Investigation of perturbed premixed flame structure using REDIM model reduction concept

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Abstract

Turbulent flames are governed by a strong and interaction between reaction and diffusion caused mainly by intensive convective mixing. The correct description of such transient combustion processes represents a challenging problem, especially for model reduction concepts. In premixed flames turbulence leads to a wrinkled or corrugated flame fronts. In the present study the performance of the Reaction-Diffusion-Manifold (REDIM) model reduction in such flame scenarios is investigated. It is examined whether the REDIM method is able to capture the transient combustion process of perturbed premixed methane-air flames.

Introduction

Recently, transient dynamics of combustion systems has attracted attention because of the importance of critical regimes of combustion for applications. This is due to the fact that for the increase of the efficiency (economy) and robustness of control of pollutants of the combustion facilities extreme (e.g. lean) conditions have to be used. Consequently, unstable (with different types of flame instabilities) and highly turbulent regimes are often in the focus of the study.

However, most combustion models (mechanisms of chemical kinetics, transport models etc.) have been mainly developed to address the stationary dynamics of the flame. This is clear because experimental and numerical investigations of reacting flows in stationary regimes are more convenient. But for developing reliable models dealing with transient combustion regimes, especially in the context of model reduction, it is very important to develop the method to compare and validate the reduced model in transient regimes.

In this work a method for comparison and validation of reduced models in transient regimes of combustion is suggested. A pre-mixed methane/air combustion system is considered in the frame of freely propagating 1D flames. Stationary propagating flames are perturbed and transient behavior leads back to the global steady state – a steadily propagating flame. The transient flame behavior is investigated both in the physical as well as in the system composition state space. In order to model the chemical reaction and turbulence interaction and to obtain physically meaningful perturbed initial solutions the so-called triplet maps are used [1]. Accordingly, initially stationary propagating laminar flames are perturbed by implementing triplet maps which can be interpreted as instantaneous perturbation of a single eddy leading to corrugated flame structures.

According to the construction of the triplet map the perturbed system states do not leave the stationary profile mapped in the system composition space. At the same time the scalar fields (species concentrations, temperature etc.) of the reacting system in physical space are changed. Thus, the magnitude of the local gradients is increased leading to dominant diffusive transport processes in the triplet mapping region. Through this, the initially stationary flame is deflected from its stationary solution profile but it relaxes to its initial state if no further perturbation is applied. This relaxation process is investigated as a suitable and physically meaningful model of transient behavior of a combustion system. In order to test the performance of the reduced model in these regimes several quantities are suggested, namely, estimation of the overall relaxation time and the time scale of the relaxation. The profiles evolving with the time are compared to the stationary profile by using the developed measure which is invariant with respect to the profile translation.

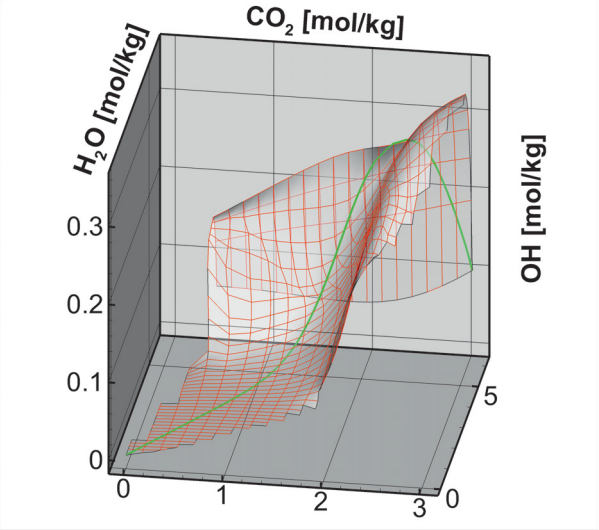

Figure 1: 2D REDIM manifold (red) with stationary system solution and 1D REDIM manifold (green) in the projection to CO_2-H_2O-OH specific mole numbers.

Both 1D and 2D (system reduced state spaces) REDIM based reduced models are compared to the detailed model transient solution. Perturbations are varied in size and location of perturbation within the stationary flame front. The accuracy of the reduced models is determined by comparing reduced and detailed transient flame structures during the relaxation processes in both state and physical space. Special attention is paid

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to the effect of the reduced model dimension on the relaxation time scale. It is shown that the reduced model accounts for processes connected to different time scales and that it is able to correctly describe the interaction of diffusion and reaction within perturbed flames typical for turbulent regimes.

REDIM based concept of model reduction

The approach used in this study, which includes the flamelets method as a limiting case, is the REDIM method [4]. It assumes that the system solution profile always belongs (stays close to) to the surface (manifold) of low dimension imbedded in the system composition state space (see Fig. 1). In the REDIM method this manifold is defined by an invariance equation as a quasi-(partial) equilibrium between fast chemical and transport processes accounting automatically only those processes which couple in the given velocity (gradients') field [4, 5].

Once the REDIM manifold is found, the system can be reduced through a reformulation of the system of governing equations [6] on this manifold. Accordingly, the suggested methodology represents a powerful and very important tool for validating the main assumption and quantifying the accuracy of the manifold's based reduced models in the transient combustion system behavior.

Implementation of perturbations

One dimensional free laminar premixed methane-air flames are considered for the investigation of turbulent effects on the inner flame structure. The influence of turbulence is represented by one dimensional eddies of different size and location within the flame front. The implementation of such turbulent eddy perturbation events can be conducted efficiently by a rearrangement of flame profiles in the form of a triplet map. Triplet maps approximate three-dimensional turbulent effects by increasing gradients through the redistribution of fluid elements along a one-dimensional domain [7]. Triplet mapping has measure preserving property, i.e. mass, energy and momentum conservation are not influenced by the rearrangement. Figure 2 depicts the mapping strategy in detail. The mapping in this study is applied in direction of the one dimensional flow. Moreover, constant pressure is assumed.

The implementation of triplet mapping in turbulent flow calculations [8, 9] incorporates frequency and eddy-size distribution of events based on different approaches [10]. In this work a single mapping event is applied instantaneously on a stationary one-dimensional free premixed flame profile (red profile in Fig. 2). The resulting perturbed profile (green profile in Fig. 2) is then used as a starting solution for detailed and reduced numerical calculations of the relaxation process towards the stationary solution. During the relaxation process no more mapping events are implemented.

Triplet mapping perturbations implemented in the study are characterized by the location in the flame front and by the eddy size. At different locations eddies of four different sizes are implemented. Then the relaxation process towards the stationary solution is investigated in composition state space and in physical space. Eddy sizes are chosen in dependence of the flame thickness [11] of the investigated system. The example eddy in Fig. 2 is characterized by its occurrence location at $(r_0 + r_0 + l)/2$ and its size l, while r_0 is left eddy boundary.

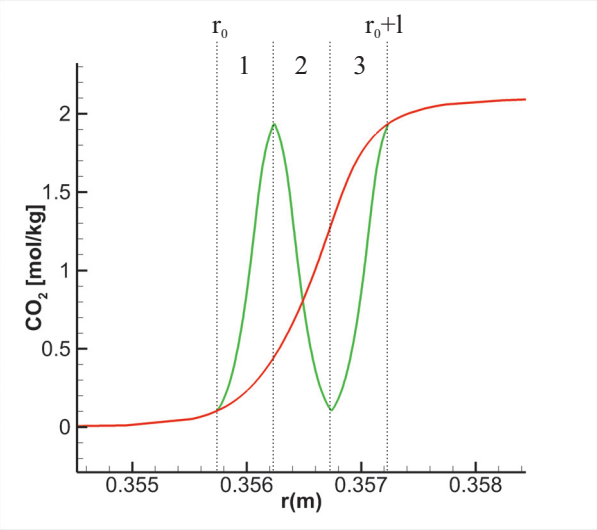


Figure 2: Triplet mapping (green profile) applied on a stationary free premixed methane-air flame profile of equivalence ratio ϕ=0.6 (red), CO_2 profile in specific mole numbers is illustrated. The segment between r_0 and r_0+l is shrunk to a third and three copies are placed on the original domain, while the middle sector is mirrored [10].

The study focuses on the relaxation process of initially implemented perturbations in form of triplet maps. One dimensional and two dimensional reduced models are compared with the detailed model regarding time scale of relaxation and relaxation time. Moreover, the reduced models are validated through a detailed analysis of the relaxation process in both composition system state space and physical space. In order to ensure comparability perturbations are applied on the same stationary profile for both detailed and reduced calculations.

It arises naturally from the formulation of the REDIM theory [3, 12] that the initial, unperturbed stationary profile (red profile in Fig. 2) is situated on both the one dimensional and two dimensional REDIM in the composition system state space (see Fig. 1). Due to the measure preserving property of triplet maps the states of the perturbed initial profile (green profile in Fig. 2) are not deflected from the manifolds. This property enables a consistent comparison of detailed and reduced relaxation processes.

Time scale analysis and relaxation time

In order to determine the time scale of the relaxation process transient solution profiles of both detailed and reduced simulations should be compared to an

unperturbed reference profile. The stationary profile (see Fig. 2) is used as a reference profile for the comparison. The comparison is based on the time dependent mean quadratic distance between the transient and the reference profiles based on species i

$$\varepsilon_i(t) = \frac{1}{N}\sum_{j=1}^{N}\frac{\sqrt{\left(\Psi_{i,j}(t) - \Psi_{i,j}^{ref}\right)^2}}{\Psi_{i,max}^{ref}}, \qquad (1)$$

where ε_i is the mean quadratic distance of the i-th scalar, N is the number of gridpoints, $\Psi_{i,j}$ is the value of the i-th scalar at the j-th gridpoint within the transient profile, $\Psi_{i,j}^{ref}$ is the corresponding reference value of the i-th scalar at j-th gridpoint and $\Psi_{i,max}^{ref}$ is the maximal reference value of the corresponding i-th scalar.

During the relaxation process a shift between the transient profiles and the reference profile in physical space is observed. Moreover, the gridpoints of both the reference profile and the transient profiles are unequally distributed because of the regridding during the numerical integration. The evaluation of $\varepsilon_i(t)$ must therefore be adapted at each time step within the solution procedure and has to be translation invariant to be used for comparison of 1D reduced, 2D reduced and detailed system solutions during the transient system behavior. This is accomplished in the following way. First, the gridpoints of the transient profile are redistributed equally at each timestep of the numerical calculation within a fixed frame in which the relaxation process takes place. The states on the redistributed grid are calculated by linear interpolation. Afterwards, the profile is shifted in physical space relative to the reference profile at each time step and $\varepsilon_i(t)$ is calculated at each frame position during the shift. Thus, a minimum value of $\varepsilon_i(t)$ can be extracted for a certain scalar i, e.g. CO_2, at each time step. In this way a quantifiable parameter of analyzing relaxation is defined which also allows a comparison between detailed and reduced calculations. The process is illustrated in Fig. 3 for a free premixed methane-air flame with the equivalence ratio of ϕ=0.6 (Fig. 2).

It is found that during the relaxation of the implemented perturbation towards the stationary solution the value for $\varepsilon_i(t)$ decreases exponentially. Therefore, the time scale of the relaxation process can be determined through the examination of $\ln(\varepsilon_i(t))$ (see Fig. 4). Accordingly, the slope of $\ln(\varepsilon_i(t))$ corresponds to the time scale of relaxation.

Although relaxation leads back towards the stationary solution, $\varepsilon_i(t) \to 0$ will not be reached due to the numerical simulation process (discretization, linear interpolation etc.). Still, a critical value for $\ln(\varepsilon_i(t))$ can be defined at which the relaxation process can be considered as completed. This represents a useful means for determining the time after which the relaxation process is practically completed. We call this time the relaxation time (see Fig. 4).

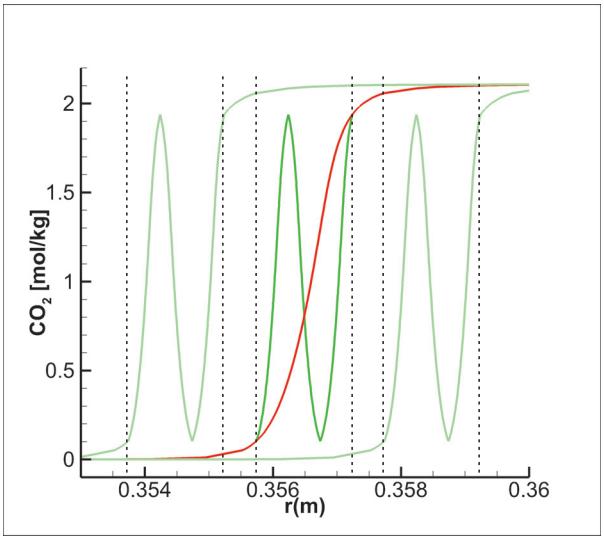


Figure 3: Shift between the transient profile (green) and the reference profile (red) at one timestep. The transient profile is re-interpolated on an equally distributed grid within a fixed frame (dashed lines) and then the frame is shifted from left to right relative to the reference profile. At each frame position $\varepsilon_i(t)$ is calculated based on the number of gridpoints within the frame. The middle frame position yields the minimum value for $\varepsilon_i(t)$ in this example.

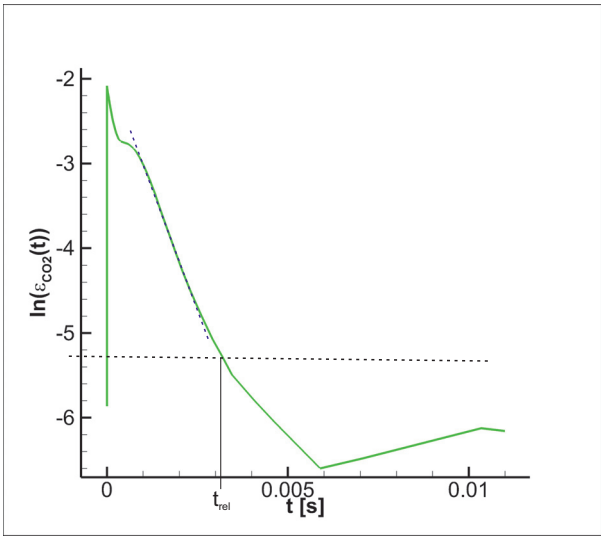


Figure 4: Decay of $\ln(\varepsilon_{CO_2}(t))$ for the eddy shown in Fig. 2. The slope of the tangent, blue dashed line represents the time scale of relaxation. The relaxation process can be considered as completed, if the black dashed line is underrun. Thus, a relaxation time t_{rel} can be defined for comparison purposes.

Results

The above methodology is applied for free laminar premixed methane-air flames of equivalence ratio ϕ=0.6 and ϕ=0.9. For both systems reduced numerical calculations are compared to detailed numerical

calculations. As a representative example the relaxation process is discussed for an eddy of size of the flame thickness and a location of occurrence within the flame profile at the position of maximum CO_2 gradient for the ϕ=0.9-system. At the chosen location the application of triplet maps leads to the maximum possible deviation from the reference profile. Thus, transient processes during relaxation can be illustrated and analyzed more clearly for this example.

Figure 5 illustrates the relaxation process in physical space for the detailed and reduced calculations. It can be observed that both the 1D and 2D reduced calculations are able to capture the highly transient processes of the detailed calculation. Due to the triplet mapping gradients are increased significantly and the relaxation process towards the stationary solution is initially dominated by strong diffusion processes.

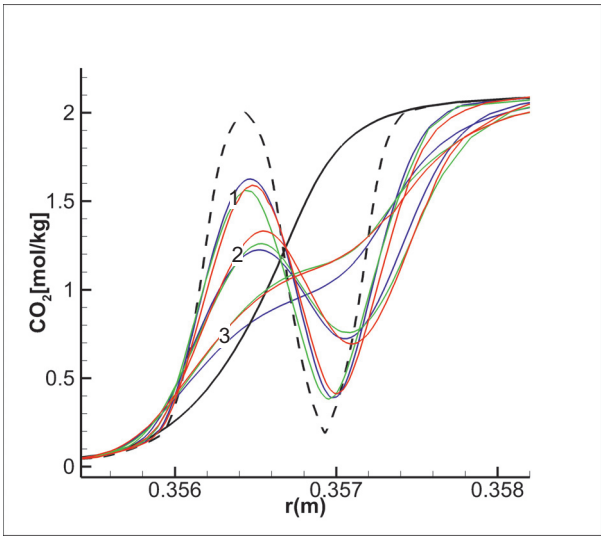


Figure 5: Relaxation process of an eddy of certain size and location of occurrence for the ϕ=0.9-system starting from the perturbed initial solution (dashed line) towards the stationary solution (black solid line). Different time steps are shown: $3 \cdot 10^{-6}$s (1), $2 \cdot 10^{5}$s (2), $6 \cdot 10^{-5}$s (3) and $5 \cdot 10^{-3}$s (stationary solution). Blue profiles: detailed calculation. Red profiles: 2D reduced calculation. Green profiles: 1D reduced calculation.

In Fig. 6 the influence of the instantaneous perturbation implemented by triplet mapping described in Fig. 5 is illustrated in projection to two dimensional state space representation (CO_2-H_2O-projection). Due to the measure preserving property of the triplet map, the states of the perturbed initial solution (dashed line in Fig. 5) are redistributed along the one dimensional profile in state space which describes the stationary solution (solid black line in Fig. 5). Moreover, the one dimensional REDIM which is used in the 1D reduced calculations also corresponds to the same profile in state space representation. That is, the relaxation process of the 1D reduced calculation (green profile in Fig. 6) occurs along the one dimensional REDIM, while the perturbed initial solution as well as the stationary solution lie on the same one dimensional green profile in state space representation in Fig. 6.

While the 1D reduced relaxation process is confined to the 1D REDIM, 2D and detailed relaxation processes lead to deviations from the one dimensional stationary solution profile in system state space representation. Caused by the instantaneous gradient increase as a consequence of the triplet mapping, strong diffusion processes firstly push 2D reduced and detailed solution profiles towards the mixing line [13]. Subsequently, relaxation processes lead to an overshoot in H_2O direction before the stationary solution state is achieved. Obviously the 2D reduced profile relaxation follows the detailed profile relaxation very well in CO_2-H_2O-projection representation.

Both the 2D reduced and the detailed relaxation remain confined to the 1D stationary solution profile, i.e. to the 1D REDIM, in the vicinity of the chemical equilibrium point. Here, the transition is dominated by fast chemical processes which relax perturbation towards the 1D system ILDM [14]. That is, in the vicinity of the equilibrium point the 1D REDIM corresponds to a 1D ILDM. Therefore, deviations from the 1D REDIM during the detailed and the 2D reduced relaxation processes occur predominantly in regimes which are characterized by a strong coupling between diffusion and chemical processes (Fig. 6).

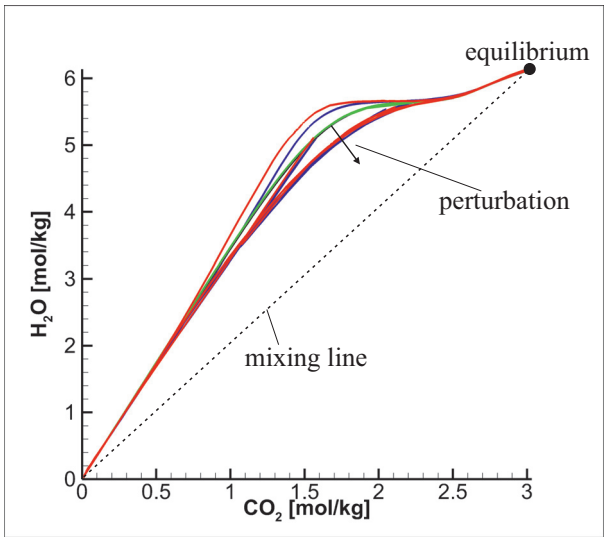


Figure 6: Relaxation process from Fig. 5 shown in 2D state space representation in CO_2-H_2O-projection. The equilibrium point denotes the state of the burnt gas. Perturbations lead to deviations towards the mixing line.

During the 2D reduced relaxation process the system solution profiles remain confined to the 2D REDIM, as Fig. 7 illustrates in CO_2-H_2O-CH_2O-projection of the state space. In comparison, detailed calculations manifest considerable deviations not only from the 1D REDIM but also from the 2D REDIM during the relaxation process. Again the influence of the instantaneous perturbation becomes visible. Detailed solution profiles are deviated from the 2D REDIM in CH_2O direction before they are relaxed back to the manifold. Still, the 2D reduced model

is able to capture the detailed relaxation process to a higher extent compared to the 1D model. Due to the hierarchical nature of REDIMs [12] the 1D REDIM is embedded in the 2D REDIM, i.e. 1D reduced solution profiles are also embedded into the 2D REDIM.

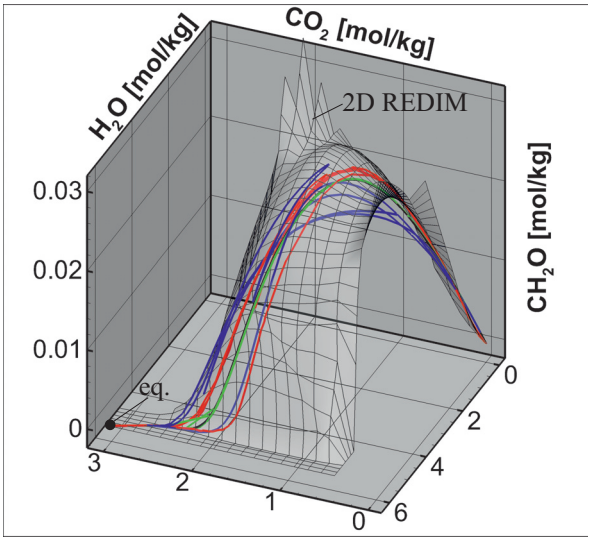


Figure 7: Relaxation process from Fig. 5 and 2D REDIM shown in 3D state space representation in CO_2-H_2O-CH_2O-projection. The equilibrium point denotes the state of the burnt gas.

As it was shown in Fig. 5 the relaxation process for the example perturbation applied on the system with equivalence ratio ϕ=0.9 can be considered as completed after less than $5 \cdot 10^{-3}$s. The relaxation of an eddy of same characteristic size and location of occurrence applied on a system with equivalence ratio ϕ=0.6 is characterized by a longer relaxation time and a lower relaxation time scale. In Fig. 8 the decay of $\ln(\varepsilon_{CO_2}(t))$ is compared for both systems for the described characteristic perturbation. It can be observed that the time scale of relaxation is much higher in the case of ϕ=0.9. Thus, the relaxation time for the same characteristic perturbation is much higher for the lean system with ϕ=0.6. The characteristic behavior for both systems is captured by both the 1D and 2D reduced models.

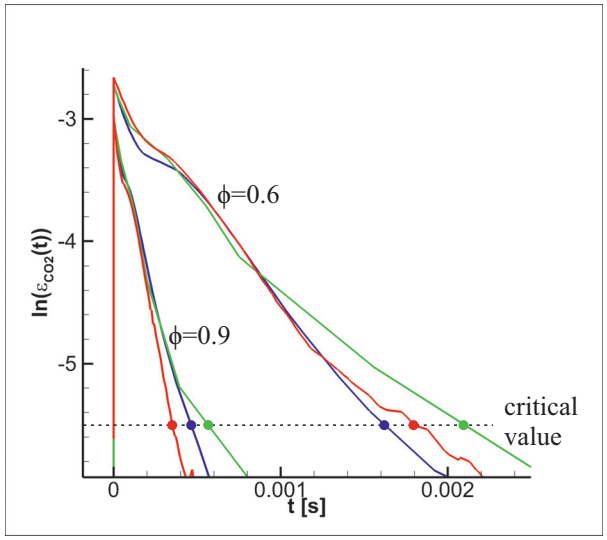
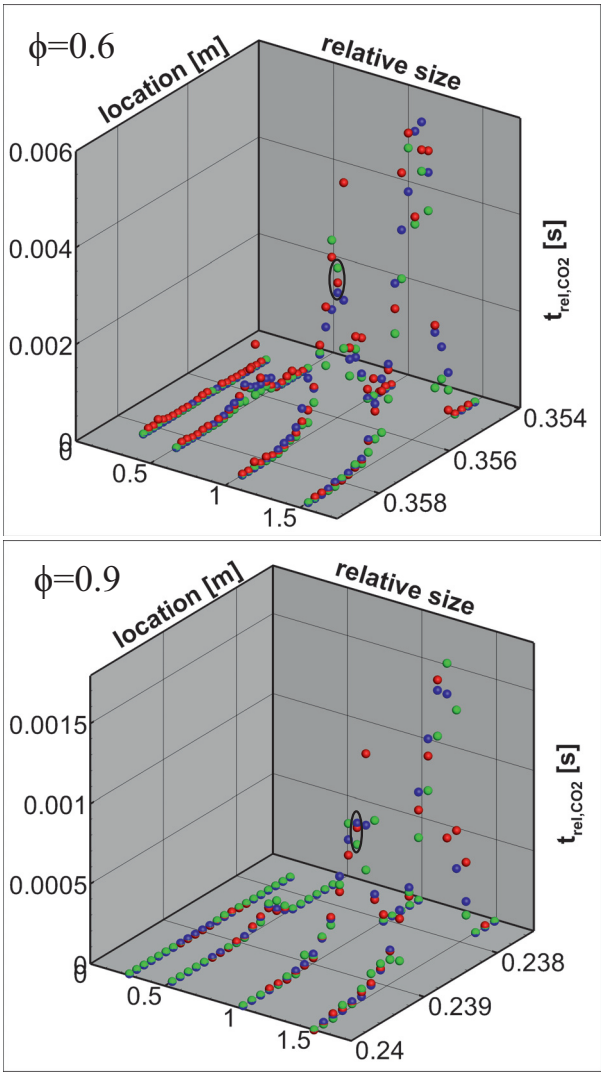


Figure 8: Decay of $\ln(\varepsilon_{CO_2}(t))$ for detailed (blue), 1D reduced (green) and 2D reduced (red) relaxation of the same characteristic perturbation (relative size and location) for two free laminar premixed methane-air flame systems of equivalence ratio ϕ=0.6 and ϕ=0.9.

As described previously (see Fig. 4) the relaxation time t_{rel,CO_2} is defined as the time elapsed when $\ln(\varepsilon_{CO_2}(t))$ becomes lower than a critical value. Here, we chose a critical value of -5.5 for the definition of t_{rel,CO_2}. Note however, that this value has no explicit physical meaning. Nevertheless, it represents a useful means for the comparison between perturbations of different sizes and locations and between the two considered systems. In Fig. 9 and 10 t_{rel,CO_2} is shown in dependence of applied eddy sizes relative to the flame thickness ζ and locations of occurrence for both systems. The marked data points correspond to the values of t_{rel,CO_2} for the example perturbations shown in Fig. 8. The flame thickness of the lean ϕ=0.6-system measures 10^{-3}m and it is nearly twice as large as the flame thickness of the ϕ=0.9-system which measures $6 \cdot 10^{-4}$m. Thus, the absolute size of the implemented eddies also differs.

It can be seen that the lean ϕ=0.6 system leads to relaxation times which are about four times higher than the relaxation times for the ϕ=0.9 system for the same relative eddy size. Moreover, it can be deducted from the illustration that eddies of the same absolute size also lead to significant longer relaxation times if they are applied on the ϕ=0.6 system.

For both systems t_{rel,CO_2} is increasing with the relative eddy size. The estimate for the global relaxation time t_{rel,CO_2} strongly depends on the location of occurrence of the applied perturbation. Surprisingly a maximum of t_{rel,CO_2} can be observed for both systems at the location of maximum CO_2 gradient (see figure caption). Once again, there is a very good agreement between reduced and detailed calculations concerning t_{rel,CO_2}.



Figures 9 and 10: Relaxation time t_{rel,CO_2} based on the decay of $ln(\varepsilon_{CO_2}(t))$ for detailed (blue), 1D reduced (green) and 2D reduced (red) simulations. Four different eddy sizes are applied, dependent on the flame thickness ζ: 0.25·ζ, 0.5·ζ, 1.0·ζ and 1.5·ζ. Locations of occurrence depend on the position of maximum gradient of CO_2 (ϕ=0.6: 0.3569m, ϕ=0.9: 0.2388m) and are equally distributed over the flame zone. For each eddy size 25 eddy locations are considered. Marked data points correspond to t_{rel,CO_2}-values from Fig. 8.

Conclusion

The ability of the REDIM based model reduction method of describing premixed turbulent combustion processes was investigated in the present study. For this purpose the relaxation process of instantaneous perturbed free laminar premixed methane-air systems of two different equivalence ratios (ϕ=0.6 and ϕ=0.9) was examined. Perturbations were implemented as triplet maps, which have measure conserving properties. The results of 1D and 2D reduced numerical calculations were validated through a comparison with detailed numerical calculations. A translation invariant quantity for the comparison of transient profiles was suggested and applied to validate the reduced models. The time scale of the relaxation process and the relaxation time were estimated based on this quantity.

A comparison of the relaxation process between reduced and detailed simulations in state and physical space showed that both reduced models captured the characteristic transition of the system solution profiles towards stationary state. Although the 1D reduced model limits the transient profile relaxation to a one dimensional domain in system state space, the relaxation process in physical space showed good agreement to the detailed relaxation process. Thus, for moderate perturbations which did not lead to extinction processes, i.e. the flamelet assumption was fulfilled, the implementation of the 1D reduced model was sufficient in order to properly describe the detailed relaxation processes.

Investigations showed that the influence of equivalence ratio and size and location of perturbations on time scale of relaxation and relaxation time was captured by both reduced models. The ϕ=0.6 system lead to significantly longer relaxation times and lower time scales of relaxation for the same characteristic perturbation.

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