

Optimization of the progress variable definition using a genetic algorithm for the combustion of complex fuels

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Abstract

In this work counterflow diffusion flamelets of n-heptane and air are used at stable and unsteady extinguishing conditions for building a thermo-chemical database for Computational Fluid Dynamics (CFD) calculations. The injectivity of the progress variable definition is achieved through an optimization process using a genetic algorithm in combination with an adequate objective function.

Keywords: tabulated chemistry, optimization, flamelet

1. Introduction

Tabulated chemistry methods present a compromise between computational cost and the ability to capture complex combustion physics in CFD simulations. These methods are suitable to describe strain or heat loss induced extinction, yet solving a handful of partial differential equations is sufficient for their application. For these reasons, they have been an attractive approach in industrial applications.

Turbulent non-autoigniting non-premixed flames subjected to intense heat loss present a particular challenge in this context, as the tabulation needs to capture 1) the effect of mixing, 2) the effect strain on stable flames, 3) the unsteady process of strain induced extinction, 4) and the effect of heat loss.

These phenomena are commonly modelled using counterflow diffusion flamelets. They represent different equivalence ratios by nature, as the mixing of pure fuel and oxidizer happens in the domain. Stable, steady state solutions can be computed at various strain rates up to the extinction point. Raising the strain beyond the extinction point, the extinction process can be represented by solving an unsteady flamelet.

Such an array of counterflow diffusion flamelets can be characterised by a mixture fraction (Z) and a progress variable (Y_c). The mixture fraction corresponds to the fraction of mass originating from the fuel inlet, thus Z represents different locations along each counterflow

flamelet. In this work, the mixture fraction is computed following Bilger [1]:

$$Z = \frac{b - b_o}{b_f - b_o}, \quad (1)$$

where $b = 2 \frac{z_C}{W_C} + 0.5 \frac{z_H}{W_H} - \frac{z_O}{W_O}$ is a linear combination of the elemental mass fractions: z of carbon: C , hydrogen: H , and oxygen: O , and the f , and o subscripts signify fuel and oxidizer respectively.

The progress variable is a linear combination of various species, it is meant to distinguish between different counterflow flamelets:

$$Y_c = \sum_{k=1}^{N_S} a_k Y_k, \quad (2)$$

with N_S : the number of species solved in the counterflow flamelet, a_k : an array of weights representing the progress variable, and Y_k : the mass fractions of different species.

An additional degree of freedom has to be introduced to account for heat loss. In counterflow diffusion flamelets lower enthalpy levels are commonly achieved by modifying the inlet temperatures of fuel and oxidizer. This is a viable option for autoigniting flamelets, as the high inlet temperatures permit large modifications, and a significant enthalpy deficit can be achieved. As this work focuses on non-autoigniting flames, the effect of lowering inlet temperatures is too limited. Additionally, a modified optically thin radiation model is used in the flamelet calculations to impose heat loss [2]. The additional source term in the enthalpy (h) equation of the

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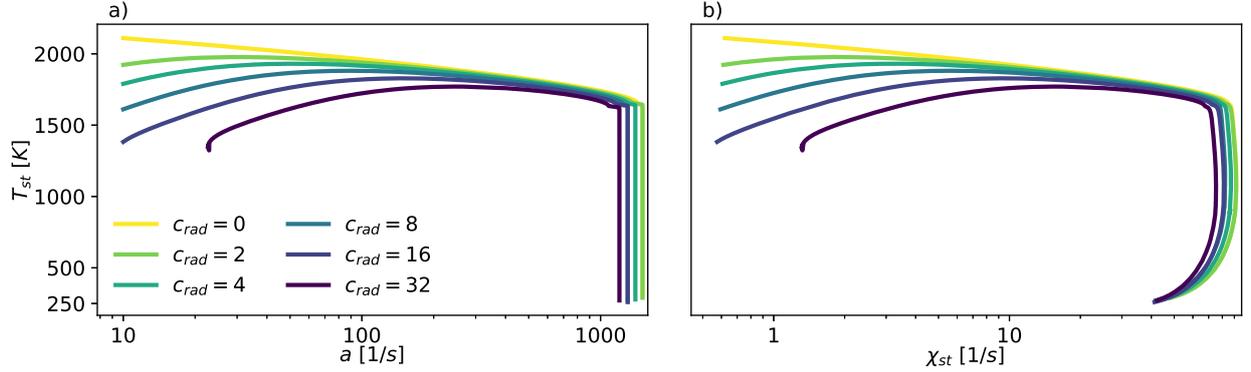


Figure 1: Temperature of the included flamelets at stoichiometric mixture fraction, as function of a) the strain rate, b) the stoichiometric scalar dissipation rate.

flamelets is:

$$S_r = -4c_{rad}k_P\sigma T^4, \quad (3)$$

where k_P is the Planck mean absorption coefficient, σ is the Stefan-Boltzmann constant, T is the temperature, and c_{rad} is a constant used for reaching different enthalpy levels. The absorption coefficient is calculated using the weighted sum of grey gasses model based on the absorption coefficients of CO_2 and H_2O .

A crucial aspect of the tabulation method is the appropriate definition of the progress variable. A good definition has to ensure, that each chemical state of the precomputed flamelets is uniquely described by the set of control variables (Z, Y_c, h), as in the CFD simulations only these control variables are solved. Thus at a given value of mixture fraction on a given enthalpy level, the progress variable has to monotonically decrease as the strain rate of steady flamelets increases, and continue monotonically decreasing in time, as the unsteady extinguishing flamelet progresses to pure mixing. In other words the progress variable has to be injective.

This works present method to improve the injectivity of the progress variable definition. The definition applied by Ma [3] is used as a reference:

$$Y_c^{ref} = \frac{4Y_{CO_2}}{W_{CO_2}} + \frac{Y_{CO}}{W_{CO}} + \frac{2Y_{H_2O}}{W_{H_2O}} + \frac{0.5Y_{H_2}}{W_{H_2}} \quad (4)$$

In section 2 the flamelet set is introduced, section 3 the genetic algorithm and its objective function is defined, in section 4 the optimized progress variable definition is tested in the CFD framework [4], finally conclusions are drawn.

2. Flamelets

The presented optimization method is developed in the context of spray combustion simulations of the Cambridge swirl flames data repository [5], in particular the n-heptane case: H1S1. In this gas turbine model flame ambient temperature liquid n-heptane is injected directly into the combustion chamber. The oxidizer is air, also supplied at an ambient temperature or 288 K. The system is open to the laboratory, thus the thermodynamic pressure is taken as 101325 Pa.

To generate the thermo-chemical database, opposing diffusion flames are computed using Chem1D [6] at stable and unsteady extinguishing conditions. The skeletal mechanism of Lu and Law [7] is used.

The database contains an "adiabatic level" of no radiative heat loss ($c_{rad} = 0$) and fuel and oxidizer temperatures of $T_f = 371.6$ K and $T_o = 288$ K respectively. Five further "levels" are added to the database at decreased enthalpy, by linearly decreasing the inlet enthalpies till a temperature of 250 K. The settings are summarised in Tab.1.

T_f [K]	T_o [K]	c_{rad}	a_{ext} [s^{-1}]	a_{uns} [s^{-1}]
371.6	288.0	0	1435	1500
350.2	280.4	2	1364	1500
327.7	272.8	4	1307	1400
303.7	265.2	8	1246	1300
278.0	257.6	16	1171	1300
250.0	250.0	32	1081	1200

Table 1: Heat loss conditions.

The computed stable and unsteady extinguishing flamelets are represented by their stoichiometric temperatures and scalar dissipation rates in Fig.1 for all 6 enthalpy levels. The the strain rates of steady flamelets are

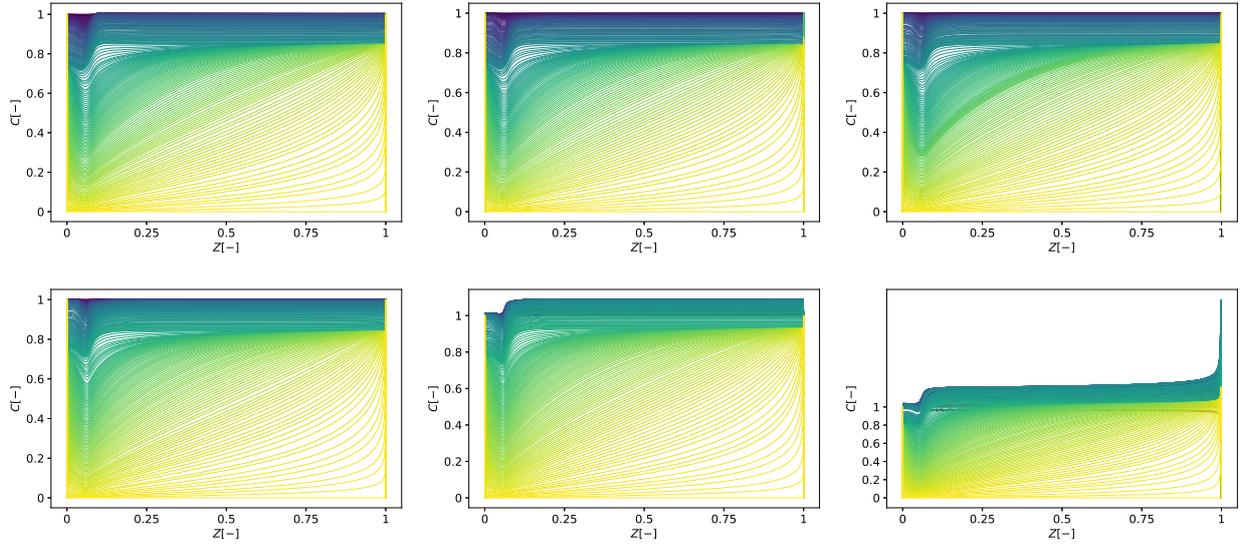


Figure 2: Reference definition Y_c^{ref} : Scaled progress variable along the flamelet

varied between $a_{min} = 10$ 1/s and the extinction point: a_{ext} , except for the lowest enthalpy level where there are no stable reacting solutions below $a_{min,6} = 22.6$ 1/s. The unsteady extinguishing flamelets are computed at a constant strain: a_{uns} , that is selected as the next whole hundred that is at least 50 1/s higher than a_{ext} .

The achieved radiative heat loss depends on the residence time of the reacting gas mixture, thus it is significantly higher at lower strain rates, as demonstrated in Fig.1. In the presence of the scaled radiative term, the stoichiometric temperatures are no longer a monotonically decreasing function of the strain rate. Instead they take a maximum value at a strain rate between a_{min} and a_{ext} . This introduces additional complexity to the progress variable optimization problem, as intermediate species recombine into final combustion products at lower temperatures.

3. Optimization method

This section describes a simple genetic algorithm for heuristic optimization based on an arbitrary objective function, and introduces an objective function designed to maximize the injectivity of the progress variable definition of the thermo-chemical database.

3.1. Genetic algorithm

The optimization method presented here is largely based on the previous work of Both [8]. Genetic algorithms are an intuitive tool for heuristic optimization of

arbitrary problems. They derive most of their concepts and jargon from biological evolution.

A group of solutions form a "population", that "reproduces" in each iteration of the algorithm. Each individual in the group represents a solution to the problem, they are identified by a genetic representation of the solution, and they are described by a single fitness function. In this work, the a subset of the a_k weights are taken directly as the genetic representation. Only those species are part of the genome, that in any of the computed flamelets at any point surpass the limiting mass fraction value of $Y_{lim} = 0.0005$, 28 species fulfil this requirement shown together with the results in Tab.2. An additional common constraint on the included species, is that the species of single component inlets is excluded, thus in the present example n-heptane is excluded from the progress variable definition. Furthermore, in case of multi-component inlets, the most abundant species is constrained such, that the progress variable is zero at the inlet. In this particular case:

$$a_{N_2} = -a_{O_2} \frac{Y_{O_2}^o}{Y_{N_2}^o}, \quad (5)$$

where $Y_{O_2}^o$ and $Y_{N_2}^o$ are the mass fractions of molecular oxygen and nitrogen in the oxidizer respectively. All considered weights are constrained to the $[-1, 1]$ interval.

In each reproductive cycle, pairs of individuals are randomly selected as parents, with a probability proportional to the fitness of the individual. The genetic rep-

resentation of the two parents goes through crossover, where parts of the two genome are taken to construct the offspring. Then the genome of the offspring goes through mutation, i.e.: random changes in the representation. This method combines the exploration and exploitation. Former corresponds to covering the search space through random mutations, while latter to preserving the well tuned segments of the genome through inheritance and crossover. Elitism is applied: i.e.: the best individual of the parent generation is preserved in place of the offspring with the lowest fitness.

The population is initialized from an initial progress variable. Then a lighter mutation is applied on all individuals to start form a sufficiently diverse population. In this process each a_k of each individual is changed with a 6% probability, the amount of change is also chosen randomly in the $[-0.05, 0.05]$ interval.

Parents are selected at random with the roulette method, where the chance of being selected is proportional to the fitness of the individuals. The crossover is executed with a 50% probability. The genome of the parents is exchanged after a randomly selected index of the a_k list. Otherwise the parents proceed without crossover.

In the mutation stage each a_k of the entire offspring generation is changed with a 10% probability, by a random amount in the $[-0.05, 0.05]$ interval.

To increase the exploitation of the best individual (elite), the three worst individual in the offspring are replaced with mutations of the elite applying the same mutation strategy as above. Finally the population is ordered again, and elite is saved in place of the worst individual.

On the present problem, the reproduction process is repeated for $N_G = 100$ generations, with a population size of $N_P = 30$.

3.2. Objective function

To assess the injectivity of the a progress variable definition, first the flamelets are interpolated on a predefined discretization in mixture fraction. For simplicity, this discretization is the same as the one applied on the complete thermo-chemical table. In the present work, a strong refinement is applied in mixture fraction around the stoichiometric point of $Z_{st} = 0.0622$. Figure 3 illustrates the step size dZ between subsequent mixture fractions, and the table index along Z . The minimum step size is located at Z_{st} and linearly increases towards pure fuel and oxidizer, thus the majority of the points are located near the stoichiometric point.

Once the flamelets are interpolated on the defined mixture fraction discretization, pseudo-premixed

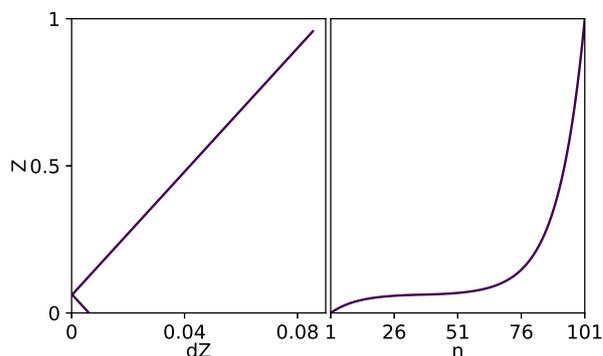


Figure 3: Discretization of mixture fraction, left: step size in mixture fraction, right: index in table.

flamelets are formed from the set of thermo-chemical states at each mixture fraction value on each enthalpy level. Each of these pseudo-premixed flamelets contains points from the extinguishing flamelet progressing backwards in time: from the pure mixing solution to the extinction point, and further points of the stable flamelets going from the extinction point towards a_{min} .

Each pseudo-premixed flamelet is assigned an objective function value that consists of two components an incentive I , and a penalty: P . The incentive is the difference between the progress variable value at the endpoints of the pseudo-premixed flamelet:

$$I = Y_c(a_{min}) - Y_c(mix). \quad (6)$$

The penalty is based on counting the total length of the pseudo-premixed flamelet in progress variable space, calculated as the sum of subsequent absolute changes in progress variable:

$$L = \sum_{i=i_{mix}}^{i(a_{min})-1} |Y_c(i+1) - Y_c(i)|, \quad (7)$$

This concept is illustrated in Fig.4.



Figure 4: Illustration of total length of pseudo-premixed flamelet in progress variable space. The penalized portions of the length are marked with red, while the black portion corresponds to the incentive: I .

The penalty associated to a pseudo-premixed flamelet

is 100 times the overlapping length:

$$P = 100(L - I). \quad (8)$$

Finally, the objective function of a pseudo-premixed flamelet is:

$$O = I - P. \quad (9)$$

The objective function of a progress variable definition is formulated as the sum of objective functions of these pseudo-premixed flamelets, thus the discretization in mixture fraction is of utmost importance, since more sparsely discretized mixture fraction regions are represented with a lower weight.

Species name	a_k
C2H2	0.08233128912763
C2H3	-0.00105796806794
C2H4	0.04586095706701
C2H6	-0.15269402988855
C3H3	-0.16623264307817
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C3H4-A	-0.19554501650256
C3H4-P	0.22495661093503
C3H5-A	0.09832301378563
C3H6	-0.03671988564438
C4H6	-0.05724568301937
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C4H8-1	0.00177123160707
C5H10-1	-0.18838496119739
C6H12-1	0.32344686533242
C7H14O2-4	0.02148094200378
C7H14O2-5	0.10971781311548
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CH2CO	-0.42817433783133
CH2O	0.13719527888134
CH3	-0.10196427077124
CH3CHO	0.36899695187240
CH4	-0.16007277163175
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CO	-0.01768170447047
CO2	0.00917666674836
H2	-0.11155287598418
H2O	0.04923159070487
N2	-0.00105237329632
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O	0.12320933586970
O2	0.00346585976861
OH	-0.21571643287272

Table 2: Optimized progress variable weights

3.3. Optimized progress variable definition

The optimization procedure was run using the flamelets illustrated in Fig.1, and resulted in the weights shown in Tab.2.

The resulting definition is illustrated in Fig.7, by comparison the definition of Ma [3] is shown on Fig.2. Both figures show the scaled progress variable along each counterflow diffusion flamelet defined as:

$$C = \frac{Y_c - Y_c(mix)}{Y_c(a_{min}) - Y_c(mix)} \quad (10)$$

The optimized progress variable definition distinguishes better between stable flamelets (marked with darker colors), as they occupy a larger portion of the $C - Z$ plane. The main improvement is on the rich side of the database, where the intuitive definition of Ma [3], results in completely overlapping flamelets.

4. Computational tests

The H1S1 n-heptane case of the Cambridge swirl flames data repository [5] is simulated with the optimized progress variable definition using the low-dissipation finite element framework presented in[4].

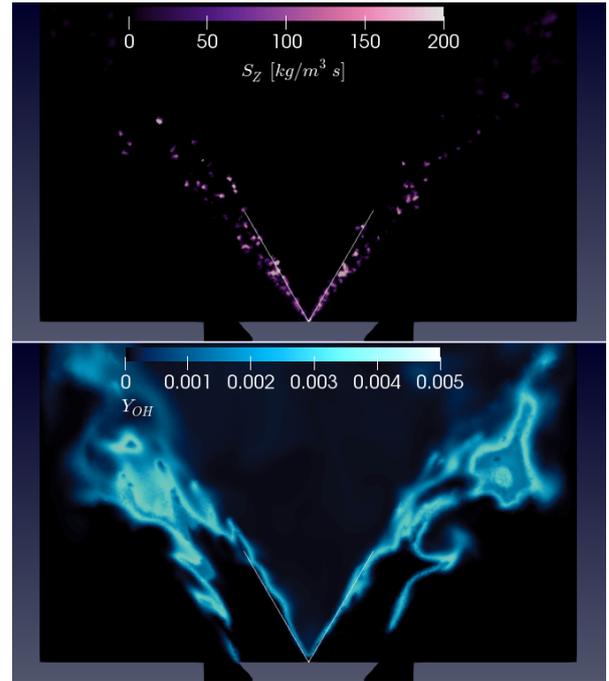


Figure 5: Instantaneous evaporative source term and the mass fraction of OH in the LES of present work.

This laboratory setup consists of an axi-symmetric bluff body surrounded by an annular air duct fitted with a swirler element. Liquid fuel is injected at the center of the bluff body directly into the flame with a 60° hollow cone injector. The setup is illustrated with instantaneous results of the large eddy simulation (LES) using the

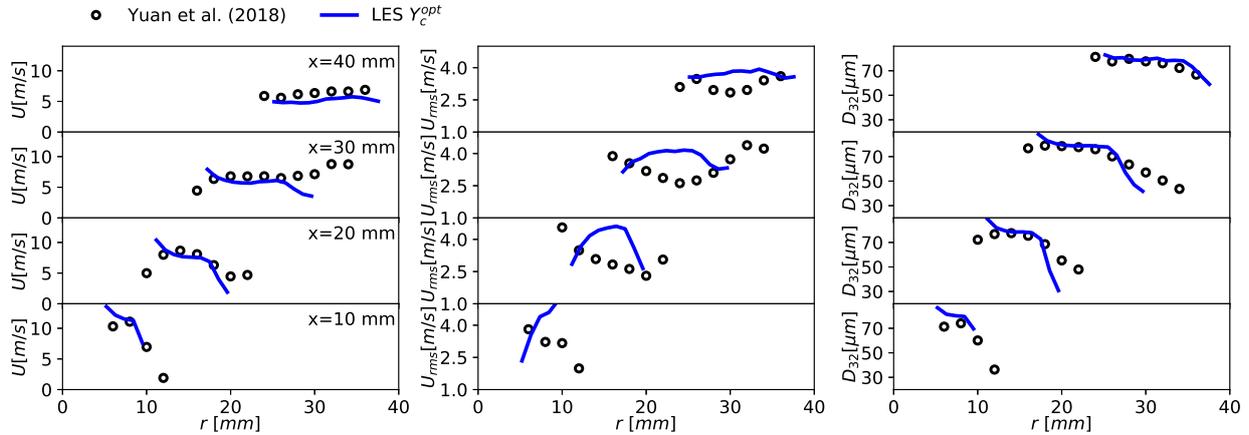


Figure 6: Comparison of phase Doppler anemometry (PDA) data of Yuan et al. [9], and the LES of present work.

optimized progress variable of present work in Fig. 5. The simulation clearly exhibits local extinction, as the OH contour is discontinuous and lifted from the bluff body. Furthermore the OH profile is clearly affected by the strong heat loss and dilution in the presence of high evaporative sources.

Comparison between the phase Doppler anemometry measurements of Yuan et al. [9] and the preliminary results of present work are shown in Fig. 6. The agreement between measurements and simulation is encouraging.

5. Conclusions

The developed optimization method clearly improves the injectivity of the progress variable definition at all mixture fractions and across all enthalpy levels.

The applied discretization in mixture fraction effectively prioritizes certain regions of the mixture fraction space, thus the injective behaviour is promoted more in regions of interest.

The optimized progress variable definition is suitable for complex applications, such as the large eddy simulation of the Cambridge swirl spray flame.

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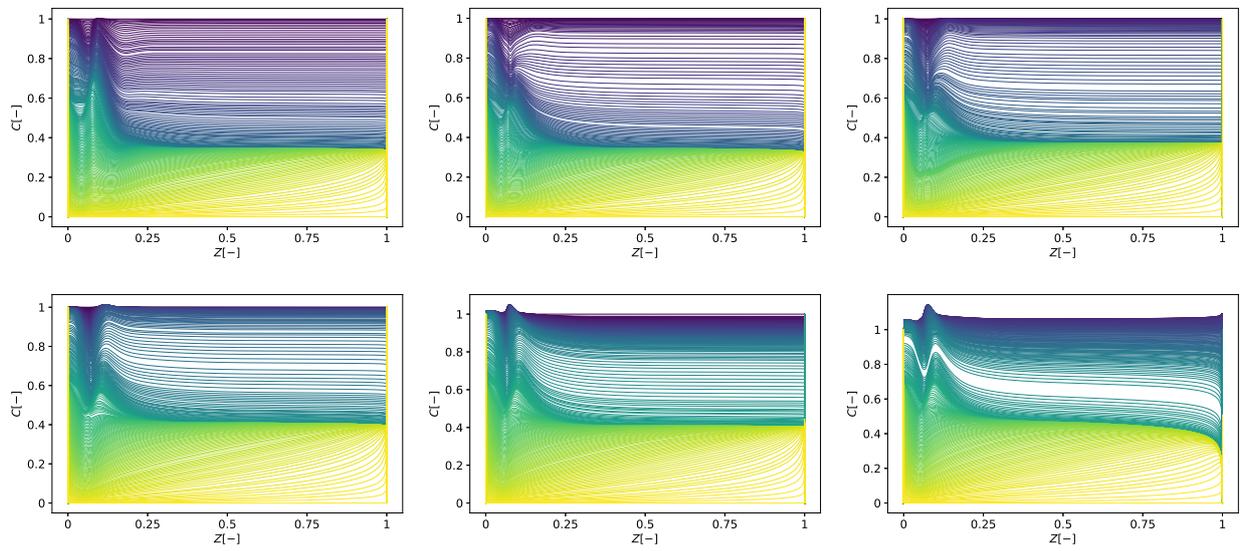


Figure 7: Optimized definition: Scaled progress variable along the flamelet