

Influence of Turbulent Mixing on Flameless Combustion and NO_x Formation

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Abstract

A numerical study of the flameless combustion process was performed to investigate the influence of turbulent mixing intensity on the combustion process and NO_x formation. The model is based on the representation of flameless combustion by a network of ideal reactors such as perfectly stirred reactor (PSR) and partially stirred reactor (PaSR). The computational results demonstrate that the combustion process as well as the NO_x formation are very sensitive to the mixing intensity. However, the total NO_x emission after complete combustion are seen to be only slightly influenced by the mixing intensity.

1. Introduction

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 ten years, scientific investigations and industrial applications have indicated that "Flameless Combustion", elsewhere called flameless oxidation (FLOX) (Wünning and Wünning, 1997), diluted (Giammartini *et al.*, 2000) or MILD (Cavaliere and De Joannon, 2004) combustion, is one of the most promising combustion technologies to meet both the targets of high process efficiency and low pollutant emissions. FLOX 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 (Plessing *et al.*, 1998). The chemical reaction zone is quite diffuse (volumetric combustion, Milani *et al.*, 2001), resulting in a heat release spread out and at the same time in a smoother temperature profile.

In order to optimize present flameless burner performances and in a view of its several applications, coming to an understanding of the physics on which this combustion regimes is based is essential, since a consistent explanation of the whole combustion process is still missing. So far, experiments (Pesenti *et al.*, 2001) and numerical (Tabacco *et al.*, 2002) studies have begun to show a strong coupling between turbulence and kinetics:

- a- Dilution with exhaust gases slows down chemical reaction rates and increases kinetics time (Tanaka and Hadsegawa, 1997)
- b- Mixing with recirculating gases increases turbulence and decreases fine scale dissipation times (Vallini *et al.*, 1999).

The result is that the characteristic times of kinetics and turbulence become comparable (Damköhler number $\cong 1$, Plessing, *et al.*, 1998) and the two phenomena are coupled with each other.

In the present work, a "Partially Stirred Reactor" (PaSR) is applied to investigate the interaction of the turbulent mixing and the combustion process as well as its impact on NO_x formation. The model is based on a combination of simple turbulent mixing approach with a detailed chemistry sub-model for fuel oxidation and NO_x formation.

2. Flameless Combustion Model

To determine the interaction of the turbulent mixing and the flameless combustion process, as well as its impact on NO_x formation in gas turbine combustor, the combustor was simulated by the flow model shown in Figure 1. The hot gases exit the first combustor chamber and enter the second combustor chamber. This second stage combustor is described as a "Partially Stirred Reactor" (PaSR), where mixing and chemical reactions occur simultaneously.

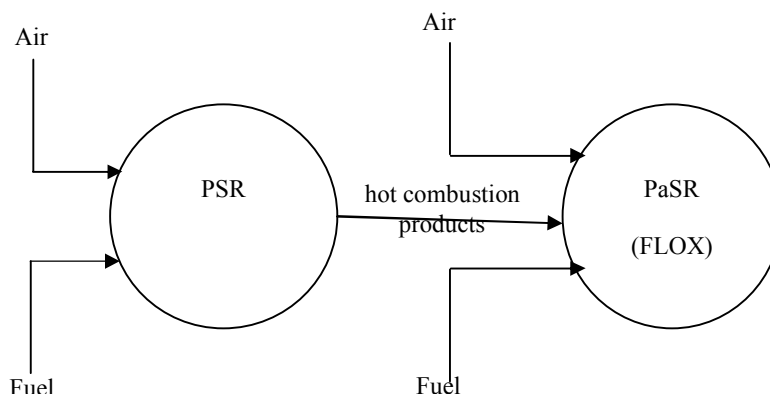


Figure1. Principle of the flameless combustion model.

3. 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_x , a full chemistry model is prohibitive. Direct numerical simulation is not feasible due to high computational costs and storage requirements. Even a probability density function (PDF) modeling approach of a “real” gas turbine combustion chamber with boundary effects, swirling inhomogeneous flow by far exceeds computational capacities. Therefore, severe simplifications have to be made to be able to study the interaction of turbulence and detailed chemistry with respect of NO_x formation. The second combustion chamber is assumed to be an ideal, turbulent, adiabatic, constant pressure, well stirred reactor. 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 (Miller *et al.*, 1996) and specially its software application PaSR is used to model the flow field that occurs in the second combustion chamber.

A detailed chemical kinetic approach is used, based on the comprehensive GRI mechanism of methane oxidation in air (Smith *et al.*, 1996).

4. Reactor Equations

The PaSR is an extension of a continuously stirred tank reactor (CSTR) model that addresses the interaction between chemical reactions and turbulence (Correa, 1993; Chen, 1997). The basic assumptions for the PaSR are similar to those of the CSTR or perfectly stirred reactor (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 τ_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, τ_{mix} . The turbulent mixing time scale is often considered to be proportional to the turbulent eddy turnover time as (Kee *et al.*, 2002):

$$\tau_{mix} = C_D \frac{\tilde{k}}{\tilde{\epsilon}} \quad (1)$$

where C_D usually treated as a constant, but its value varies for different flow configurations, as suggested by Pope (1981) C_D is set to 2.0. The ratio of turbulent kinetic energy to its dissipation rate, $\tilde{k}/\tilde{\epsilon}$, represents the time scale of the energy-containing eddies which characterize the turbulent mixing action.

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:

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

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:

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

and so is the energy equation for a particle is:

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

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, τ_R , is calculated as:

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

(For more details, the reader can consult the PaSR Application user manual (Kee *et al.*, 2002)).

5. Initial Conditions

The inlet gas compositions and temperatures used in the present study are listed in Table 1. The pressure is fixed at 1 atm. The only parameter varied in this study is the characteristic turbulent mixing time, τ_{mix} . It corresponds to the degree of mixing intensity in the reactor. Numerical simulations are performed for $\tau_{\text{mix}} = 0$ s, $\tau_{\text{mix}} = 50$ ms and $\tau_{\text{mix}} = 100$ ms.

Table 1. Inlet conditions for the numerical simulations.

	Gas	Flow rate (kg/s)	Temperature (K)	Composition (% vol.)
1st Combustor (PSR model)	Natural Gas	12,5	770	CH ₄ 94,5%; C ₂ H ₆ 1,2%; C ₃ H ₈ 0,4%; N ₂ 2,3%; O ₂ 0,6%
	Air	545,5	770	O ₂ 20,7%; N ₂ 77%; H ₂ O 1,58%; CO ₂ 0.0%
2nd Combustor (FLOX) (PaSR model)	Natural Gas	4,0	1300	CH ₄ 94,5%; C ₂ H ₆ 1,2%; C ₃ H ₈ 0,4%; N ₂ 2,3%; O ₂ 0,6%
	Air	558,0	1300	O ₂ 12,5%; N ₂ 74%; H ₂ O 8,77% CO ₂ 3.7%

6. Results and Discussion

In this section, we discuss the influence of the turbulent mixing on the chemical kinetics under flameless combustion conditions. In order to demonstrate the influence of turbulent mixing on the chemical reactions, we vary the turbulent mixing time, τ_{mix} . From the limiting case of the PSR (i.e., $\tau_{\text{mix}} = 0$ s), we move to realistic turbulent time scales, $\tau_{\text{mix}} = 100$ ms, which corresponds to very fast mixing, and an intermediate mixing time, $\tau_{\text{mix}} = 50$ ms, which is slow mixing.

Figure 2 shows the time evolution of the estimated mean of OH mass fraction. With increased mixing time τ_{mix} , ignition delay times decrease significantly (the ignition delay time is defined as the time elapsed between $\tau_{\text{res}} = 0$ s and the sudden increase in OH mass fraction). The combustion process, which is very short in the PSR case, is stretched for less intense mixing and the OH peak concentration are much lower.

Figures 3 and 4 plot the time evolution of estimated means of NO and NO₂ in PSR case and PaSR model for different turbulent mixing times. It can be seen that, the mean NO_x mass fraction, after complete combustion, depends 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 NO_x emissions.

Figures 5 and 6 represent the time evolution of estimated means of carbon dioxide (CO₂) and carbon monoxide (CO), respectively, 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 radicals reached their equilibrium concentrations and mass fraction of CO₂ its maximum value: during ignition carbon monoxide is formed and then oxidized to CO₂.

7. Conclusions

A partially stirred reactor (PaSR) model has been developed to study the influence of turbulent mixing intensity on the combustion process and NO_x formation under flameless combustion conditions. The computational results show that the combustion process as well as the 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. The ignition delay is shorter but the residence time to achieve complete combustion increase significantly. Total NO_x emissions after complete combustion are 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 NO_x emissions.

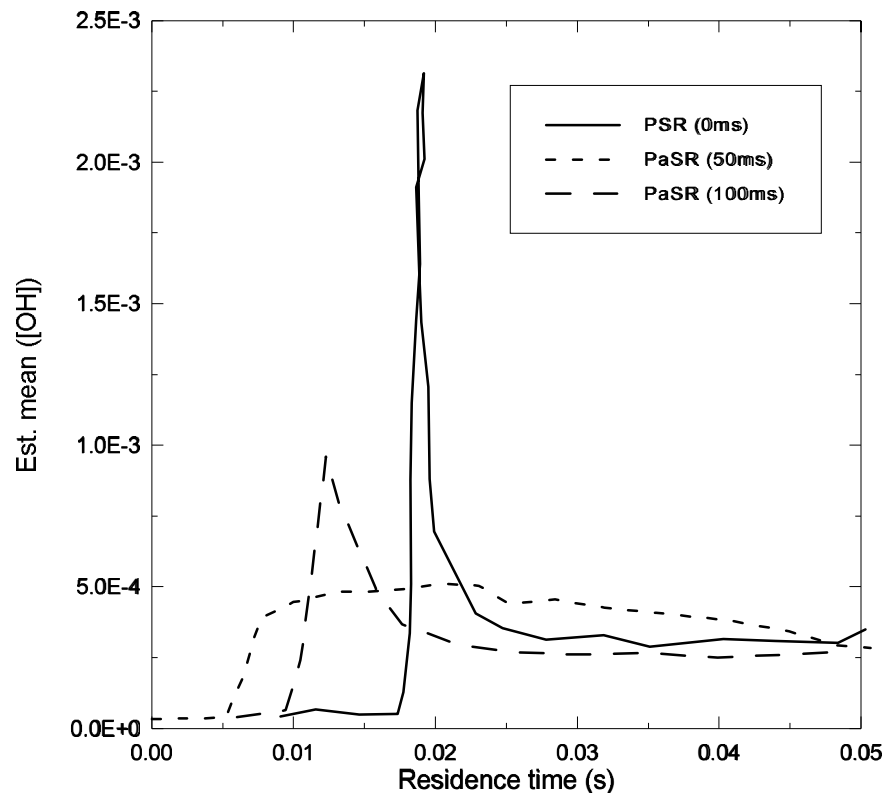


Figure 2. Time evolution of estimated mean of OH mass fraction in the PSR and PaSR cases.

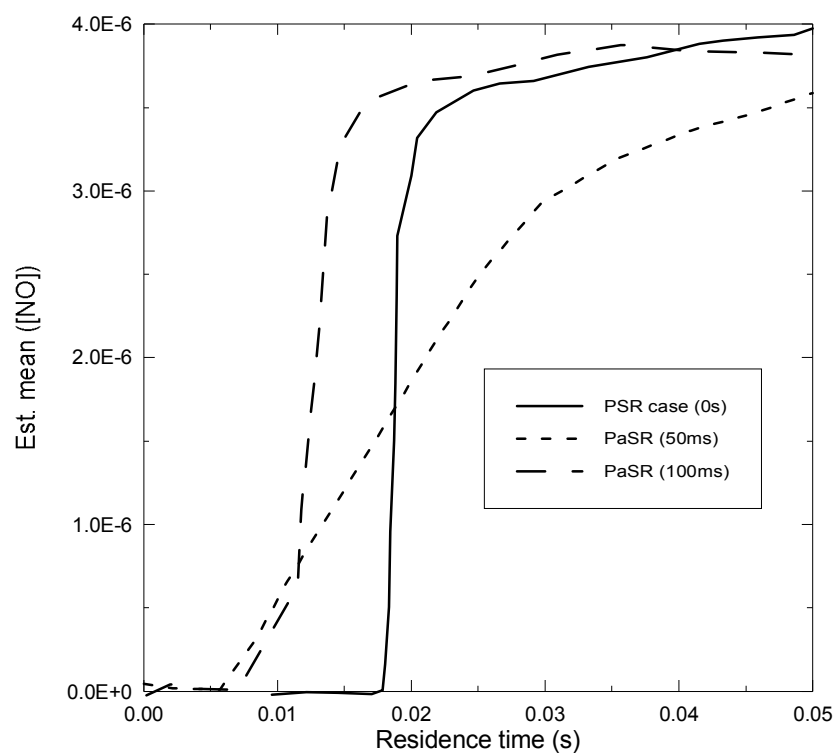


Figure 3. Time evolution of estimated mean of NO mass fraction in the PSR and PaSR cases.

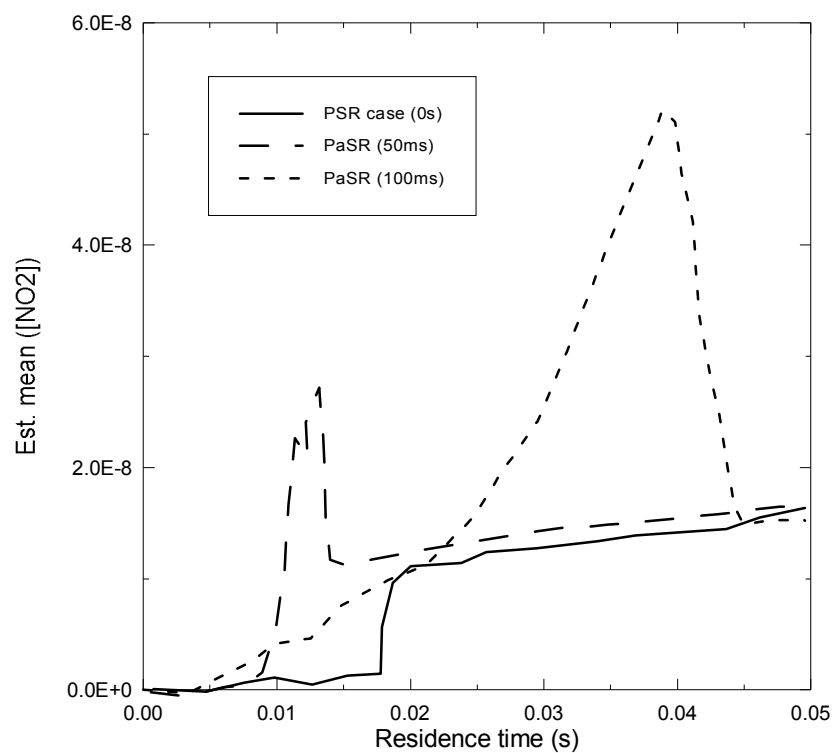


Figure 4. Time evolution of estimated mean of NO₂ mass fraction in the PSR and PaSR cases.

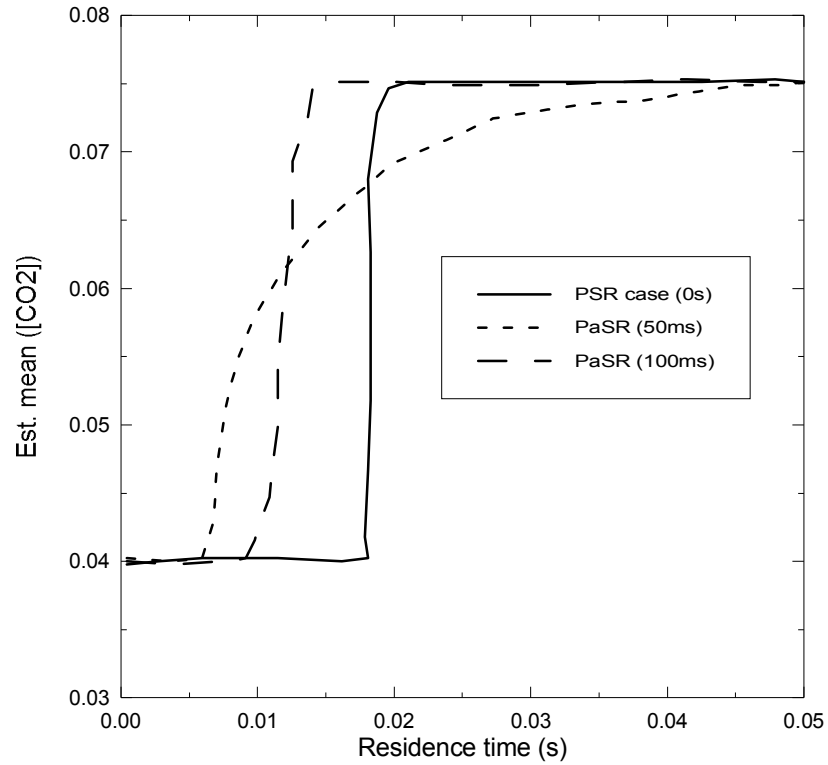


Figure 5. Time evolution of estimated mean of CO₂ mass fraction in the PSR and PaSR cases.

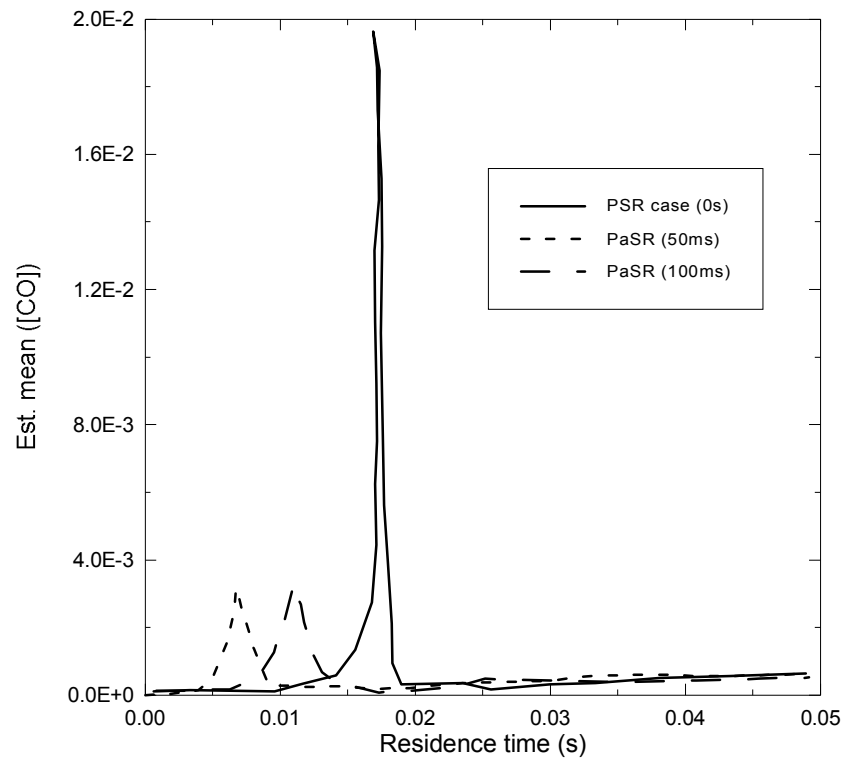


Figure 6. Time evolution of estimated mean of CO mass fraction in the PSR and PaSR cases.

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Author Biographies

Dr. Mohamed Sassi received his B.S. from The University of Rochester in 1995, and then his MS in 1997 and Ph.D. in 1990 from The University of California at Berkeley, all in mechanical engineering with specialization in combustion and thermal sciences. Since then he has worked as a Research Engineer for the account of Electricite de France (EDF) for five years on optical diagnostics for combustion and plasma processes, and in 1995 he joined a school of engineering in Tunisia as Associate Professor and Chairman of the Energetics Department, and then as full Professor and Director of Studies until August 2004, when he joined The Petroleum Institute of Abu Dhabi as a joint Chemical/Mechanical Faculty member. His research interests have always been in experimental and numerical modeling of turbulent combustion, pollutant formation and control, and electrical plasma processes.

Dr. Hmaeid Benticha received his B.S. (1979) in Physics from The Faculty of Sciences in Tunisia, and then his M.S. (1984) and his 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 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.

Dr. Mohamed Hamdi received his diplomat of engineering (2000), his M.S. (2001) and his Ph.D. (2005) all in energetics engineering from The School of Engineering in Monastir, Tunisia. He is now an Assistant Professor in The Institute of Applied Sciences and Technology in Sousse, Tunisia, where he continues to work on his research in combustion pollutant formation and control and flameless combustion within his former research group in Monastir, Tunisia.