A versatile coupled progress variable / REDIM model for auto-ignition and combustion: Parameterization, Coupling and Implementation Strategies

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Abstract

In previous work, we presented a coupled model, which unifies the advantages of a progress variable model (PVM) for auto-ignition in media of very weak scalar gradients, and of a model based on the reaction diffusion manifold approach (REDIM) for reaction coupled with diffusive transport. Both models correspond to different low-dimensional manifolds in state space. In this paper, we discuss the parameterization of the models' manifolds, especially of the reaction progress, as well as a simple, robust method for coupling both models, by introducing an additional dimension, namely a normalized strength of spatial gradients. The implementation and behaviour of this coupled model is shown. Exemplary one-dimensional numerical simulations of an auto-igniting hot-spot transitioning into a propagating flame are performed, both with fully detailed calculation and by employing the coupled reduced chemistry, respectively.

Introduction

Many models for the simplified, reduced treatment of chemical reactions in CFD simulations exist (e.g. ILDM [1, 2], REDIM [3, 4], GQL [5], FGM [6, 7], flamelet concept [8], flamelet-prolongation of ILDM [9], CSP [10], QSSA [11] or progress variable models [12–14]). These models provide pre-calculated chemical source terms as functions of some set of reduced variables. One could attribute most of the existing models either to the case where the system's behavior is governed by the coupling of chemistry with molecular transport, or to the case where no such coupling exists and solely the chemical reaction is important, without essential influence of transport (e.g, the case of homogeneous auto-ignition). But in practical combustion scenarios, the strength of this coupling varies in a wide range, mostly residing between these two extremes. Examples for this behavior can be found in stratified combustion, or in situations like hot-spot auto-ignition where an initially nearly-homogeneous system becomes increasingly affected by diffusive transport of thermal energy and chemical species due to the build-up of scalar gradients by chemical reactions.

In this paper, we refer to a progress variable model (PVM) [12, 15], describing chemical reactions without any influence of transport effects, and to a model based on the reaction diffusion manifold approach (REDIM) [3, 4, 16], covering situations with interaction of chemistry and diffusion. In order to couple both models, we presented a unified model in previous work [15]. With this approach, a combined application of both models is possible. One approach to alleviate this coupling is a unified parameterization of both manifolds. For physical variables (e.g. conserved quantities like mixture fraction or enthalpy), this is not problematic. But for chemical progress variables(s), this is non-trivial, since the models rely on different definitions of these progress variables.

Using a consistent parameterization for both models, the combined use of the models is strongly alleviated.

In a first, simple approach towards coupling the models, an additional dimension, namely a normalized strength of spatial gradients, is introduced into the unified model. This variable physically represents the strength of diffusive transport.

The implementation and behaviour of the unified model is later shown and validated by exemplary one-dimensional calculations of a hot-spot with detailed transport and detailed and reduced chemistry, respectively.

Parameterization

In preparation of the coupling of the PVM and REDIM-based model, we use a uniform parameterization of the models' manifolds. As mentioned above, this is straightforward for physical variables (e.g. mixture fraction Z, enthalpy h, pressure p). In contrast, the parameterization of the reaction progress is challenging. Common candidate variables for reaction progress are temperature, mass fractions of certain chemistry-sensitive species (e.g. of CO_2), or linear combinations of them. This approach is very problem-dependent, and could cause conflicts with the requirements of a progress variable [12, 17]. Applying an automated formulation [17] of the progress variable, one could satisfy these requirements. The exact physical definition, however, is still problem-dependent.

For the PVM, we introduced an alternative parameterization, based on the specific entropy s and the entropy $\dot{s}_{\text{prod}}$ produced by chemical reactions [15, 18], respectively. Temporal integration over a trajectory from initial state (denoted by index 0) to chemical eqilibrium (denoted by index ∞) and normalization leads to the progress variable χ and its source term $\dot{\chi}$ as a function of time t:

$$\chi(t) = \frac{\int_{t_0}^{t} \dot{s}_{\text{prod}}(t^*)\, dt^*}{\int_{t_0}^{t_\infty} \dot{s}_{\text{prod}}(t^*)\, dt^*} \tag{1}$$

$$\dot{\chi}(t) = \frac{\dot{s}_{\text{prod}}(t)}{\int_{t_0}^{t_\infty} \dot{s}_{\text{prod}}(t^*)\, dt^*} \tag{2}$$

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Since $\dot{s}_{\text{prod}} > 0$ according to the second law of thermodynamics, χ is guaranteed to be monotonically increasing along the integration path. For systems without transport of heat or mass, $\int \dot{s}_{\text{prod}}\, \mathrm{d}t$ is identical to the local increase of the system's entropy.

Even if transport processes are essential (like for the REDIM), integrating the term $\dot{s}_{\text{prod}}$ over any path in state space will lead to a variable that is monotonically increasing along this path. The result is, however, no more identical to the system's entropy. Nevertheless, the progress variable bears a relatedness to chemical entropy production also in this case. Note that the actual physical meaning of χ and its entropy-relatedness are irrelevant for a later use of the model in CFD applications.

Starting with a 2-dimensional REDIM with its original parameterization given by $\boldsymbol{\theta} = [\xi, Z]$ the manifold is reparameterized. The reaction progress variable χ calculates by integration along lines of constant mixture fraction Z:

$$\chi\left(\xi, Z\right) = \frac{\int_{\xi_0}^{\xi} \dot{s}_{\text{prod}}\left(\xi^*, Z\right) \cdot \left(\dot{\xi}^*\right)^{-1} \mathrm{d}\xi^*}{\int_{\xi_0}^{\xi_\infty} \dot{s}_{\text{prod}}\left(\xi^*, Z\right) \cdot \left(\dot{\xi}^*\right)^{-1} \mathrm{d}\xi^*} \quad (3)$$

$$\dot{\chi}\left(\xi, Z\right) = \frac{\dot{s}_{\text{prod}}\left(\xi, Z\right)}{\int_{\xi_0}^{\xi_\infty} \dot{s}_{\text{prod}}\left(\xi^*, Z\right) \cdot \left(\dot{\xi}^*\right)^{-1} \mathrm{d}\xi^*} \quad (4)$$

with $\dot{\xi}$ beeing the source term of the initial reaction progress parameterization ξ.

In both cases this finally yields χ, by which the reaction progress of both the PVM and REDIM are tabulated. Also, the chemical source term for this variable is obtained:

$$\dot{\chi}_{\text{chem}} = f\left(\chi\right) \quad (5)$$

Coupling Strategy

Both PVM and REDIM rely on low-dimensional manifolds in state space, to which the dynamics of the system is limited. However, the different model assumptions underlying these approaches yield different manifolds. To perform a coupling of the models, a smooth transition between the manifolds is desired. This transition should be in directions of the fast chemical subspace [15]. Employing the global quasi-linearization approach (GQL) [5] to identify these fast subspaces, the matrix $\boldsymbol{M}_s$ describing the slow subspace can be identified and a reduced state $\boldsymbol{\theta}$ (indicated by index PVM or REDIM) can be projected from the PVM manifold onto the REDIM manifold, or vice versa:

$$\boldsymbol{M}_s \boldsymbol{\Psi}_{\text{PVM}}\left(\boldsymbol{\theta}_{\text{PVM}}\right) = \boldsymbol{M}_s \boldsymbol{\Psi}_{\text{REDIM}}\left(\boldsymbol{\theta}_{\text{REDIM}}\right) \quad (6)$$

$\boldsymbol{\Psi}$ denotes the detailed state of the PVM or the REDIM, respectively.
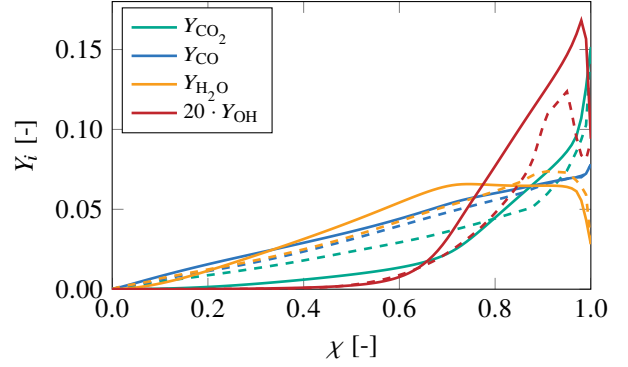

Figure 1: Mass fraction of major and minor species over progress variable based on entropy produced by chemical reaction. $\phi = 1$, $T = 1000\,\text{K}$, $p = 10\,\text{bar}$. solid: PVM, dashed: REDIM

In a first attempt the matrix $\boldsymbol{M}_s$ can be defined as a line of zeros with the columns corresponding to CO_2 or H_2O set to one. Assuming that entropy is only noticeably produced by chemical reaction within the slow subspace, reaction progress variable can be defined according to equation 1 (PVM) and 3 (REDIM). Figure 1 shows major species (CO_2 and H_2O) and minor species (CO and OH) as a function of this progress variable for an equivalence ratio $\phi = 1$, $T = 1000\,\text{K}$ and $p = 10\,\text{bar}$. It is seen that at $\chi = 0$ and $\chi = 1$, the scalars for REDIM and PVM match; these points correspond to the same physical states, namely unburned mixture and chemical equilibrium, respectively. Overall, the species mass fractions considered as functions of the progress variable are described by similar curves.

According to the consistent parameterization of the PVM and REDIM manifolds (including reaction progress based on entropy produced by chemical reaction) the projection simplifies and it holds $\boldsymbol{\theta}_{\text{PVM}} = \boldsymbol{\theta}_{\text{REDIM}} = \boldsymbol{\theta}$.

Furthermore, we introduce a new dimension α which describes a normalized distance in state space between the PVM-manifold and the REDIM manifold. α is normalized to the interval $[0, 1]$, with $\alpha = 0$ corresponding to points on the PVM-manifold (resulting from chemical reaction without dissipative transport) and $\alpha = 1$ corresponding to points on the REDIM-based manifold (strong coupling of reaction and dissipation). The points described by $0 < \alpha < 1$ notionally correspond to states between the manifolds, and the transition from 0 towards 1 for α would in this picture correspond to an increased importance of dissipative processes for the reacting system. This will not necessarily match the exact physical behaviour; however, the focus here is on obtaining a practical, simple and robust model that can incorporate both auto-ignition and flame propagation.

The variables delivered by the model $\boldsymbol{F}\left(\boldsymbol{\theta}\right)$ are then computed by linear interpolation between the PVM and REDIM:

$$\boldsymbol{F}\left(\boldsymbol{\theta}\right) = \left(1 - \alpha\right) \cdot \boldsymbol{F}_{\text{PVM}}\left(\boldsymbol{\theta}\right) + \alpha \cdot \boldsymbol{F}_{\text{REDIM}}\left(\boldsymbol{\theta}\right) \quad (7)$$
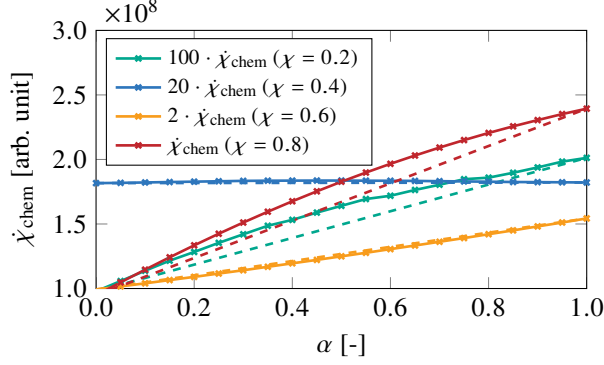
Figure 2: Source term of progress variable interpolated between PVM and REDIM (varying χ). $\phi = 1$, $T = 1000\,\mathrm{K}$, $p = 10\,\mathrm{bar}$. solid: source term calculated from interpolated state, dashed: interpolated source term

Figure 2 shows the chemical source term of the progress variable $\dot{\chi}_{\mathrm{chem}}$ interpolated from the models (dashed) and calculated from the interpolated state vector (solid), respectively. The deviation in the whole range is very small.

The consistent parameterization of both models is not mandatory, but facilitates this coupling and makes it computationally faster, since the projection of states from one manifold to the other manifold is straight-forward.

Implementation

In the following, a practical implementation of the coupled model will be demonstrated and tested.

Calculations for both model calculation and validation (PVM and REDIM) relied on detailed chemical kinetics, and were performed with the in-house code INSFLA [20] for reacting flows in one-dimensional systems. A mechanism for toluene reference fuel (TRF) [21] was used. Table 1 shows the composition of the fuel, which corresponds to an octane number of 95.

Table 1: Composition of the toluene reference fuel (TRF)

	C_8H_{18}	C_7H_{16}	$C_6H_5CH_3$
vol-%	82.08	7.92	10.00
mol-%	76.99	8.35	14.66

For the coupled model used in this work the parameter range in progress variable was set to $0.0 < \chi < 1.0$, in pressure to $10\,\mathrm{bar} < p < 63\,\mathrm{bar}$ and in mixture fraction according to an equivalence ratio to $0.5 < \phi < 3.3$. Instead of the specific enthalpy, the temperature T_{ub} of the corresponding unreacted mixture (index *ub* stands for *unburned*) was used as a tabulation parameter in the range of $500\,\mathrm{K} < T_{\mathrm{ub}} < 1250\,\mathrm{K}$.

The gradient estimate [3] for REDIM was taken from detailed calculations of non-premixed, adiabatic, isobaric flames of different stretch rates.

To ensure the normalized progress variable ($0 < \chi < 1$) describing the same *unreacted* ($\chi = 0$) and *burned* ($\chi = 1$) state for both models, the chemical equilibrium was calculated [22] and used to complete the temporal trajectory and the line of constant mixture fraction, respectively, when computing the progress variable (see equation 1 and 3).

In a first attempt the temperature gradient was used to estimate the strength of spatial gradients α for the coupling in the reduced calculations. Based on the temperature gradients of detailed calculations α was normalized with a factor of 10^5 and limited to the interval $[0, 1]$.

Validation

In order to validate the reduced chemical kinetics of the coupled model, without side-effects of modeling transport processes in the reduced state space, the system of conservation equations for the detailed state $\boldsymbol{\Psi}$ was solved [11]:

$$\frac{\partial \boldsymbol{\Psi}}{\partial t} = S\left(\boldsymbol{\Psi}\right) - \boldsymbol{v}\,\mathrm{grad}\left(\boldsymbol{\Psi}\right) + \frac{1}{\rho}\,\mathrm{div}\left(\boldsymbol{D}\,\mathrm{grad}\left(\boldsymbol{\Psi}\right)\right) \quad (8)$$

Here $\boldsymbol{v}$ denotes the flow velocity, ρ the density and $\boldsymbol{D}$ the generalized diffusion matrix [23]. For the following calculations Le = 1 and equal diffusivities were used. This yields $\boldsymbol{D} = \boldsymbol{I} \cdot d$, with the diffusion coefficient d. Nevertheless, these simplifications are not mandatory for the application of the coupled model.

The chemical source term $S\left(\boldsymbol{\Psi}\right)$ was computed from the source term of the progress variable and the Jacobian of the detailed state vector, both delivered by the coupled model:

$$S\left(\boldsymbol{\Psi}\right) = \dot{\chi}\frac{\partial \boldsymbol{\Psi}}{\partial \chi} \quad (9)$$

For both detailed and reduced calculation an initial profile was created with homogeneous pressure $p = 15\,\mathrm{bar}$ and homogeneous species composition corresponding to an equivalence ratio $\phi = 1$. Temperature was set to $T = 1000\,\mathrm{K}$ with a 20 K hot-spot at the left side of the calculating domain. Figure 3 shows the initial temperature profile.
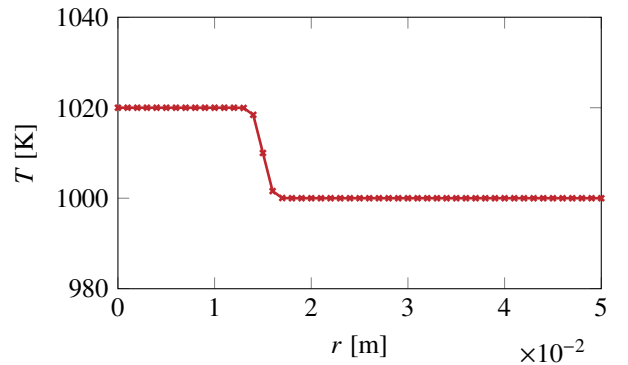

Figure 3: Initial temperature profile for a 1020 K hot-spot embedded into a 1000 K ambience. $\phi = 1$, $p = 15\,\mathrm{bar}$.
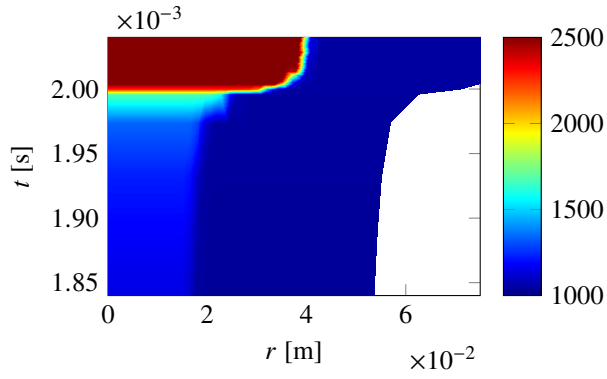
Figure 4: Detailed calculation: Temporal evolution of a 1020 K hot-spot embedded into a 1000 K ambience. $\phi = 1$, $p = 15$ bar. The colorbar shows temperature in K
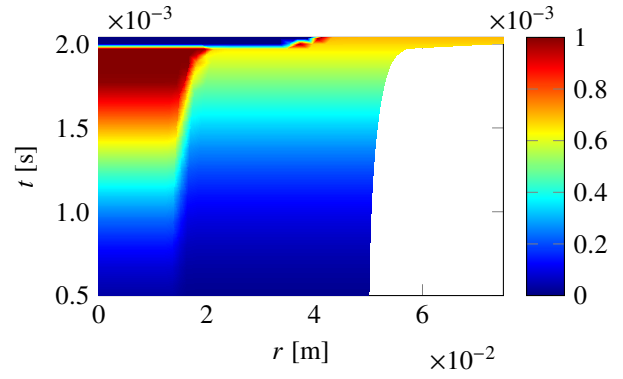

Figure 6: Detailed calculation: Temporal evolution of a 1020 K hot-spot embedded into a 1000 K ambience. $\phi = 1$, $p = 15$ bar. The colorbar shows massfraction of CH_2O
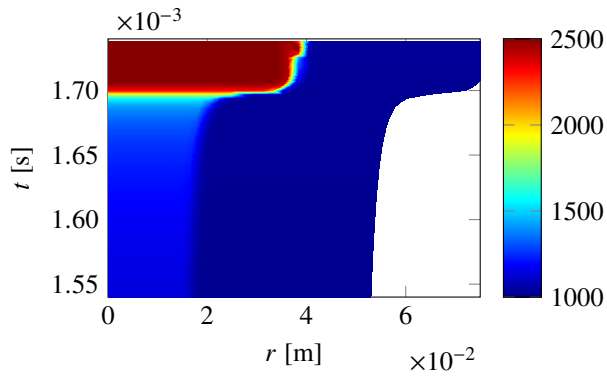

Figure 5: Reduced calculation: Temporal evolution of a 1020 K hot-spot embedded into a 1000 K ambience. $\phi = 1$, $p = 15$ bar. The colorbar shows temperature in K
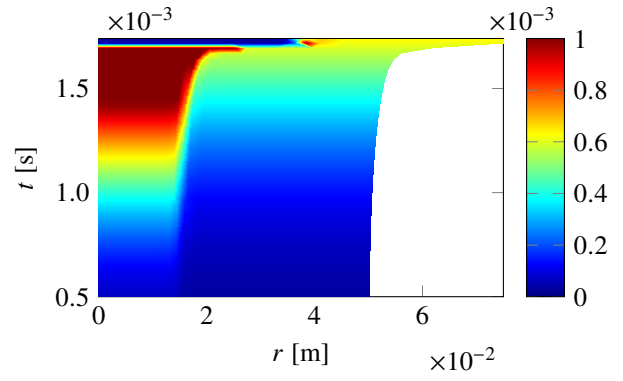

Figure 7: Reduced calculation: Temporal evolution of a 1020 K hot-spot embedded into a 1000 K ambience. $\phi = 1$, $p = 15$ bar. The colorbar shows massfraction of CH_2O

Figure 4 and 5 show the temporal evolution of the temperature profile for detailed and reduced calculation, respectively. It can be seen, that the hot part of the profile ignites and as a result of the rise in temperature the volume expands. Then a flame propagates from the ignited hot-spot into the cooler surrounding. These phenomenons are all well represented by the reduced calculation. The ignition of the hot-spot takes place within 2,0 ms for the detailed and 1,7 ms for the reduced calculation, respectively. So it differs by 15 %.

Figure 6 and 7 show the temporal evolution of mass fraction CH_2O for detailed and reduced calculation, respectively. CH_2O is produced in the early stage of ignition, so the highest values are on the left side of the calculating domain before ignition. Also the cooler right side of the doamin starts to ignite and a rise in CH_2O mass fraction is noticeable. As it is consumed in later stages of ignition, the lowest values are in the burned area. Apart from deviation in ignition delay (as mentioned above) the reduced calculation matches very well with the detailed results in these terms. This means, that not only the temperature rise of ingnition and flame propagation but also the pre-ignition phase and the evolution of minor species (like CH_2O) is captured very well by the coupled model.
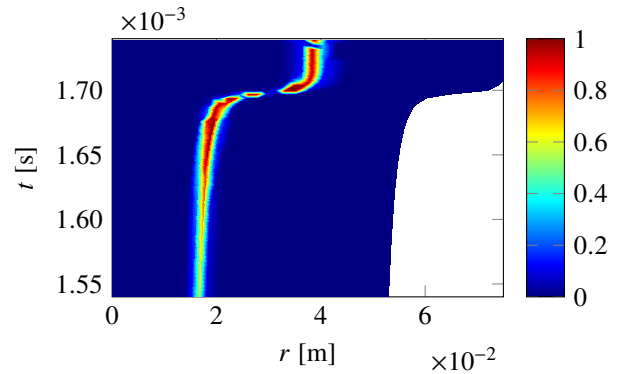

Figure 8: Reduced calculation: Temporal evolution of a 1020 K hot-spot embedded into a 1000 K ambience. $\phi = 1$, $p = 15$ bar. The colorbar shows normalized strength of spatial gradients

Figure 8 shows the normalized strength of spatial gradients α, which represents the application of the PVM and REDIM in the coupled model. In a wide range of the domain α has values near zero and the reduced calculation is dominated by the PVM. But as the hot-spot starts to ignite, temperature rises and local gradients develop the REDIM

model gets more influence until flame propagation is fully dominated by REDIM.

Conclusion

In this work we introduced, discussed and tested a versatile coupled model which aims at describing both auto-ignition and flame propagation in a unified framework. The starting point are exsting dedicated models for auto-ignition (Progress variable model, PVM) and for flame propagation (Reaction diffusion manifold, REDIM).

By introducing a consistent parameterization for both the PVM-manifold and the REDIM-based manifold, we got a simple and robust projection for states from one manifold onto the other. Additionally, this projection comes close to the GQL-directions, which are physically motivated. Furthermore the normalized strength of spatial gradients was introduced. This property is used to perform the coupling of both models, by linear interpolating between them.

We show results from both detailed and simplified simulations (the latter using the coupled model) of a hot-spot igniting and subsequently developing into a propagating flame, as a test case for the coupled model. Although we got small deviations (i.e. in ignition delay), the results are reasonable. Besides the spatial and temporal evolution of temperature, also the production rate of minor species (like CH_2O) in the early phase of ignition is captured very well by the model.

Acknowledgements

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