



Assessment of chemical time scale for a turbine burner

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ABSTRACT. Understanding the relationship between chemical kinetics and turbulent mixing characteristic time scales provides the necessary knowledge to establish the type of combustion regime, which, furthermore, helps grasping the main characteristics of the flame physics. One of the most convenient tools for evaluating the turbulence/chemistry interaction is provided by the analysis of the Damköhler number field distribution. Literature survey provides several examples of Damköhler number computation, mostly regarding single global chemical reaction. The present work aims at applying this procedure for the calculation of the chemical time-scale (and thus of the Damköhler number) for the two-step kinetic mechanism of Westbrook and Dryer used in the simulation of gas reheat inside a turbine stage. Based on this methodology, we may be able to establish which chemistry-turbulence interaction model is more appropriate for a specific simulation (finite-rate eddy dissipation concept, flamelet approach, etc.). The research has set forth important variations of the Damköhler number (in the order of hundreds of units) throughout the flow domain. In the wake of the injector where the turbulent intensity is high and the incipient incomplete mixing prohibits fuel ignition, the flow is completely controlled by turbulence and Damköhler number is low. Hence, the appropriate turbulence/chemistry model could very well be an eddy dissipation concept type. Similar approach should be chosen for the rotor-stator passage, also. Conversely, in the rotor passage, due to the blocking effect of the walls and the strong interactions between fluid tensions and pressure, the turbulence intensity is diminished and the appropriate fuel oxidizer mixing triggers ignition and flame sustainability.

KEYWORDS: turbine burner, Damköhler number, chemical time scale

NOMENCLATURE

Latin I – spatial scale D - thermal diffusivity Da - Damköhler number k – turbulent kinetic energy K_r - kinetic constant of the reaction rate R – chemical source term Re – Reynolds number Z - mixture fraction Z'' - mixture fraction fluctuation

- $\begin{array}{l} Y-mass \ fractions \\ Greek \\ \delta \ \ thickness \ of \ the \ flame \ front \\ \epsilon \ \ turbulent \ dissipation \ rate \\ \nu' \ \ turbulent \ intensity \end{array}$
- $\tau\,$ time scale
- $\boldsymbol{\chi}$ scalar dissipation rate
- $\boldsymbol{\omega}$ turbulence eddy frequency
- Subscripts f – flow





c - chemical I – integral scale st – stoichiometric

1 INTRODUCTION

Interaction between turbulent mixing and chemical kinetics is the key aspect in combustion modeling as it determines the combustion regime. Therefore, a fundamental understanding of turbulence/chemistry interactions in reacting systems may provide the needed insight into the physics of the flame, allowing an appropriate selection or development of physical models. The Damköhler number (Da) represents the ratio of the time scales of the flow (τ_f) and of the chemical reactions (τ_c)

t - turbulent

), respectively. Large Damköhler values are associated with turbulent mixing controlled flames, while low Damköhler values corresponds to chemically controlled flames. In the latter case, the system behaves like a perfectly stirred reactor in which reactants and products are quickly mixed by turbulence but the characteristic time scale is imposed by the chemistry. The calculation of the local Damköhler number requires proper definitions of the flow and chemical time-scales. Usually, the flow time scale for turbulent conditions is given in terms of the integral time-scale, although several other possibilities are considered in literature (e.g. Taylor scales, Kolmogorov scale). The assessment of the chemical time-scale is quite challenging, especially in the case of complex kinetic mechanisms. Furthermore, the diffusion flame poses supplementary difficulties compared to the premixed combustion.

Literature survey provides several examples of Damköhler number computation, mostly regarding single global chemical reaction. A method for considering more complex kinetic schemes was proposed by Fox [1] who defined the chemical time-scale in terms of the inverse of the eigenvalues of the Jacobian matrix of the source term. The present work aims at applying this procedure for the calculation of the chemical time-scale (and thus of the Damköhler number) for the two-step kinetic mechanism of Westbrook and Dryer used in the simulation of gas reheat inside a turbine stage.

The knowledge of chemical time-scale may help the choice of a proper time discretization for transient numerical models, such as those based on Large Eddy Simulations techniques. Also, based on this methodology, we may be able to establish which chemistry-turbulence interaction model is more appropriate for a specific simulation (finite-rate eddy dissipation concept, flamelet approach, etc.).

2 **REVIEW OF DAMKÖHLER NUMBER CHARACTERIZATION**

Depending on the provision of the reactants and on the combustion process, the flame types can be classified in two basic flame types, the premixed and the non-premixed flames. Premixed combustion occurs if fuel and oxidizer are mixed before they enter the reaction zone. In the non-premixed combustion regime fuel and oxidizer are injected separately from each other. In that case fuel and oxidizer are mixed during the combustion process.

2.1 NON-PREMIXED FLAMES

As non-premixed flames do not exhibit inherent propagation speeds they cannot flash back. That is why non-premixed injection is often used due to safety reasons. As diffusion is the rate controlling process in these flames, a common expression is also diffusion flame. The flame fronts are more complex than for premixed flames, as they cover the entire range of equivalence ratio from 0 for pure air to 1 for pure fuel. Combustion takes place near stoichiometric mixture composition. Non-premixed flames can be found in early diesel engines, aircraft gas turbines or H2-LOx rocket combustion engines to name a few.

The time needed for convection and diffusion, both being responsible for turbulent mixing, is typically much larger than the time needed for most of the combustion reactions to occur. So turbulent mixing and chemical reactions are the rate limiting processes. They are related through the dimensionless Damköhler number Da, where

$$Da = \frac{\tau_f}{\tau_c}$$

(1)

The decision of the most relevant flow and chemical time scales which control the flame structure is important in obtaining meaningful parameters which describe the system. When defining the Damköhler number for premixed flames, the flow time scale (τ_f) is generally defined by the ratio of the turbulent





length scale to the turbulent intensity (I/v'), which is proportional to the integral time scale ($\tau_I = k/\epsilon$) being the largest turbulent time scales in the system. In contrast to premixed flames distinct regime definition for non-premixed combustion is difficult. The definition of a characteristic flame velocity such as that of pre-mixed combustion is not available [2], thus complicating the calculation of a reaction time scale. Non-premixed flames exhibit multiple flow scales which may evolve temporally as well as have dependence on spatial coordinates, and burner flow conditions this results in multiple choices for definition of the flow scales. Many authors suggest the use of the inverse of the stoichiometric scalar dissipation rate for the definition of a local mixing time [2, 3]

$$\tau_m = 1 / \chi_{st} = \left(2D \left| \overline{\nabla Z_{st}''} \right|^2 \right)^{-1}$$
(2)

Additionally, literature shows the non-premixed Damköhler number being calculated using τ_I and τ_K , the Kolmogorov mixing time which is the scale of the smallest eddies in the system where energy is dissipated to heat [4]. Another possibility would be using the Batchelor scale (τ_B) which is the time scale associated to the largest scales at which non-premixed streams remain segregated [1]. The assumption that the Batchelor and Kolmogorov time scales are equal for gases leads to the definition of Batchelor length scale [5]. Hence, four definitions of the Damköhler number for non-premixed combustion yield depending on the choice of the mixing time: the integral Damköhler number $(Da_I)_I$ the local mixing Damköhler number (Da_m), which uses the local mixing time τ_m , the Kolmogorov (Da_n) and Batchelor Damköhler number (Da_B), which are equivalent for gases. Several authors have attempted to characterize non-premixed combustion regimes using various diagrams. Poinsot and Veynante [3] considered that diffusion flames regimes can be analysed based on two characteristic ratios: (1) a length scale ratio of integral (I_0) and diffusive scales (I_d) and (2) a time scale ratio of the turbulence integral characteristic time (τ_I) and the chemical time (τ_c). A relationship between the Damköhler number based on the mixing time scale (corresponding to the local non-premixed flame structure) and that based on integral time scale (τ_{T}) (corresponding to the global structure of the turbulent non-premixed flame) can be established as:

$$Da_{I} = \frac{\tau_{I}}{\tau_{c}} = \frac{\tau_{I}}{\tau_{\eta}} \frac{\tau_{\eta}}{\tau_{c}} \cong \frac{\tau_{f}}{\tau_{\eta}} \frac{\tau_{m}}{\tau_{c}} = \frac{\tau_{I}}{\tau_{\eta}} Da_{m} \approx \sqrt{\operatorname{Re}_{t}} Da_{m}$$
(3)



Figure 1: Non-premixed combustion diagram adapted from [3].

On a log-log plot of coordinates $Da_I - Re_t$, constant mixing Damköhler number Da_m corresponds to lines of slope 1/2. For large Damköhler numbers, i.e. for fast chemistry, the flame is very thin, and the reactive layer is thinner than the diffusion layer, which is assumed to be equal to the Kolmogorov size, which is the size of the smallest eddies. In this region the laminar flamelet assumption (LFA) can be





implemented. It is defined as the Flamelet region as the flame occurs as laminar flame elements. With respect to Eq. 3 this condition may be expressed as $Da_m > Da^{LFA}$, where Da^{LFA} depends only on the local flame structure and does not take into account vortex time scales. For a longer chemical time scale, the thickness of the reactive layer becomes equal to the Kolmogorov length scale. In this case, a departure from laminar flame structures and unsteady effects is expected. This condition may be expressed as $Da_m > Da^{EXT}$. The regime of unsteady effects and extinction is divided where the flame Damköhler number is equal to the Damköhler number at extinction, Da^{EXT} . For large chemical scales and small Damköhler numbers, extinction occurs. These conditions are depicted in Fig. 1. The regime of turbulent non-premixed flames has been discussed in several papers [6][7][8][9]. Another attempt to characterize non-premixed flames has been performed by Peters [2]. He plots the ratio of the mixture fraction variance $\sqrt{Z''^2}$ and the diffusion thickness $(\Delta Z)_F$ against the time scale ratio of the scalar dissipation rate at quenching χ_q to the conditional Favre mean scalar dissipation rate $\widetilde{\chi}_{st}$. The mixture fraction Z is a conserved scalar, which is 1 in the fuel stream, and 0 in the oxidizer stream. For $\chi_q > \chi_{st}$, three regimes can be detected, the separated flamelet region, the connected flame zones and the connected reaction zones. The line $\sqrt{Z''^2} / (\Delta Z)_F = 1$ distinguishes between the separated flamelet and the connected flame zones. In the separated flamelet regime, the mixture fraction fluctuations are so large that they extend to sufficiently lean and rich mixtures. So the diffusion layers and thus the reaction zones are broken up. For $\sqrt{Z''^2}/(\Delta Z)_F < 1$ the mixture fraction variance is too small to be able to break up the flame zones. In that case there might be intense mixing or partial premixing. The determination of chemical time scales for turbulent combustion systems is particularly difficult as detailed reaction mechanisms are often required for adequate description of the combustion process. A definition of the laminar flame velocity s_L , used for the calculation of $\tau_c (= \delta / s_L)$ doesn't exist for non-premixed combustion. The chemical time τ_c is determined from several different methods including activation energy asymptotics [10], global chemistry assumption [11] or the critical scalar dissipation rate at quenching $\tau_q = 1/\chi_q$ has been used for estimation of τ_c with complex chemistry

cases [4]. At this time a clear definition for τc for complex chemistry systems involving detailed kinetic mechanisms is needed, and it is the focus of this work. In most cases a global chemistry assumption is made to simplify the estimation of τ_c . An example of this is given by Kuo [12] where the following definition is used

$$Da_I = \left(\frac{\nu K_r^2}{\varepsilon}\right) \tag{4}$$

where v is the kinematic viscosity, ε is the dissipation of turbulent kinetic energy, and K_r is the kinetic constant of the global reaction. On the other hand, Fox [1] provides a method for considering more complex kinetic schemes, suggesting that the chemical time-scale can be defined in terms of the eigenvalues of the NxN Jacobian matrix **J** of the chemical source terms, whose elements J_{ij} , for an isothermal case, are given by :

$$\mathbf{J}_{ij} = \frac{\partial R_i}{\partial Y_i} \tag{5}$$

Chemical time-scales can then be associated to each eigenvalues as:

$$\tau_{ch} = \frac{1}{|V_{ch}|} \tag{6}$$

where V_{ch} is the eigenvalue vector from the eigenvalue decomposition of **J**. In a complex kinetic scheme, for which the time-scales can range over several orders of magnitude, the slowest chemical time-scale should be chosen for the estimation of the Damköhler number:

$$\tau_c = \max(\tau_{ch}) \tag{7}$$





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Upon determination of an appropriate expression for τ_c and τ_f , the evaluation of the Damköhler number can easily allow identification of the predominant combustion regime, hence the selection of the appropriate turbulent combustion model. Turbulent combustion models are generally well suited for: (1) high Damköhler numbers where mixing dominates the process or (2) low Damköhler numbers where chemistry dominates the physics and finite rate chemistry models are required. An example of a high Damköhler number model is the Steady Laminar Flamelets Model (SLFM) which uses the mixture fraction variable as well as the mixture fraction variance to describe the flame as an ensemble of steady laminar diffusion flames under going various strain rates which are all well characterized by the two transported variables. In lower Damköhler flows turbulent structures can enter the flame pre-heating zone and further mix and distort the flame front, these unsteady effects require a modeling approach with higher coupling between the chemical reactions and the turbulent mixing. A model such as Eddy Dissipation Concept (EDC) transports the species involved in a detailed reaction mechanism, and treats the flame as an ensemble of perfectly stirred reactors (PSR) where the PSR residence time is a function of the local mixing time scales. This allows for a more complex chemistry tracking approach, while coupling the turbulent structures to the chemistry physics.

3 TURBINE BURNER MODEL

Turbine combustion is a relatively recent concept, and the amount of work published in the open literature is presently quite limited. A turbine-combustor is defined as a turbine in which fuel is injected and burned. The process of combustion in the turbine is called *in situ* reheat. A comparison of the Brayton, regenerative Brayton, Ericssson, Carnot, and isothermal expansion, isentropic compression cycles, concludes that the Ericsson cycle has the highest thermal efficiency and highest dimensionless net work, therefore it should be the prime candidate for GTE cycle [13]. A second option is the isothermal expansion, isentropic compression cycle whose thermal efficiency and net work are better than those of the Brayton and regenerative Brayton cycles. Thermodynamic cycle analysis has been carried out for both continuous combustion [14] and for inter-stage combustion [15], using component efficiencies based on typical, real-life values. These studies demonstrate performance gains related to lower fuel consumption, higher specific thrust, and enhanced operational speed and compressor pressure ratios for both turbojet and turbofan engines. In addition, a CFD analysis based on the RANS equations coupled with a two-step, global, finite rate model for methane combustion [16] showed for a land-based GTE a power increase of up to 5.1% in a four-stage turbine combustor with a 2% mass flow rate of fuel [17].

3.1 CFD COMPUTATIONAL MODEL AND RESULTS

The computational model is based on a CAD model inspired from a true one row turbine with 26 stator vanes and 61 rotor blades that expands 8.1 kg/s burnt gas from 911 KPa total pressure and 1263 K total temperature. The rotation speed of the rotor wheel is 22000 RPM. The injection concept is somehow similar to the one illustrated in Fig. 1b, but in our particular case we used a perforated pipe placed at mid-pitch in the stator row passage (Fig. 2).



Figure 2: Turbine burner computational domain and typical mesh slice at half span.





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The flow and combustion are modelled by the Reynolds-averaged Navier-Stokes equations coupled with the species transport equations. Two sets of data were obtained using different mesh grid sizes and turbulence models. In the first run, we used a rather coarse grid with almost 500000 nodes and the scale adaptive shear stress transport (SST-SAS) turbulence model. In the second run, almost 2500000 nodes were employed in conjunction with detached eddy simulation (DES) turbulence model [18]. In both cases the chemistry turbulence interaction is described in terms of finite rate eddy dissipation concept (FREDC). The choice we have taken was to increase the inlet total temperature at 1550 K to succeed in firing up the flow of injected pure methane using the two-step, global, finite rate chemical mechanism of Westbrook and Dryer [19]. This increase amounts to the modern combustors usual outlet temperature.

Inlet and outlet planes are represented by straight arrows while the periodic faces are indicated by circling arrows. In middle of the stator passage there is the injection pipe. To reduce the computational effort we have chosen to select only a section of full turbine stage 3D model (see Fig. 2) containing one vane passage and two rotor passages. In this case, the uneven number of blades leads to a pitch ratio close to unity (0.85). The simulation was performed in ANSYS CFX simulation environment. The composition of the inlet burnt gas is given by the mass fraction distribution computed from equilibrium calculations at the given inlet temperature: $y_{CO2} = 0.064$, $y_{CO} = 10^{-6}$, $y_{O2} = 0.152$, $y_{H2O} = 0.035$, $y_{N2} =$ 0.751. The fuel inlet velocity is 50 m/s and 350 K is its static temperature. The turbulence intensity for both inlets was 5%. The global time step was $9 \cdot 10^{-5}$ s per passing period (cycle). Herein, the passing

period is defined as the time requested for the rotor to travel a distance equal to the stator pitch length at mid span.

After 50 simulation cycles, the data was exported to an in-house code to compute Damköhler number field distribution. The exported data contained the molar concentrations of the species from the chemical mechanism (CH₄, CO, CO2, H₂O, O₂), the turbulence eddy frequency and the reaction rates. According to the turbulence models used, the turbulence eddy frequency (ω) [s⁻¹] is one of the quantities directly modelled based on appropriate transport equation. Based on the molar concentrations and the reaction rates we were able to perform the computation of the Jacobian from Eq. 5.

3.2 **DATA ANALYSIS**

The major goal of the simulations was the evaluation of the feasibility of the new turbine-burner concept. However, due to the highly strained flow, the stability of the combustion process is questionable with respect to the unsteadiness induced by the rotor-stator interaction. The broad range of time scales associated with this type of flows overtakes the average computational capabilities, especially for engineering purposes. On the other hand, an experimental model of the turbine burner capable of providing some insights on the main parameters of the flow and reliable data for burning characteristics of the flow was not available. In these circumstances, the most simple and computational less expensive turbulence-chemistry interaction mechanism was FREDC based on the two-step WD2 reaction mechanism. However, we have discovered some inconsistencies among the temperature and reaction rates field distributions. Although combustion seems to start in the wake of the injection pipe as confirmed methane oxidation rate distribution (Fig. 3), the temperature peeks in the rotor wheel close to the pressure side of the rotor blades (Fig. 4). All contours are displayed at half span. The distribution field of carbon monoxide oxidation rate shows the same characteristics as the temperature field inducing the idea that temperature distribution is controlled by the slowest reaction. This trend is confirmed on both coarse mesh and fine mesh sets of data. The distributions of the turbulent integral time scale for the two sets of data are represented in Fig. 5 and Fig. 6. It is apparent that mesh refinement did not produce sensible variations in the time scale of the flow. With respect to the chemical time scale distributions depicted in Fig. 7 and Fig. 8, slight differences are apparent in the wake of the injection pipe. A finer mesh leads to an increase of the chemical time scale from $\sim 10^{-5}$ to $\sim 10^{-4}$ downstream the fuel inlet. However, the Damköhler number for both sets of data ranges (Fig. 9 and Fig. 10) is consistently greater than unity ($Da_1 > 1$) in the wake of the injection pipe which advocates the fulfilment of the conditions associated with steady flamelet assumptions regime of the non-premixed combustion. Consequently, we have performed a third simulation using PDF flamelet approach based on a mechanism consisting of 17 species and 55 reactions without NOx. The major species are CH, CH₂O, CH₃, CH₄, CO, CO₂, H, H₂, H₂O, H₂O₂, HO₂, N2, O, O₂, OH, ³CH₂. The skeletal mechanism was taken from [20].







Figure 3: Methane oxidation rate distribution.



Figure 4: Temperature distribution.



Figure 5: Logarithm base 10 of the coarse mesh integral time scale.

Figure 6: Logarithm base 10 of the fine mesh integral time scale.

The new results in the steady flamelet approach are described in Fig. 11 based on the temperature field contours at mid-span of the turbine stage. At theoretical level, these results are much more promising as they depict the development of the flame right in the wake of the injection pipe with its associated normal temperature increase which peeks in the 2300 K. A most interesting and somehow unexpected aspect is the comparison between the area averaged temperature at outlet from the turbine stage based on the FREDC model and PDF model (Fig. 12). In this case, the differences are within 10-15 K which is somehow indiscernible from an experimental measurement point of view.



Figure 7: Logarithm base 10 of coarse mesh chemical time scale.

Figure 8: Logarithm base 10 of fine mesh chemical time scale.



Figure 9: Coarse mesh Damköhler number (*Da*_I).

Figure 10: Fine mesh Damköhler number (*Da_I*).



Figure 11: Temperature field for the PDF flamelet approach.



Figure 12: Time evolution of the area averaged temperature at the turbine outlet.

The differences between the time averages of the area averages of the outlet temperatures is even less, on the order of only 4 K. It seems that WD2 mechanism (which is a global two-step chemical mechanism) yields almost the same global averaged outlet temperature and, from this point of view, can produce confusing conclusions.

4 CONCLUSIONS

The broad range of time scales associated with the combustion inside a turbine stage overtakes the average combustion models' capabilities, especially for engineering purposes. To gain some insight into the problem of turbine combustor, several iterative simulations are required to get closer to a physically acceptable solution. In the lack of any experimental measurements, for the given conditions and physical models, it seems that the flamelet approach yields the most suitable and physically meaningful





results. Even so, it is out of the question the possibility of discerning between the two combustion models only based on global averaged measured quantities.

ACKNOWLEDGEMENT

This research was funded by the by the Joint Applied Research Project PN-II-PT-PCCA-2013-4, with the support of ANCS, CNDI – UEFISCDI, project no. 286/2014.

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