

REDIM simplified chemistry for the simulation of counter-flow diffusion flames with oscillating strain rates

C. Yu¹, F. Minuzzi², U. Maas¹

¹ Institute of Technical Thermodynamics, Karlsruhe Institute of Technology (KIT), Germany

² Reactive Fluid Mechanics Group, National Institute for Space Research (INPE), Brazil

1 Introduction

In many practical combustion devices such as gas turbines and internal combustion engines, combustion always occurs under transient conditions [1]. Such transient conditions lead to a complex behavior of flame structure and thermo-kinetic quantities. Over the last decades, many efforts have been made to investigate the transient behavior of flames [2,3,4]. Among these investigations is the transient behavior under time-dependent strain rates. In e.g. [4] Darabiha et al. applied a sinusoidal strain rate oscillation and discussed the response of flame structures using complex chemistry for hydrogen-air counter-flow diffusion flames.

In order to study the dynamic behavior of flames, numerical modeling is required and based on the solution of the governing conservation equations for mass, species, momentum and energy [5,6]. Based on detailed chemistry one must solve a large number of conservation equation for species which results in a high computational cost [6], making model reduction desirable. In this work, the Reaction-Diffusion Manifolds (REDIM) reduction method [7], is applied to simplify the chemical kinetics. In this method, the dynamics of system is constrained to a low-dimensional attracting slow manifold in the composition space. In this work, we investigate the applicability of REDIM reduced chemistry to counter-flow diffusion flames with oscillating strain rates, showing that REDIM reduced chemistry can indeed represent the response of flames to oscillating strain rates.

2 Brief review of Reaction-Diffusion Manifolds (REDIM)

The thermo-kinetic states in a reacting system with n_{sp} species can be described by a state vector $\psi = (h, p, \phi_1, \phi_2, \dots, \phi_{n_{sp}})^T$, where h is the specific enthalpy, p the pressure, $\phi_i = w_i/M_i$ the specific mole number of species i (w_i is the mass fraction and M_i the molar mass). Then the evolution of thermos-kinetic states can be represented by the following equation [6]:

$$\frac{\partial \psi}{\partial t} = \mathbf{F}(\psi) - \mathbf{v} \cdot \text{grad}(\psi) + \frac{1}{\rho} \text{div}(\mathbf{D} \cdot \text{grad}(\psi)) \quad (1)$$

where $\mathbf{v}$ is the flow velocity, ρ the density, $\mathbf{F}$ the n -dimensional source term and $\mathbf{D}$ the $n \times n$ -dimensional matrix of the transport coefficients. The target in the concept of low-dimensional manifolds is to describe the original full thermo-kinetic states $\boldsymbol{\psi}$ by a m_s -dimensional manifold with $m_s \ll n$ [6,7]. This can be achieved due to the existence of fast time scales that the system dynamics is governed by m_s slowest modes and thus m_s -dimensional manifolds in the state space [6]. Such a manifold $\mathcal{M}$ is defined as

$$\mathcal{M} = \{ \boldsymbol{\psi} : \boldsymbol{\psi} = \boldsymbol{\psi}(\boldsymbol{\theta}), \quad \boldsymbol{\psi} : R^{m_s} \rightarrow R^n \}, \quad (2)$$

here $\boldsymbol{\theta}$ is the vector of reduced coordinates with m_s dimension. As proposed in [7], the Reaction-Diffusion Manifolds (REDIM) can be obtained by solving the following system of partial differential equations (PDEs) to their steady state:

$$\frac{\partial \boldsymbol{\psi}}{\partial t} = (\mathbf{I} - \boldsymbol{\psi}_{\boldsymbol{\theta}} \cdot \boldsymbol{\psi}_{\boldsymbol{\theta}}^+) \cdot \left\{ \mathbf{F}(\boldsymbol{\psi}) - \frac{1}{\rho} [(\mathbf{D} \cdot \boldsymbol{\psi}_{\boldsymbol{\theta}} \cdot \boldsymbol{\kappa})_{\boldsymbol{\theta}} \cdot \boldsymbol{\kappa}] \right\} \quad (3)$$

where $\boldsymbol{\psi}_{\boldsymbol{\theta}}^+$ is a generalized Moore-Penrose pseudo-inverse of $\boldsymbol{\psi}_{\boldsymbol{\theta}}$. $\boldsymbol{\kappa} = \text{grad}(\boldsymbol{\theta})$ is the gradient of reduced coordinates, which must be estimated and supplied to solve the PDEs.

For the numerical simulation, only m_s conservation equations for $\boldsymbol{\theta}$ are needed to be solved, and all other thermo-kinetics quantities can be obtained through a look-up algorithm based on a stored table of $\boldsymbol{\psi}(\boldsymbol{\theta})$. In the simulation of laminar cases the equation systems in terms of $\boldsymbol{\theta}$ read:

$$\frac{\partial \boldsymbol{\theta}}{\partial t} = \boldsymbol{\psi}_{\boldsymbol{\theta}}^+ \cdot \left\{ \mathbf{F}(\boldsymbol{\psi}(\boldsymbol{\theta})) + \frac{1}{\rho} \text{div}(\mathbf{D} \cdot \boldsymbol{\psi}_{\boldsymbol{\theta}} \cdot \text{grad}(\boldsymbol{\theta})) \right\} - \mathbf{v} \cdot \text{grad}(\boldsymbol{\theta}) \quad (4)$$

From a numerical point of view, to solve the PDEs (Eq.3) one needs: (i) a gradient estimation $\boldsymbol{\kappa}$; (ii) a boundary condition; (iii) a initial condition/profile; (i) is a crucial point in the implementation of REDIM. However, as already shown in [7], the REDIM does not depend much on this gradient estimation for manifolds with higher dimensions. (ii) defines the application regime of the final REDIM reduced chemistry. (iii) is the least important point, because any reasonable initial condition can be applied and has no influence on the accuracy of the REDIM reduced chemistry.

The counter-flow diffusion flame used in this work has a composition of 25% methane and 75% air in the fuel stream with 292 K and pure air in the oxidizer stream with 294 K. This mixture is the same as that in the Sandia Flame [8]. Therefore, a 2D-REDIM was built for this specific case.

In Fig.1, we show in the left figure the initial profiles for Eq.3 used in this work. Blues lines are the flamelet solution based on detailed chemistry. The left most and right most flamelets enclose the application regime, defining the boundary condition. The middle flamelet supplies the gradient estimation for Eq.3. The red mesh grid in the left figure defines the initial profile/condition, which is obtained by a simple linear interpolation between three flamelets. After integrating eq.3, one obtains the stationary solution representing the REDIM reduced chemistry in the right figure (red mesh grid). Furthermore, we also plot several stable (blue lines) and extinguishing flamelets (green lines) in the right figure, showing that the REDIM reduced chemistry (red mesh grid) and the stable and extinguishing flamelets almost overlap with each other, so that REDIM can indeed describe the flame state quite well.

To summarize, the construction of REDIM requires very little knowledge of the studied system. One only needs determine the application range for boundary condition and any one initial condition to solve the Eq.3. Although the gradient estimation is required, the REDIM is not much sensitive to it and a simple and reasonable gradient estimation is sufficient.

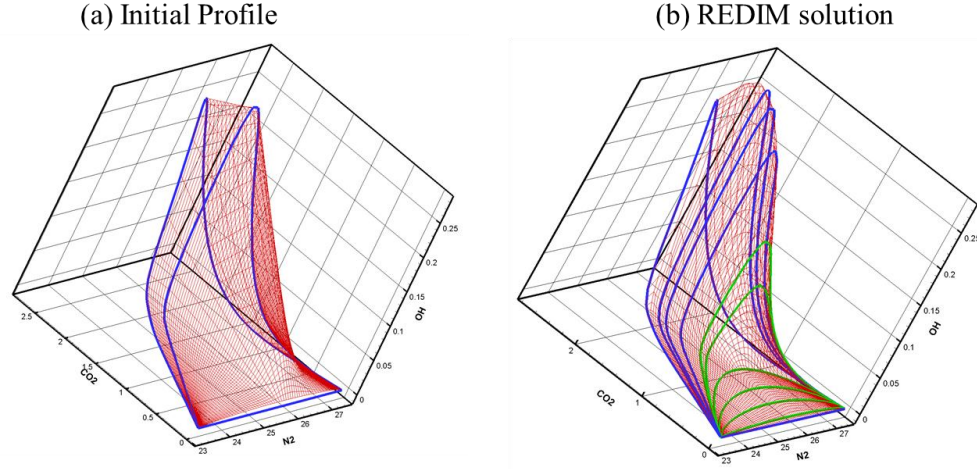


Fig. 1 (a) the initial profile (red mesh grid) for the integration of REDIM; (b) the REDIM reduced chemistry (red mesh grid); Blue lines: flamelets define the boundary conditions and supply the gradient estimation; Green lines: stable and extinguishing flamelets based on detailed chemistry.

3 Steady Counter-flow diffusion flames

A 2D-REDIM reduced chemistry cf. Fig.1 (right figure) is applied. The computational time for the calculation using 2D REDIM reduced chemistry is only 6% of the time using detailed chemistry. Fig.2 shows the maxima of temperature and mass fractions of CO_2 and OH over strain rates. The quenching strain rate for detailed chemistry $a_{\text{quenching}}^{\text{detail}} = 648 \text{ s}^{-1}$, and the quenching strain rate for REDIM reduced chemistry $a_{\text{quenching}}^{\text{redim}} = 610 \text{ s}^{-1}$. It can be observed clearly that at low strain rates ($a < 400 \text{ s}^{-1}$) REDIM reduced chemistry agree with detailed chemistry very well, while at high strain rates noticeable deviations can be seen. Such deviations, however, can be decreased if one uses a better gradient estimation or increases the dimension of the REDIM reduced chemistry.

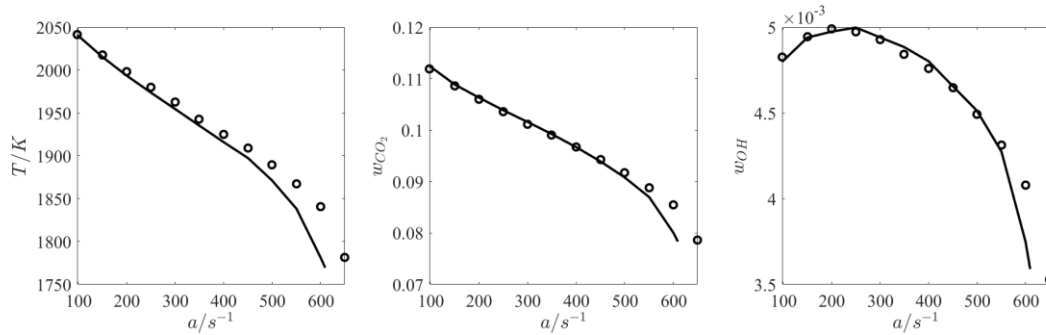


Fig. 2 Maxima of temperature and mass fractions of CO_2 and OH over strain rate a/s^{-1} . Circles: detailed chemistry solution; Lines: REDIM reduced chemistry solution.

4 Test case for oscillating strain rates

In this work, the strain rates a are assumed to vary continuously as a sine function: $a(t) = a_0 - A \cdot \sin(2\pi f \cdot t)$, where a_0 is the mean value of the strain rates, A the amplitude and f the

frequency. Three oscillating cases will be studied. We will consider one case with strain rates far from the quenching limit (case 1), one case with strain rates near the quenching limit (case 2) and one case with strain rates exceeding the quenching limit (case 3):

- 1) Case 1: the mean value is selected to be $a_0 = 200 \text{ s}^{-1}$ and the amplitude to be half of the mean value $A = a_0/2 = 100 \text{ s}^{-1}$, ensuring that for the whole oscillating phase flames are far from quenching limit. The frequency is set to be 10 Hz, 200 Hz and 500 Hz.
- 2) Case 2: the mean value is selected to be $a_0 = 400 \text{ s}^{-1}$ and the amplitude to be again half of the mean value $A = a_0/2 = 200 \text{ s}^{-1}$. In this case, the maximal reachable strain rate ($a = 600 \text{ s}^{-1}$) is then close to the quenching limit. The frequency is set to be 10 Hz, 200 Hz and 500 Hz.
- 3) Case 3: we keep the frequency to be 10 Hz and the mean value to be $a_0 = 400 \text{ s}^{-1}$. However the amplitude is set to be $A = 230 \text{ s}^{-1}$ (for which extinction occurs only for REDIM reduced chemistry) and $A = 300 \text{ s}^{-1}$ (for which extinction occurs for both detailed and REDIM reduced chemistry) (see Fig.2).

Note that, although in the following context only temperature profiles are shown due to space limitations, species concentrations are also checked and the same conclusions can be drawn.

5 Results and Discussion

In Fig.3, we first show the temporal development of temperatures for different frequencies for case 1 (mean value $a_0 = 200 \text{ s}^{-1}$ and $A = 100 \text{ s}^{-1}$). We can observe clearly that for this case which flames are far from the quenching limit), temperature profiles from REDIM reduced chemistry and detailed chemistry correspond to each other very well. The only noticeable deviation occurs when the minimal temperatures are reached. For example at around $t = 0.075 \text{ s}$ for 10 Hz, minimal temperature for detailed chemistry is 1936 K and for REDIM reduced chemistry is 1929K. However, such differences are relative small.

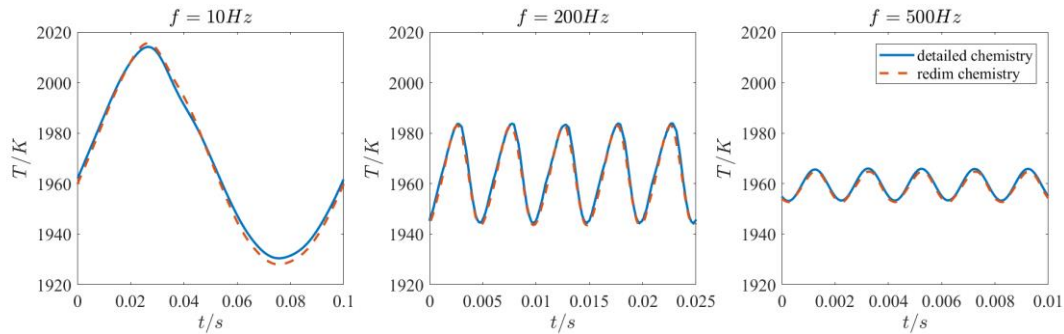


Fig. 3 time history of temperatures under harmonic oscillation strain rates with different frequencies for case 1 (mean value $a_0 = 200 \text{ s}^{-1}$ and $A = 100 \text{ s}^{-1}$).

Figure 4 shows the time development of temperatures for different frequencies for case 2 (mean value $a_0 = 400 \text{ s}^{-1}$ and $A = 200 \text{ s}^{-1}$). For this case, the REDIM reduced chemistry agrees with detailed chemistry very well where strain rates are far from quenching limit (temperature higher than mean value). However, the deviations become large when strain rates are close to the quenching limit. The largest deviations can be observed at around e.g. $t = 0.075 \text{ s}$ for 10 Hz or $t = 0.009 \text{ s}$ for 200 Hz where the

instantaneous strain rates are the closest to the quenching limit. This observation is consistent with the results shown in Fig.2, that for temperatures deviations between results from detailed chemistry and from REDIM reduced chemistry become large for the strain rates above 500 s^{-1} . Furthermore, the deviations become smaller with increasing frequencies.

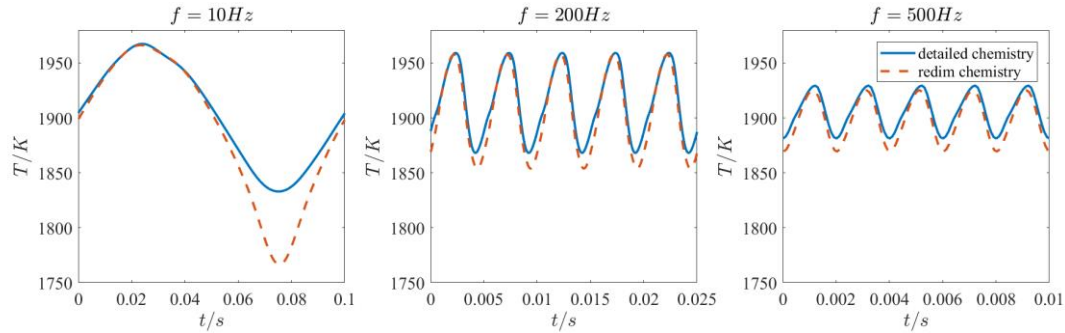


Fig. 4 time history of temperatures under harmonic oscillation strain rates with different frequencies for case 1 (mean value $a_0 = 400 \text{ s}^{-1}$ and $A = 200 \text{ s}^{-1}$).

In Fig.5, we show the results for case 3. The left most figure shows the oscillating strain rates for case 3, and the middle and right figures show the temperature profiles. For $A = 230 \text{ s}^{-1}$ (middle figure) the extinction occurs for REDIM chemistry, while no extinction for detailed chemistry. This is because the peak strain rates are very close to the quenching limit and the REDIM chemistry predicts the extinction earlier than detailed chemistry (compared to Fig.2 and left figure in Fig.5). Therefore we observe that the detailed chemistry predicts stable flames while REDIM chemistry causes extinction at around 0.07 s. However, we must emphasize here that we use a simple gradient estimation to construct the REDIM reduced chemistry in this work. If we use a more detailed gradient estimation, such deviation can be removed and our test showed that profiles based on REDIM reduced chemistry agree those with detailed chemistry again [9].

If one further increases the amplitude ($A = 300 \text{ s}^{-1}$) so that for both detailed and REDIM chemistry extinction process happen (red line in left figure in Fig.5), we see again a good agreement between detailed and REDIM chemistry (right figure in Fig.5). As REDIM chemistry has a smaller quenching strain rate, the extinction of flame predicted by REDIM chemistry runs earlier than detailed chemistry. However, time for detailed chemistry that flame is completely extinct is around 0.069 s and this time for REDIM chemistry is around 0.063 s. Thus the corresponding relative errors for REDIM chemistry is only around 8% compared to detailed chemistry, which is of an acceptable accuracy.

5 Conclusion

In this work, the Reaction-Diffusion Manifolds (REDIM) reduced chemistry has been applied for the simulation of counter-flow diffusion flame under harmonic oscillating strain rates with different frequencies. For oscillating strain rates far from quenching limit, REDIM reduced chemistry predicts the dynamic behaviors very well compared to detailed chemistry. For oscillating strain rates near to the quenching limit, noticeable deviation can be observed at the position where maximal strain rates are reached. However, such deviations decrease with increasing frequencies. For the cases where instantaneous strain rates exceed the quenching limit, REDIM reduced chemistry predicts the extinction process earlier than detailed chemistry with 8% time deviations, which is in acceptable accuracy. All

results show the applicability of REDIM reduced chemistry to represent the dynamic behaviors of unsteady flames quite well.

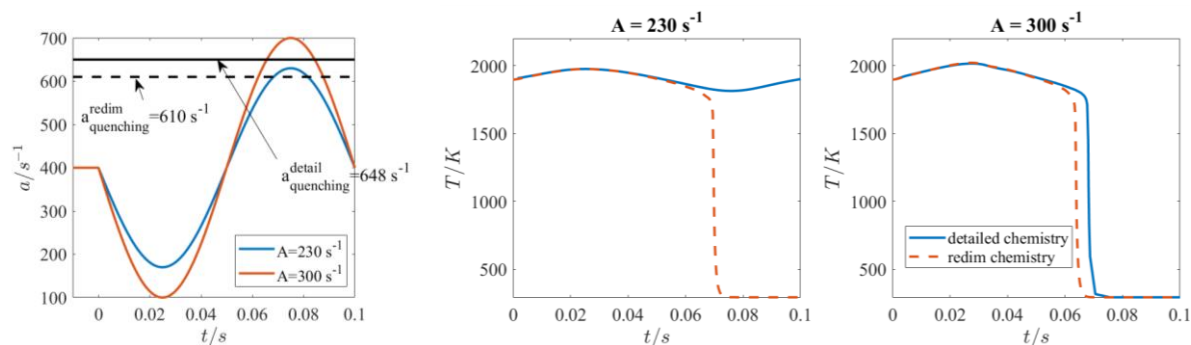


Fig. 5 left: time history of strain rates over one period. Middle and right figure: time history of temperatures under harmonic oscillation strain rates with different amplitudes. Blue: detailed chemistry; Red: REDIM chemistry.

6 Acknowledgement

Financial support by the DFG within the DFG/MOST project MA 1205/26 is gratefully acknowledged. F.Minuzzi acknowledges financial support from CAPES – Brazil, under the context of the PNPD program. The authors thank Prof. Dr. T.Ueda from Keio University for helpful discussions.

References

- [1] F.E.C. Culick, M.V.Heitor, J.Whitelaw. (1997). Unsteady Combustion. AIAA Journal 35(5): 920.
- [2] C.J.Sung, J.B.Liu, C.K.Law (1995). Structural Response of Counterflow Diffusion Flames to Strain Rate Variations. Combustion and Flame 102: 481-492.
- [3] T.M.Brown, R.W.Pitz, C.J.Sung (1998). Oscillatory stretch effects on the structure and extinction of counterflow diffusion flames. Symposium (International) on Combustion: 703-710.
- [4] N.Darabiha (1992). Transient Behaviors of laminar counterflow Hydrogen-Air diffusion flames with complex chemistry. Combustion Science and Technology 86: 163-181.
- [5] J.Warnatz, U.Maas, R.W.Dibble (1996). Combustion, Vol 3, Springer.
- [6] T.Turanyi, A.S.Tomlin (2016). Analysis of kinetic reaction mechanisms. Springer.
- [7] V.Bykov, U.Maas (2007). The extension of the ILDM concept to reaction diffusion manifolds. Combustion Theory and Modelling, 11(6):839-862.
- [8] R.S.Barlow, J.H.Frank (1998). Effects of turbulence on species mass fractions in methane/air jet flames, Symposium (International) on Combustion, 27 (1): 1087-1095.
- [9] C.Yu, F.Minuzzi, U.Maas. publication in preparation.