. Base case parameters

Parameter	Value
Inlet air temperature (K)	800
Inlet hydrogen temperature (K)	300
Inlet air mass flow rate (kg/s)	0.12
Inlet hydrogen mass flow rate (kg/s)	0.05
Operating pressure (atm)	10

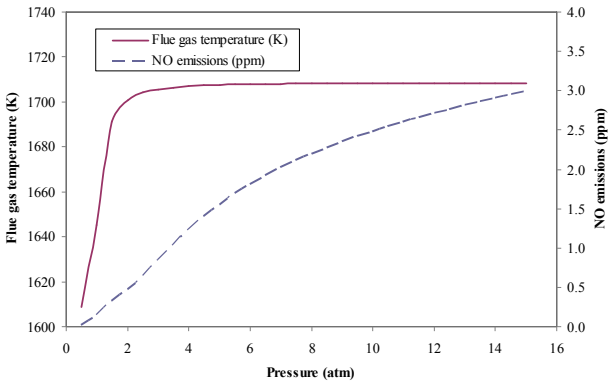

Fig. 3. Effect of pressure on NO emissions and flue gas temperature

Effect of Inlet Air Temperature: The temperature of preheated inlet air plays an important role in NO emission and the flue gas temperature. Our simulation results indicate that NO emission is greatly influenced by high temperatures of the preheated inlet air. It is seen in Fig. 4

that at temperatures higher than self-ignition temperature of the inlet mixture, the NO emission increases sharply. Combustor temperature in flameless combustion should not exceed about twice the self-ignition temperature [*e.g.*, Cavaliere et al. 2004]. Therefore, flameless conditions are no longer present for inlet air temperatures higher than 800 K. As a result, there is a sharp increase in NO emissions for these conditions.

Effect of EGR: As shown in Fig. 5, there is a reduction of NO by increasing the amount of EGR. It is observed in our simulations that the percentage of EGR does not influence the exhaust gas temperature considerably; however, it reduces the mixing zone temperature and homogenises the temperature of the combustion chamber.

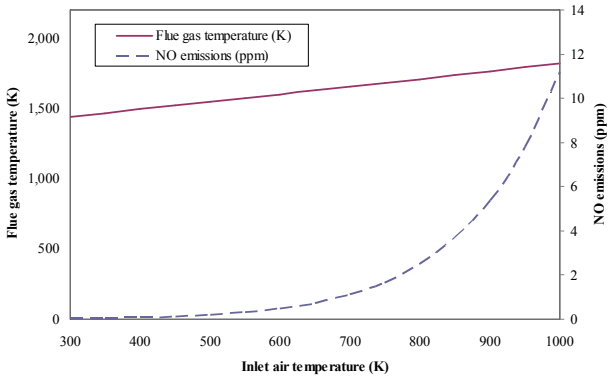

Fig. 4. Effect of inlet air temperature on NO emissions and flue gas temperature

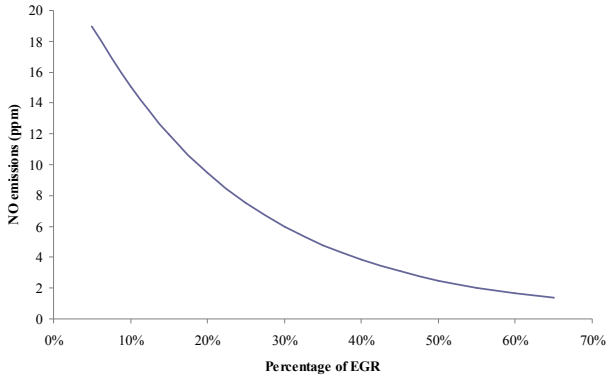

Fig. 5. Effect of EGR percentage on NO emissions

Effect of Equivalence Ratio: The hydrogen mass fraction is varied to examine the effect of inlet mixture equivalence ratio. The simulation results reveal that the equivalence ratio of the inlet mixture has a significant effect on NO emission and on the flue gas temperature. These results are given in Fig. 6. It is observed that in the base case conditions and equivalence ratios

near it, NO emission is notably low. However, for higher equivalence ratios flameless combustion conditions no loner exist and hence NO emissions increase sharply.

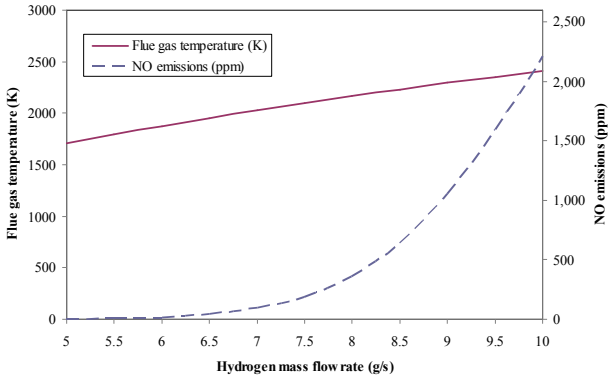

Fig. 6. Effect of equivalence ratio on NO emissions and flue gas temperature

CONCLUSIONS

Flameless combustion is modelled in the combustor of a gas turbine using a network of ideal reactors including PSR and PFR. Hydrogen is selected as the fuel due to its low pollutant emissions. Effects of the main parameters of the gas turbine combustor are studied; these include operating pressure, preheated inlet air temperature, EGR percentage, and inlet mixture equivalence ratio.

It is observed that the operating pressure, equivalence ratio and inlet air temperature have influences on NO emissions. An increase in equivalence ratio increases NO emissions more significantly compared to other parameters, while the operating pressure shows a moderate effect on NO emissions. On the other hand, NO emissions decrease by an increase in EGR percentage, although EGR does not influence the flue gas temperature. However, the flue gas temperature is increased by an increase in any of the other three parameters.

Study of these parameters on combustion illustrates that pollution emissions are extremely low at flameless combustion conditions. It is also observed that homogeneous temperature distribution exists in the combustor at these conditions.

BIBILOGRAPHY

Adachi, S., Iwamoto, A., Hayashi, S., Yamada, H. and Kaneko, S. [2007], Emissions in combustion of lean methane-air and biomass-air mixtures supported by primary hot burned gas in a multi-stage gas turbine combustor, *Proceedings of the Combustion Institute,* Vol. 31, pp. 3131-3138.

Arghode, V.K. and Gupta, A.K. [2011], Investigation of forward flow distributed combustion for gas turbine application, *Applied Energy,* Vol. 88, pp. 29-40.

Cavaliere, A. and Joannon, M.D. [2004], Mild combustion, *Progress in Energy and Combustion Science,* Vol. 30, pp. 329-366.

Colorado, A.F., Herrera, B.A. and Amell, A.A. [2010], Performance of a flameless combustion furnace using biogas and natural gas, *Bioresource Technology,* Vol. 101, pp. 2443-2449.
Duwig, C., Stankovic, D., Fuchs, L., Li, G. and Gutmark, E. [2008], Experimental and numerical study of flameless combustion in a model gas turbine combustor, *Combustion Science and Technology,* Vol. 180, pp. 279-295.
Galletti, C., Parente, A., Derudi, M., Rota, R. and Tognotti, L. [2009], Numerical and experimental analysis of NO emissions from a lab-scale burner fed with hydrogen-enriched fuels and operating in Mild combustion, *International Journal of Hydrogen Energy,* Vol. 34, pp. 8339-8351.
Heil, P., Toporov, D., Forster, M. and Kneer, R. [2010], Experimental investigation on the effect of O2 and CO2 on burning rates during oxyfuel combustion of methane, *Proceedings of the Combustion Institute*.
Kee, R.J., Coltrin, M.E. and Glarborg, P. [2003], *Chemically Reacting Flow: Theory and Practice*, John Wiley and Sons, Hoboken, New Jersey.
Lupant, D., Pesenti, B., Evrard, P. and Lybaert, P. [2007], Numerical and experimental characterization of a self-regenerative flameless oxidation burner operation in pilot-scale furnace, *Combustion Science and Technology,* Vol. 179, pp. 437-453.
Mancini, M., Schwöppe, P., Weber, R. and Orsino, S. [2007], On mathematical modelling of flameless combustion, *Combustion and Flame,* Vol. 150, pp. 54-59.
Schaffel, N., Mancini, M., Szlek, A. and Weber, R. [2009], Mathematical modeling of mild combustion of pulverized coal, *Combustion and Flame,* Vol. 156, pp. 1771-1784.
Swithenbank, J., Poll, I., Vincent, M.W., and Wright, D.D. [1973], Combustion design fundamentals, *Fourth Symposium (International) on Combustion*, pp. 627.
Tabacco, D., Innarella, C. and Bruno, C. [2002], Theoretical and numerical investigation on flameless combustion, *Combustion Science and Technology,* Vol. 174(7), pp. 1-35.
Turns, S.R. [2006], *An Introduction to Combustion*, Second ed, McGraw-Hill.
Wunning, J.A. and Wunning, J.G. [1997], Flameless oxidation to reduce thermal NO-formation, *Progress in Energy and Combustion Science,* Vol. 23, pp. 81-94.
Yu, Y., Wang, G., Qizhao, L., Chengbiao, M. and Xianjun, X. [2010], Flameless combustion for hydrogen containing fuels, *International Journal of Hydrogen Energy,* Vol. 35, pp. 2694-2697.