



The analysis of chemical time scales in a partial oxidation flame



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ABSTRACT

Time scale analysis is a well-established method in combustion science to identify slow and fast processes, but is also required for multi-scale modeling of turbulence–chemistry interaction. Models such as flamelet are based on scale separation arguments, which require a suitable definition of chemical time scales. In this article we study different time scale definitions. Two definitions previously published in the literature as well as two new definitions are investigated in detail. Most time scales require the computation of the eigenvalues of the chemical Jacobian, which is computationally expensive especially for larger chemical reaction mechanisms. One of the new definitions also requires the Jacobian of the chemical source term, whereas the computation of the second newly proposed time scale is computationally straight-forward since neither one is needed. We evaluate the four methods on a simple one-step reacting system and a partial oxidation flame which combines an oxy-fuel type reaction and a fuel-rich reforming post flame zone. Most of the considered time scale definitions provide similar results whereas the computational effort differs significantly.

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1. Introduction

Combustion systems are objects of governmental regulations and a “validated, predictive, multi-scale, combustion modeling capability to optimize the design and operation of evolving fuels in advanced engines for transportation applications” is required, cf. [1]. The term “multi-scale”, i.e. the coexistence of different time and/or length scales, illustrates one major characteristic of combustion. In the absence of transport processes, combustion chemistry leads to a system of stiff ODEs. The term “stiff” usually refers to a large difference between the largest and the smallest eigenvalues of the Jacobian. A number of model reduction methods are based on time scale respectively eigenvalue analyses. The Intrinsic Low Dimensional Manifold (ILDM) method [6,7] is based on the evaluation of slow time scales and defines a subspace significantly smaller than the original. Another example is the Computational Singular Perturbation (CSP) method [8,10,9] to identify the fast reaction subspace. CSP is able to analyze the dynamics and identify fast and slow time scales [2,11,12]. Here, the slow and thus characteristic time scales are driving the process whereas the fast time scales become exhausted. Najm et al. [11] give a short summary on the application of the CSP in reactive flows. In the Level Of Importance (LOI) method [4,5,3] individual species time scales are important when identifying steady-state species in skeletal mechanism development.

For the simulation of turbulent combustion using either RANS or LES methods, the modeling of turbulence–chemistry interaction (TCI) is a major topic, by e.g. providing a suitable closure for the chemical source term. Both turbulence (from integral to Kolmogorov) and chemistry are characterized by a large range of time and length scales. Many models such as flamelet use the assumption of scale separation between turbulence and chemistry and allow a decoupling of the solution methods, cf. the books [33–35,1,36–38] for comprehensive reviews of multi-scale combustion methods. Time and length scales are also used to define characteristic numbers such as Karlovitz (Ka) or Damköhler (Da) and they are used to identify different regimes.

From this discussion, it becomes apparent that a suitable definition for the chemical time scale is of fundamental importance. This holds especially when chemistry is coupled to transport processes, see e.g., [17,13,15,16] for applications using a combined analysis. When considering rather slow processes such as fuel-rich reforming, the definition of a feasible and characteristic time scale is not straightforward due to the absence of a well defined reaction-zone. For this purpose, the present investigation focuses on the application and comparison of different characteristic chemical time scale definitions using both a simple test problem and a partial oxidation flame with three distinctively different regions. In this article, two new definitions for a time scale are introduced. Their ability to represent the characteristic time scale and thus to retain the system’s dynamics is analyzed. In addition, two established definitions from the literature are compared to the new definitions. In our first example, the time scale analysis is applied to a simple test problem including a global one-step reaction. In the second example, a set

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of homogeneous reactor setups derived from a previously investigated partial oxidation flame with a CO₂ diluted fuel stream and pure CO₂ as oxidizer is considered. These are chosen in order to investigate significantly different reaction dynamics due to varying equivalence ratios. Oxy-fuel processes can lead to significantly different reaction dynamics. The use of pure CO₂ as oxidizer increases the flame temperature and thus the reaction velocity [18]. On the other-hand, a dilution with CO₂ significantly decreases the flame temperatures and thus the reaction speed [19]. Further, the chosen oxy-fuel composition at high equivalence ratios enforces partial oxidation reactions, which exhibit much slower dynamics [16]. Thus, an oxy-fuel composition in fuel lean, stoichiometric and fuel rich mixture is used to study the time scales definitions within different system dynamics.

A description of the mathematical formulation of the time scale definitions is presented in Section 2. The test problem and the corresponding results are presented in Section 3. The partial oxidation flame used as a suitable test case for the different definitions of time scales is presented in Section 4. Results and a discussion can be found in Sections 5 and 6 summarizes the results.

2. Mathematical fundamentals of time scale analysis

Most definitions of time scales are based on the evaluation of the eigenvalues of the Jacobian matrix of the chemical source term. This is a standard method in linear algebra, cf. e.g., [20]. However, we briefly summarize the fundamentals of eigenvalue analysis and its specific application in Section 2.1 and present the different time scales in the following subsections of Section 2.2. Throughout this paper $\|\cdot\|$ stands for the Euclidean vector or matrix norm, respectively.

2.1. Jacobian matrix and eigenvalues

The temporal evolution of mass fractions and temperature of a reacting chemical system is described by the ordinary differential equation

$$\frac{d}{dt} \begin{bmatrix} Y \\ T \end{bmatrix} (t) = \dot{\omega}(Y_1, \dots, Y_{n_{sp}}, T), \quad (1)$$

$$\begin{bmatrix} Y \\ T \end{bmatrix} (0) = \begin{bmatrix} Y_0 \\ T_0 \end{bmatrix}, \quad (2)$$

with the vector of species mass fraction $Y = (Y_1 \dots Y_{n_{sp}})^\top$. In the reaction system, the conservation of all elements must be ensured. Thus, the number of elements n_e such as H or O represents the minimum number of linearly dependent equations. When evaluating the eigenvalues of this system, we find at least n_e trivial eigenvalues [21].

The Taylor expansion of $\dot{\omega}$ with respect to Y^0 at Y^e reads

$$\dot{\omega}(Y^e) = \dot{\omega}(Y^0) + D\dot{\omega}(Y^e - Y^0) + \mathcal{O}((Y^e - Y^0)^2), \quad (3)$$

and by the linearity of the differential operator we have

$$\frac{d}{dt}(Y^e - Y^0) = D\dot{\omega}(Y^e - Y^0) + \mathcal{O}((Y^e - Y^0)^2).$$

The matrix $D\dot{\omega} := (D\dot{\omega}_{ij})_{i,j=1,\dots,n_{sp}} = \frac{\partial \dot{\omega}_i}{\partial Y_j}(Y^0)$ is the Jacobian of $\dot{\omega}$ at time t_0 . By setting $E := (Y^e - Y^0)$ and dropping all high-order terms we obtain that $E(t)$ is the solution of the linear ordinary differential equation with constant coefficients

$$\frac{d}{dt} E(t) = D\dot{\omega} E(t), \quad (4)$$

$$E(t_0) = E_0. \quad (5)$$

By a simple computation we find that

$$E(t) = e^{(t-t_0)D\dot{\omega}} E_0, \quad (6)$$

is the unique solution of Eqs. (4) and (5) where $E_0 = Y^e - Y^0$ is the initial value. Note that $\exp(t - t_0)D\dot{\omega}$ is the matrix exponential function, which is defined by its Taylor series. A popular approach to an analytical solution of Eqs. (4) and (5) is to transform $D\dot{\omega} = VDV^{-1}$, where, in general, V is formed by a non-orthogonal eigenvector basis while D is a tridiagonal matrix.

2.2. Time scales

In the following section, different time scale approximations previously established in the literature and two new ones proposed here are described in detail.

Note that there is a general difference between the first two definitions, which are often used in mechanism reduction methods and the last two definitions. The first two approaches split the time scales into two subsets. One subset forms the fast and thus dissipative time scales. The remaining time scales result in a subset of relevant time scales. Now, we are interested in one single time scale, which can be seen as the characteristic time scale of the chemical system to be compared to the time scales of e.g. the flow problem. In order to select such a single characteristic time scale, an appropriate criterion needs to be defined. This selection is carried out by first identifying a “relevant subspace” of the system’s dynamics and second using the fastest of them as characteristic time scale. Introduced by Caudal et al. [14], the relevant subspace is formed by the minimal set of eigenvectors such that $\|(\sum_{i \in I} \alpha_i v_i) - \dot{\omega}\|$ is smaller than some $\varepsilon > 0$. In contrast, in the ILDM method, the subspace is formed by the eigenvectors related to the small eigenvalues, i.e. to slow processes/larger time scales. A characteristic time scale can then be found in this reduced system as the inverse of the largest eigenvalue related to the eigenvectors, which span the ILDM.

The last two definitions result in a single time scale only, which is assumed to represent the characteristic time scale and thus the system’s dynamics. In the following, 4 algorithms are presented, which approximate the characteristic time scale for a particular reaction system.

2.2.1. Eigenvalue time scale

We recall in the following section the methodology presented in Caudal et al. [14] for the calculation of time scales based on eigenvalue analysis and make the same assumptions concerning the mathematical characteristics such as e.g. the algebraic/geometric multiplicity of the eigenvalues and their eigenvectors. However, it is important to note that in a complex reaction mechanism, the algebraic and geometrical multiplicity of the eigenvalues, which is here assumed to be one can differ. Nevertheless, the solution of the decomposition of the matrix, as shown in the previous section, can still be found by a Jordan decomposition. For a discussion in more detail, see [20].

Again, we transform (6) into a more convenient form by setting $D\dot{\omega} = VDV^{-1}$, where $V = \{v_1, \dots, v_{n_{sp}}\}$ is a matrix of eigenvectors and D is a diagonal matrix with $D_{ii} = \lambda_i$ and the eigenvalues and eigenvectors are in general complex valued. The assumptions in [14] simplify the analysis performed in the following. For real valued eigenvalues, $E_i = (E_0)_i e^{(t-t_0)\lambda_i}$ describes the exponential evolution of the i th component. At $t = t_0$ we have the characteristic velocity λ_i . For complex valued eigenvalues, the eigenvectors are also complex. By splitting the system into a real and a complex part and further by using a complex-to-real transformation we obtain a system in the new eigenvector basis

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