

A Tangential Stretching Rate Index to analyze Ignition Phenomena

M. Valorani*, S. Paolucci†, E. Martelli‡, T. Grenga†

*Sapienza University of Rome, Rome, Italy

†University of Notre Dame, South Bend, Indiana

‡Second University of Naples, Caserta, Italy

Abstract—We introduce an index to analyze numerical datasets simulating ignition in reactive systems. The index is obtained by combining the concepts of stretching rate in dynamical systems with the CSP method, and is validated with reference to a planar model of branched-chain reactions and to a test case involving hydro-carbon oxidation kinetics.

I. INTRODUCTION

Ignition of hydrocarbon fuels is controlled by branched chain-reactions and its complexities increase with the length/size of the fuel molecule. A time scale analysis of auto-ignition in spatially homogeneous systems, carried out by either the Computational Singular Perturbation (CSP) Method [1], [2] or Chemical Explosive Mode Analysis (CEMA) [3], pointed out that a distinguishing feature of the explosive behavior is the emergence of positive eigenvalues during both chain-branching and thermal ignition. To explore details of ignition with the simplest possible model, we consider a planar (2D) model: an isothermal branched-chain explosion model proposed by Williams. We analyzed Williams' model by means of (i) the local tangential stretching rate (TSR) [4], and (ii) a normalized index measuring the relative contribution of each mode to TSR. We first present the theory for the TSR and its validation with reference to Williams' model and the propane/air system.

II. TANGENTIAL STRETCHING RATE: THEORY

The point dynamics of a chemical kinetic system is described by a set of ODEs $\frac{d\mathbf{z}}{dt} = \mathbf{g}(\mathbf{z})$, $\mathbf{z}(0) = \mathbf{z}_0$, $\mathbf{z} \in \mathbb{R}^N$. The state vector \mathbf{z} stands for the species concentration vector, $\mathbf{g}(\mathbf{z}) = S\mathbf{r}(\mathbf{z})$ the species reaction rate vector, S the stoichiometric coefficients matrix, $\mathbf{r}(\mathbf{z})$ the net reaction rates vector, and \mathbf{z}_0 the initial concentrations vector. Consider a scaled measure $\mathbf{v}(t)$ of the difference between two trajectories emanating from two nearby initial conditions, \mathbf{z}_1 , and \mathbf{z}_2 . The vector dynamics of $\mathbf{v}(t) := \lim_{|\underline{\varepsilon}| \rightarrow 0} (\mathbf{z}_2(t) - \mathbf{z}_1(t))/|\underline{\varepsilon}|$, is described by the set of ODEs:

$$\frac{d\mathbf{v}}{dt} = J_{\mathbf{g}}(\mathbf{z}) \mathbf{v}, \quad \mathbf{v}(0) = \mathbf{1}, \quad (1)$$

where $J_{\mathbf{g}} := \partial \mathbf{g}(\mathbf{z}) / \partial \mathbf{z}$ is the Jacobian matrix of \mathbf{g} , and $\mathbf{1}$ is a unit vector at \mathbf{z}_0 taken along any direction. The time

evolution of the norm $v = \sqrt{\mathbf{v}^T \cdot \mathbf{v}}$ obeys the ODE:

$$\frac{dv}{dt} = \left(\frac{\mathbf{v}^T \cdot J_{\mathbf{g}} \cdot \mathbf{v}}{v^2} \right) v, \quad v(0) = 1. \quad (2)$$

The rate at which v grows/shrinks is governed by the (local) rate of stretching of the dynamics, $\omega_{\tilde{\mathbf{u}}}$, evaluated along the direction identified by the unit vector $\tilde{\mathbf{u}} := \mathbf{v}/v$ and defined as:

$$\omega_{\tilde{\mathbf{u}}} := \tilde{\mathbf{u}}^T \cdot J_{\mathbf{g}} \cdot \tilde{\mathbf{u}}. \quad (3)$$

We introduced the TSR by setting $\tilde{\boldsymbol{\tau}} := \mathbf{g}/g$, with $g = |\mathbf{g}|$, and $N-1$ normal stretching rates. Defining the unit normal vector as $\tilde{\mathbf{n}}(\mathbf{z}) = \{\tilde{\boldsymbol{\tau}}_2(\mathbf{z}), -\tilde{\boldsymbol{\tau}}_1(\mathbf{z})\}$, we have

$$\omega_{\tilde{\boldsymbol{\tau}}} := \tilde{\boldsymbol{\tau}}^T \cdot J_{\mathbf{g}} \cdot \tilde{\boldsymbol{\tau}}, \quad \omega_{\tilde{\mathbf{n}}} := \tilde{\mathbf{n}}^T \cdot J_{\mathbf{g}} \cdot \tilde{\mathbf{n}}. \quad (4)$$

Now: $J_{\mathbf{g}} = A\Lambda B$, with left and right normalized eigenvector matrices $A = \{\mathbf{a}_j\}_{j=1,N}$ and $B = \{\mathbf{b}^i\}_{i=1,N}$, and eigenvalue matrix $\Lambda = \{\lambda_j^i\}_{i,j=1,N}$. The unit vector $\tilde{\boldsymbol{\tau}}$ can be rewritten after projecting the vector field over the right eigenvector basis as $\tilde{\boldsymbol{\tau}} = \frac{\mathbf{g}}{g} = \frac{1}{g} \sum_{i=1}^N \mathbf{a}_i f^i$, with $f^i := \mathbf{b}^i \cdot \mathbf{g}$, and $g = \sum_{i=1}^N \mathbf{a}_i f^i$. We now have

$$\begin{aligned} \omega_{\tilde{\boldsymbol{\tau}}} &= \tilde{\boldsymbol{\tau}}^T \cdot J_{\mathbf{g}} \cdot \tilde{\boldsymbol{\tau}} = \frac{1}{g^2} (\mathbf{g}^T A \Lambda B \mathbf{g}) = \frac{\mathbf{g}^T}{g^2} \sum_{i=1}^N \mathbf{a}_i \lambda_i (\mathbf{b}^i \cdot \mathbf{g}) \\ &= \frac{\mathbf{g}^T}{g^2} \sum_{i=1}^N \mathbf{a}_i \lambda_i f^i = \frac{1}{g^2} \sum_{i=1}^N (\mathbf{g}^T \cdot \mathbf{a}_i) \lambda_i f^i = \sum_{i=1}^N W_i \lambda_i, \end{aligned} \quad (5)$$

where $\omega_{\tilde{\boldsymbol{\tau}}}$ is the weighted average of the eigenvalues with weights that depend on the normalized mode amplitudes and on the degree of co-linearity of the eigenvectors \mathbf{a}_i with respect to the vector field \mathbf{g} .

III. TEST CASES

A. Williams' Model

Williams' model [5] consists of a system of three irreversible isothermal branched-chain reactions: $\text{R} \rightarrow \text{C}$ (init), $\text{R} + \text{C} \rightarrow \alpha \text{C} + \text{P}$ (prop), $\text{C} \rightarrow \text{P}$ (term), where R=reactants, C=intermediates, P=products. After normalization, the evolution of R (x_1) and P (x_2) is described by:

$$x_1' = -x_1 - x_1 x_2,$$

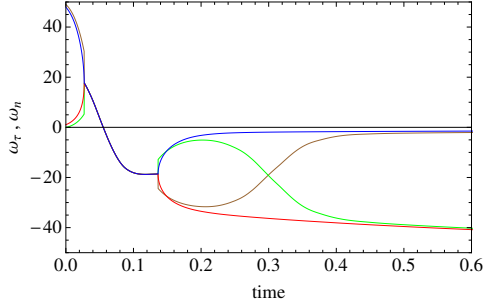


Fig. 1. Williams' model: $\tilde{\omega}_{\tau}$ (brown), $\tilde{\omega}_{\bar{n}}$ (green) and the real part of eigenvalues λ_1 (red), λ_2 (blue).

$$\begin{aligned} \epsilon \mathbf{x}'_2 &= \mathbf{x}_1 + (\alpha - 1)\mathbf{x}_1\mathbf{x}_2 - \gamma\mathbf{x}_2, \\ \gamma \mathbf{x}'_3 &= \gamma\mathbf{x}_2 + \mathbf{x}_1\mathbf{x}_2, \\ (\mathbf{x}_1(0), \mathbf{x}_2(0), \mathbf{x}_3(0)) &= (1, 0, 0). \end{aligned}$$

Figure 1 compares the evolution of the tangential (brown) and normal (green) stretching rates with respect to variations of the real parts of the eigenvalues. We observe that ω_{τ} follows the fast eigenvalue (positive (blue) in the first phase, negative (red) in the last phase) up to time $t = 0.2$. In the interval $t = 0.2-0.45$, the two stretching rates switch between the eigenvalues, so that after $t = 0.45$, ω_{τ} follows the slow eigenvalue (blue). The opposite trend is followed by the normal rate. The striking finding is that ω_{τ} undergoes a smooth transition from the fast to the slow scale occurring in the time range $t = 0.2 - 0.4$. and in so doing it tracks the controlling time scale at all times, independently of any user-defined error threshold.

B. Propane/Air Curran Mechanism

We analyze (Fig. 2) the branched-chain/thermal, adiabatic isochoric, auto-ignition of propane/air oxidation (Curran mechanism [6]) with the TSR, for initial conditions $p=1$ atm, $T=1000\text{K}$, and a stoichiometric mixture. After a short transient, ω_{τ} becomes coincident with λ_{a+} ; a bit sooner than the merging of the two positive eigenvalue, ω_{τ} departs from λ_{a+} . In fact, ω_{τ} begins to sense the “most energetic” dissipative scales until equilibrium, when it becomes coincident with one particular negative eigenvalue. Next, we define a Participation Index of the i -th mode to the TSR as: $P_i^{\omega_{\tau}} = W_i |\lambda_i| / \sum_{j=1}^N |W_j |\lambda_j||$. Modes with a large $P_i^{\omega_{\tau}}$ contribute the most to the development of the most energy containing time scale and form the active sub-space. Figure 3 shows the modes mostly contributing to the active sub-space for the propane/air mechanism ($P_i^{\omega_{\tau}} > 10^{-2}$). It can be noted that at sample #170 of Fig. 2, only two modes (one with an eigenvalue with negative real part and the other with an eigenvalue with positive real part), are above the selected tolerance. We can also apply the CSP criterion [7] to find the number of exhausted modes M .

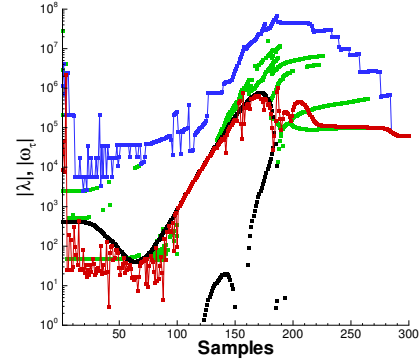


Fig. 2. TSR analysis for propane; eigenvalues with positive real parts (black); first non-exhausted mode (blue); ω_{τ} (red) , modes in active subspace (green).

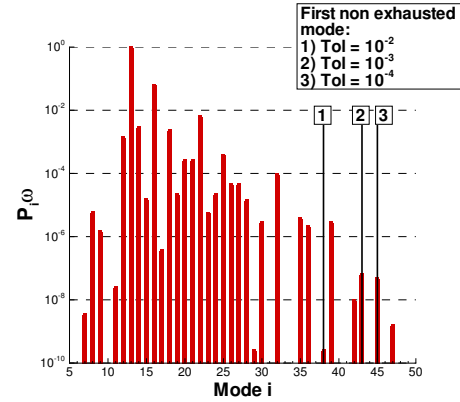


Fig. 3. Participation Index and first non-exhausted mode for different tolerances for sample #170 (see Fig. 2).

The picture shows that, the modes just slower than the first non-exhausted mode, $M+1$, do not contribute much to ω_{τ} .

IV. CONCLUSIONS

The Tangential Stretching Rate concept is a proper characteristic chemical time scale. It is the most relevant during both the explosive and relaxation regimes, is intrinsic to the dynamics, and, as such, it can be identified without the need of ad-hoc assumptions.

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