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# Influence of turbulent mixing intensity on the MILD combustion and the pollutant formation

Hamdi Mohamed\* and Bentîcha Hmaeid

## Abstract

Moderate or intense low-oxygen dilution (MILD) combustion has been acknowledged as one of the most interesting combustion technologies to meet both the targets of high process efficiency and low pollutant emissions. Therefore, the potential for its implementation in gas turbine combustors is investigated in recent research activities. In the MILD combustion regime, we find that the characteristic times of kinetics and turbulence become comparable and the two phenomena are coupled with each other. In this work, a partially stirred reactor is applied to investigate the influence of the turbulent mixing intensity on the combustion process as well as its impact on NO<sub>x</sub> formation. The proposed model is based on a combination of simple turbulent mixing approach with a detailed chemistry sub-model for methane oxidation and NO<sub>x</sub> formation. The computational results demonstrate that the combustion processes as well as the pollutant formation are very sensitive to the mixing intensity. However, the total NO<sub>x</sub> emissions after complete combustion are seen to be only slightly influenced by the mixing intensity.

**Keywords:** MILD combustion, Turbulent mixing intensity, Gas turbine combustion, Pollutant formation, NO<sub>x</sub> emissions

## Background

Pollutant emissions from combustion systems have created increasing environmental concerns. Industrial gas turbine emissions have potentially many different climatic effects such as atmospheric ozone production and destruction, changes in composition of greenhouse gases, alterations of cloud properties and coverage, etc.

Hence, in order to overcome the conflict of interests between energy saving and pollutant emission reductions, alternative combustion concepts are needed. New modes of combustion have been recently introduced in gas turbines, including lean premixed combustion, staged combustion, catalytic combustion and rich-quench-lean combustion. In the last 10 years, scientific investigations and industrial applications have indicated that flameless combustion, elsewhere called flameless oxidation [1], diluted [2], or moderate or intense low-oxygen dilution (MILD) [3] combustion, is one of the most promising combustion technologies to meet both the targets of high

process efficiency and low pollutant emissions. MILD combustion is based on large recirculation of the hot combustion products allowing stable combustion in vitiated air. In this regime, combustion occurs with spontaneous ignition, and it appears to develop without a visible and audible flame [4]. The chemical reaction zone is quite diffuse (volumetric combustion [5]) resulting in a heat release spread out and at the same time in a smoother temperature profile.

Plessing et al. [4] investigated the mixing process inside a laboratory-scale furnace fitted with a FLOX burner using laser techniques to simultaneously measure temperature and OH radical. By analyzing the reaction zone, they found that the reaction rate is slow compared with the mixing rate, giving a low Damköhler number. They concluded that MILD combustion could be modeled as a well-stirred reactor.

In conventional flames, the chemical kinetics occurs much faster than the mixing, whereas under MILD conditions, the combustion is controlled by both kinetics and the mixing. As an extension to this, in a furnace environment, MILD combustion may be likened to a well-stirred reactor (WSR) as the chemical time scales

\* Correspondence: hamdimh@yahoo.fr

Laboratoire d'Etudes des Systèmes Thermiques et Énergétique, Ecole Nationale d'Ingénieurs de Monastir, University of Monastir, Monastir 5000, Tunisia

becoming larger in relation to the turbulence time scales [4]. The link between MILD combustion and a well-stirred reactor may tend to indicate that this regime should be readily modeled, since a well-stirred reactor is well-defined. Recently, Hamdi et al. [6] studied the possibility of integration of the flameless combustion mode to an adiabatic combustor, typically used in gas turbine engines by means of a specific zero-dimensional loop reactor model. They illustrated clearly that the flameless combustion appears as a promising technique for industrial gas turbine combustor applications, even at high operating temperatures and pressures.

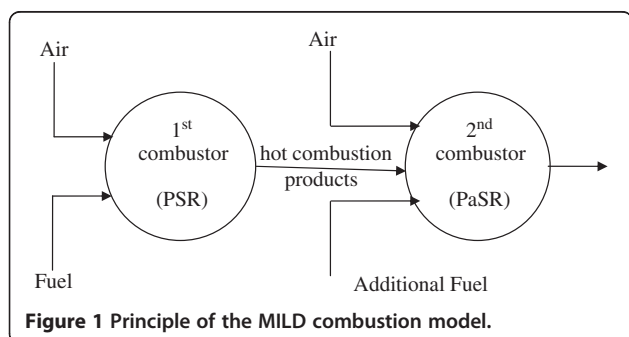
The interaction between the turbulence and the chemistry in describing the nature of MILD combustion is expected to play a significant role however [7], so the analogy to a WSR may not always be applicable. Kraft et al. [8] investigated numerically the influence of varying intensities of turbulent mixing on NO<sub>x</sub> formation using a partially stirred plug flow reactor model describing the combustion process of methane in tubular flow reactor. By analyzing the sensitivity of reaction paths to various degrees of mixing intensities, they found that the formation pathways of NO formation are sensitive to the mixing intensities.

The main aim of this work is to deepen the influence of turbulence-chemistry interaction on MILD combustion process as well as its impact on the pollutant emissions. Throughout this study, we use the complex finite rate chemistry scheme GRI3.0 for methane and NO<sub>x</sub> formation [9], and a simple partially stirred reactor (PaSR) model to account for the turbulence effect on the combustion.

## Methods

### MILD combustion model

To determine the interaction of the turbulent mixing and the MILD combustion process as well as its impact on pollutant formation in gas turbine combustor, the combustor was simulated by the flow model shown in Figure 1. The flow model proposed in this work stimulates the 'sequential combustor system' where a second combustion chamber is employed after the first stages of the turbine. This form of oxidation leads to the MILD combustion at a second chamber. The hot gases exit the first combustor



chamber and enter the second combustor chamber. This second stage combustor, representing the MILD combustion process, is described as a 'PaSR,' where mixing and chemical reactions occur simultaneously.

### Numerical simulation approach

Modeling the interaction of a complex set of chemical reactions and high Reynolds number turbulent fluid flow typical for gas turbine combustion is a challenging task. If the emphasis is on the formation of pollutants such as NO<sub>x</sub>, a full chemistry model is prohibitive. Direct numerical simulation is not feasible due to high computational costs and storage requirements. Therefore, severe simplifications have to be made to be able to study the interaction of turbulence and detailed chemistry with respect to NO<sub>x</sub> formation. The first combustion chamber is assumed to be an ideal, turbulent, adiabatic, constant pressure, perfectly stirred reactor (PSR). It is assumed that there are no boundary effects, and the turbulence created at the inlet is homogeneous, isotropic, and stationary. Then, the second combustion chamber is described as a PaSR. The widely available CHEMKIN package [10] and specially its software application PaSR [11] are used to model the flow field that occurs in the second combustion chamber.

The PaSR is an extension of a continuously stirred tank reactor (CSTR) model that addresses the interaction between chemical reactions and turbulence [12,13]. The basic assumptions for the PaSR are similar to those of the CSTR or PSR. The major difference between a PSR and a PaSR lies in the treatment of the molecular mixing inside the reactor. In a PSR, the contents of the reactor are well-mixed by assuming high-intensity turbulent stirring action, and the only influence from fluid dynamics is controlled by the reactor residence time  $\tau_R$ . Unlike the PSR, a PaSR allows fluid dynamics to control the extent of the mixing and, consequently, the chemical reactions by means of an additional parameter: the scalar mixing time,  $\tau_{mix}$ . The turbulent mixing time scale is often considered to be proportional to the turbulent eddy turnover time as follows [11].

$$\tau_{mix} = C_\phi \frac{\tilde{k}}{\bar{\epsilon}} \quad (1)$$

where  $C_\phi$  usually treated as a constant, but its value varies for different flow configurations.

Lindstedt et al. [14], Cao et al. [15], and Christo and Dally [16] reported similar requirement for adjusting  $C_\phi$  when using the joint PDF approach. Typically,  $C_\phi$  values of no higher than 3 are reported in the literature, but they found that for MILD flames a higher value is required. Thus, it was necessary to increase the value of  $C_\phi$  from the default value of 2, as suggested by Pope [17], to 3 to stabilize the flame.

The composition and temperature in the PaSR are described by a probability density function (PDF). This composition PDF is a subset of the joint velocity-composition PDF because the flow field in the PaSR is assumed to be spatially homogeneous. Velocity fluctuations are also ignored, that is, the PDF is over scalars only, but is not a delta function in scalar space because reactants, intermediates, and products are not mixed at the molecular level.

The PaSR consists of an adiabatic chamber having  $M$  inlet streams and one outlet. Steady flows of reactants are introduced through the inlets with given gas compositions and temperatures. The reactor pressure is assumed to be constant.

The overall mass balance for the gas mixture inside the PaSR is as follows:

$$\frac{d(\langle \rho \rangle V)}{dt} = \sum_{i=1}^M \dot{m}_i - \dot{m}_0 = 0 \quad (2)$$

where  $\dot{m}_i$  is the mass flow rate of the  $i^{th}$  inlet, and  $\dot{m}_0$  is the through-flow mass flow rate.

The average properties of the PaSR are obtained from the ensemble of particles inside the reactor. Each particle is regarded as an independent PSR and interacts with others only through the molecular mixing process. Therefore, the conservation of energy and species is applied to an individual particle rather than to the reactor.

The species equation for a particle is then similar to that of a PSR:

$$\frac{dY_k^{(n)}}{dt} = \frac{1}{\dot{m}_0 \tau_R} \sum_{i=1}^M \{ \dot{m}_i (Y_{i,k} - \langle Y_k \rangle) \} + \frac{W_k \dot{\omega}_k^{(n)}}{\rho^{(n)}} \quad (3)$$

and so is the energy equation for a particle:

$$\frac{dT^{(n)}}{dt} = \frac{1}{C_p^{(n)} \dot{m}_0 \tau_R} \sum_{i=1}^M \dot{m}_i \left( \sum_{k=1}^{k_g} Y_{i,k} (h_{i,k} - \langle h_k \rangle) \right) - \sum_{k=1}^{k_g} \frac{W_k \dot{\omega}_k^{(n)} h_k^{(n)}}{\rho^{(n)} C_p^{(n)}} \quad (4)$$

In the above equations, the angled bracket ( $\langle \rangle$ ) indicates the ensemble average that we use to approximate the density-weighted average in the simulation. The average residence time of the reactor,  $\tau_R$ , is calculated as follows:

$$\tau_R = \frac{\langle \rho \rangle V}{\dot{m}_0} \quad (5)$$

### Initial conditions for the numerical simulations

The inlet gas compositions and temperatures used in the present study are listed in Table 1. The pressure is fixed at 1 atm, and the residence time in the reactor is fixed to 100 ms. In all the computations, the combustion was supposed to proceed adiabatically (i.e.,  $Q_{loss} = 0$ ). A value of 1 ms was chosen for the time step of the Monte Carlo simulation. We used 1,000 stochastic particles in the PaSR calculations in order to correctly predict the statistics of the computed scalars. The only parameter varied in this study is the characteristic turbulent mixing time  $\tau_{mix}$ . It corresponds to the degree of mixing intensity in the flow reactor. Numerical simulations are performed for  $\tau_{mix} = 0, 25, \text{ and } 50$  ms for which the characteristic physical and chemical times are the same order of magnitude.

### Results and discussion

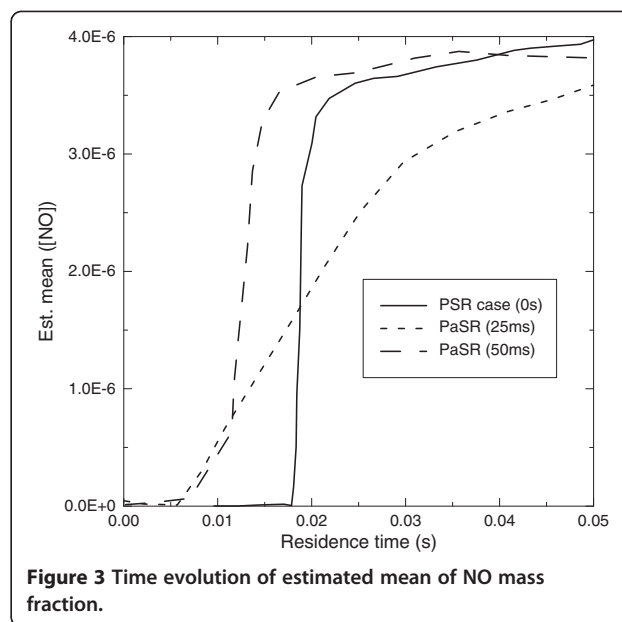
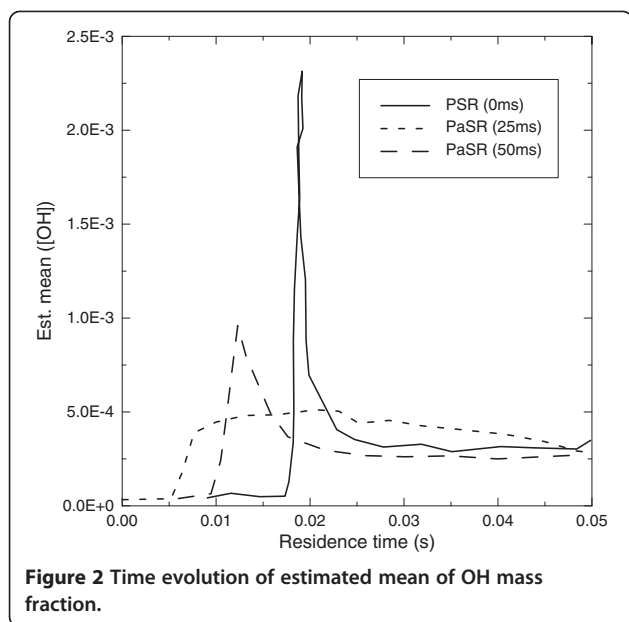
In the following section, we discuss the influence of the turbulent mixing intensity on the chemical kinetics under MILD combustion conditions. In order to demonstrate the influence of turbulent mixing intensity on the chemical reactions, we vary the turbulent mixing time  $\tau_{mix}$ , from the limiting case of the PSR (i.e.,  $\tau_{mix} = 0$  s), which corresponds to very fast mixing; we move to realistic turbulent time scales  $\tau_{mix} = 50$  ms, which is slow mixing, and an intermediate mixing time  $\tau_{mix} = 25$  ms.

As we mentioned earlier, the turbulence times are about the same order as the characteristic time for chemical reactions to guarantee that both processes influence each other. This will be demonstrated with the time evolution of the statistical moments estimated from the approximation of the PDF for the important chemical species as well as two-dimensional marginal PDF. Additionally, the estimations of the overall production of NO from the chemical source term of each particle will give insight on how reaction paths will vary.

Figure 2 shows the time evolution of the estimated mean of OH mass fraction. We note that the mixing

**Table 1 Inlet conditions for the numerical simulations**

Combustor	Gas type	Flow rate (kg/s)	Temperature (K)	Composition (%vol)
First combustor (PSR model)	Natural gas	12.5	770	CH <sub>4</sub> 94.5, C <sub>2</sub> H <sub>6</sub> 1.2, C <sub>3</sub> H <sub>8</sub> 0.4, N <sub>2</sub> 2.3, O <sub>2</sub> 0.6
	Air	545.5	770	O <sub>2</sub> 20.7, N <sub>2</sub> 77, H <sub>2</sub> O 1.58, CO <sub>2</sub> 0.0
Second combustor (FLOX) (PaSR model)	Natural gas	4.0	1,300	CH <sub>4</sub> 94.5, C <sub>2</sub> H <sub>6</sub> 1.2, C <sub>3</sub> H <sub>8</sub> 0.4, N <sub>2</sub> 2.3, O <sub>2</sub> 0.6
	Air	558.0	1,300	O <sub>2</sub> 12.5, N <sub>2</sub> 74, H <sub>2</sub> O 8.77, CO <sub>2</sub> 3.7

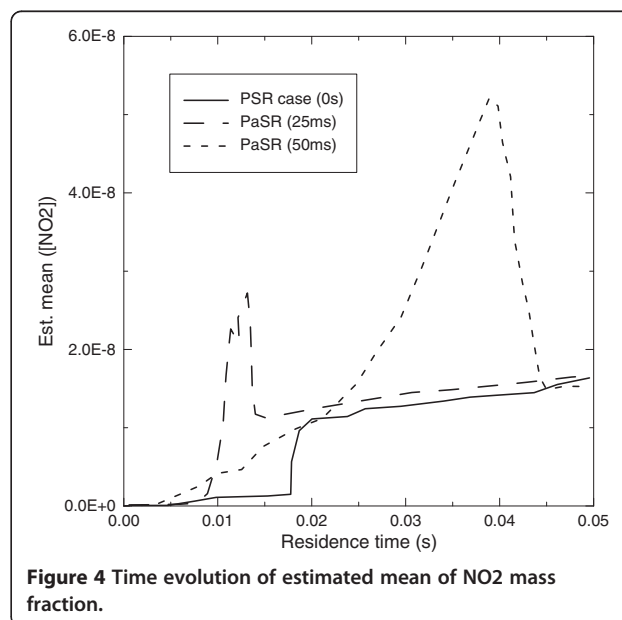


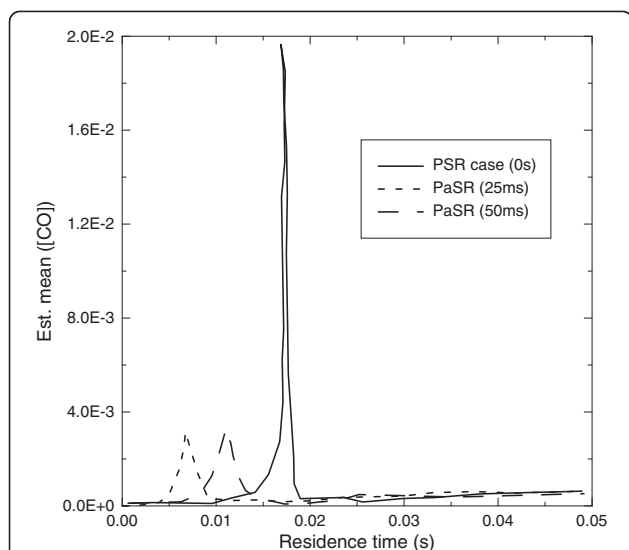
time has a significant influence on the auto-ignition delay time: with increasing mixing time  $\tau_{mix}$ , ignition delay times decrease significantly (the ignition delay time is defined as the time elapsed between  $\tau_{res} = 0$  s and the sudden increase in OH mass fraction). The distribution of the mean mass fraction of OH radical is strongly influenced by the mixing intensity. A rapid increase in the OH concentration signals that ignition takes place. Due to the reduction of the mixing intensity (i.e., higher mixing time), the presence of OH radical is shifted to an earlier point in time. Moreover, the sharp peak present in the diagram of the OH concentration for the PSR case (i.e.,  $\tau_{mix} = 0$  s) is broadened, meaning that the ignition process is distributed over a longer interval. The combustion process, which is very short in the PSR case, is stretched for less intense mixing, and the OH peak concentration is much lower. Our results agree qualitatively with those obtained by Correa and Dean [18] for the auto-ignition of lean n-heptane/air mixtures using an initial temperature of 1,000 K. They explained the decreasing of the auto-ignition delay with the increase of the mixing time arguing that the rich particles lead the ignition process because of their intrinsic shorter ignition delays, in agreement with the results of Chen [13]. These results are of capital importance for the understanding of the MILD combustion regime since it can be considered as a continuous auto-ignition [3].

Figures 3 and 4 plotted respectively the time evolution of estimated means of NO and NO<sub>2</sub> in PSR case and PaSR model for different turbulent mixing times. It can be seen that the ignition delay time is shorter, but the residence time, to achieve complete burnout, increases significantly. Nevertheless, total NO<sub>x</sub> emissions after

complete burnout are influenced only slightly or even tend to decrease with less intense mixing. This is in contrast to the common expectation that imperfect mixing in the combustion process leads to overall higher NO<sub>x</sub> emissions. This result is similar to that obtained by Kraft et al. [8] for the combustion of methane in a tubular flow reactor.

We note that the ignition delay time can be defined as the time needed by the system to increase its temperature of 10 K in comparison with the inlet temperature [19]; therefore, the time evolution of mass fraction of OH radical at varying intensities of turbulent

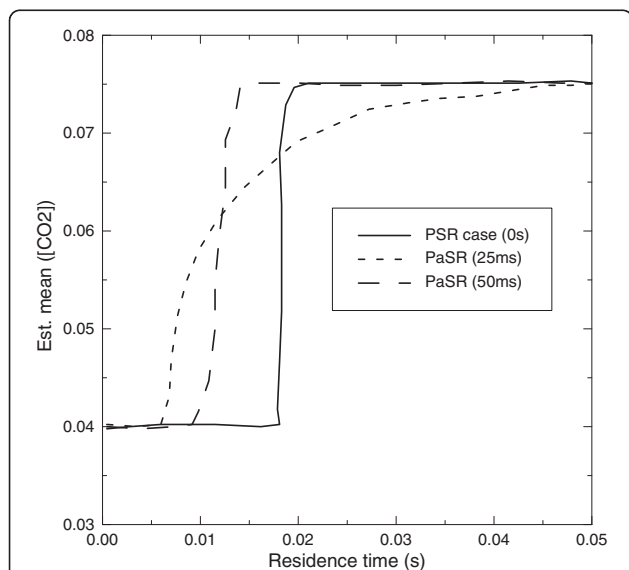




**Figure 5** Time evolution of estimated mean of CO mass fraction.

mixing, given in Figure 2, can give an idea on the influence of the mixing intensity on the combustion temperature and, therefore, their influence on  $\text{NO}_x$  formation. Figure 2 shows that the effect of mixing times on the ignition delay (i.e., on the temperature) becomes less discernible at large mixing times.

Figures 5 and 6 represent respectively the time evolution of estimated means of carbon monoxide (CO) and carbon dioxide ( $\text{CO}_2$ ) in PSR case and PaSR model for different turbulent mixing times. Figures 5 and 6 show that in all cases, the combustion process is fully completed within the residence time of 50 ms, and all



**Figure 6** Time evolution of estimated mean of  $\text{CO}_2$  mass fraction.

radicals reached their equilibrium concentrations and mass fraction of  $\text{CO}_2$  its maximum value. During ignition, carbon monoxide is formed and then oxidized to  $\text{CO}_2$ .

## Conclusion

In the present work, computational results are presented for natural gas combustion at gas turbine relevant MILD combustion conditions: A PaSR model has been developed to study the influence of turbulent mixing intensity on the combustion process and pollutant emissions. The computational results show that the combustion processes as well as the  $\text{NO}_x$  formations are very sensitive on the mixing intensity. With increasing turbulent mixing time (i.e., decreasing mixing intensity), the combustion process is stretched out. Total  $\text{NO}_x$  emissions after complete combustion depended only slightly on the mixing intensity. This is in contrast to the common expectation that imperfect mixing in the combustion process leads to overall higher  $\text{NO}_x$  emissions.

## Competing interests

The authors declare that they have no competing interests.

## Authors' contributions

HM carried out the simulation and calculation of data and drafted, interpreted, and corrected the manuscript. BH participated in the organization and presentation of the results and corrected the draft manuscript. All authors read and approved the final manuscript.

## Authors' information

HM received his Diploma of Engineering (2000), his M.Sc. (2001), and Ph.D. (2005), all in Energetic Engineering from the National School of Engineering in Monastir, Tunisia. He is now an assistant professor in the Preparatory Institute for Engineering Studies of Monastir, Tunisia where he continues to work on his research in combustion pollutant formation and control and MILD combustion within his former research group in Monastir, Tunisia. BH received his B.Sc. (1979) in Physics from the Faculty of Sciences in Tunisia and his M.Sc. (1984) and Ph.D. (1986) from the University of Paris VII, France, both in Physics with a specialization in reactive flows. Since 1988, he has been with the National School of Engineering in Monastir, Tunisia where he is teaching and doing research in the areas of thermodynamics, combustion of gaseous premixed and diffusion flames, pulverized solid particle jet combustion with radiative transfer, and air pollutant formation and control.

Received: 30 May 2012 Accepted: 29 August 2012

Published: 18 September 2012

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doi:10.1186/2251-6832-3-22

**Cite this article as:** Mohamed and Hmaeid: Influence of turbulent mixing intensity on the MILD combustion and the pollutant formation. *International Journal of Energy and Environmental Engineering* 2012 **3**:22.

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