

Transient Interactive Flamelets with Tabulated Chemistry

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1 Introduction

Incorporating chemistry and accounting for turbulence-chemistry interactions in Computational Fluid Dynamics (CFD) calculations is challenging. In order to achieve industrially acceptable simulation times, while still accounting for chemistry, and effects of the turbulent flow-field on the chemistry, methods based on transient flamelets [1] and a flamelet progress variable have been proposed [2]. In this work we present a method that facilitates for running a high number of transient flamelets on-line with the CFD code. Our method relies on a progress variable parameterization of the chemistry, where chemical enthalpy is chosen as the progress variable, as suggested in Ref. [2]. In the following we outline the modifications to the method proposed in Ref. [2]; discuss the differences between a parameterization employing homogeneous reactor calculations and a parameterization based on transient flamelet calculations; show the applicability of the model in both a stand-alone transient flamelet configuration, and in CFD using a constant volume spray chamber test case.

For brevity we do not elaborate further on the flamelet model itself. Instead the reader is referred to Ref. [1] and references therein for further details.

2 Progress variable method – tabulation and implementation

In Ref. [2] a normalized progress variable for the whole flamelet was defined according to:

$$C(\tau) = \frac{\int_0^1 \sum_{i=1}^{N_s} h_{298,i}(Y_i(Z),\tau) dZ - \int_0^1 \sum_{i=1}^{N_s} h_{298,i,u}(Y_i(Z),0) dZ}{\int_0^1 \sum_{i=1}^{N_s} h_{298,i,b}(Y_i(Z),\tau_\infty) dZ - \int_0^1 \sum_{i=1}^{N_s} h_{298,i,u}(Y_i(Z),0) dZ}, \quad (1)$$

where C is the flamelet progress at time τ , $h_{298,i}$ is the chemical enthalpy for species i , the subscript u denotes unburned state, the subscript b denotes quasi-steady burning state, N_s is the total number of species, and $Y_i(Z)$ the mass fraction of species i at mixture fraction coordinate Z . The formulation allowed for deriving a transport equation in physical space where the progress C was decoupled from mixture fraction Z . Here we focus on how a progress variable approach can be used to speed up the flamelet solver step, where we need to retain a dependency of mixture fraction on the progress variable source term. We note that we can formulate a transport equation for chemical enthalpy (sum over the product of species mass fraction and corresponding chemical enthalpy) and apply the flamelet transform to obtain an equation for chemical enthalpy in mixture fraction space. Assuming unity Lewis numbers, and keeping only the leading order terms, the following equation is obtained in mixture fraction space for chemical enthalpy:

$$\frac{\partial h_{298,tot}}{\partial \tau} = \frac{\rho \chi}{2} \frac{\partial^2 h_{298,tot}}{\partial Z^2} + \omega_{h_{298,tot}}, \quad (2)$$

where $h_{298,tot}$ is the total chemical enthalpy, $h_{298,tot} = \sum_{i=1}^{N_s} h_{298,i} Y_i$, ρ the density, χ the scalar dissipation rate, Z mixture fraction and $\omega_{h_{298,tot}}$ the total chemical enthalpy source term. It may now be recognized that two possibilities exist for pre-tabulating the required source term: a) adiabatic constant pressure reactor calculations; and b) transient flamelet calculations. Both methods have been applied, using the same discretization practice for generating the resulting table in mixture fraction and chemical enthalpy space. When producing the table through transient flamelet calculations, scalar dissipation rate is considered during the tabulation process, and is thereby an additional tabulation parameter. Tabulation performed calculating constant pressure reactors assumes that scalar dissipation acts only on the reaction progress through Eq. (2), while it does not influence the chemical composition for each mixture fraction.

The resulting tables contain, in addition to the source term for the chemical enthalpy, NASA polynomial coefficients and mean molecular weight as function of enthalpy (sum of chemical and thermal enthalpy), pressure, mixture fraction, scalar dissipation at stoichiometric mixture fraction, and the chemical enthalpy itself. Species mass fractions for selected species are stored and may be retrieved from the table in a post-process step. It should be observed that emissions such as soot and NOx may not be taken directly from the table as the chemistry governing emission formation processes is slow. Instead, emissions need to be calculated using a tabulated source-term approach [3].

Implementation of Eq. (2) in a transient flamelet solver is straightforward and results in a decrease of scalars to be solved by the 1D-solver to only one, assuming no pressure change and no heat losses. Instead of computing species source terms, only the chemical enthalpy source term and mean molecular weight need to be retrieved for all mixture fraction grid points at each solver call, which drastically decreases the computational time required to advance the flamelet solver. Density, required in Eq. (2), is computed assuming ideal gas knowing the pressure and the mean molecular weight.

Implementation of a library based transient flamelet solver employing chemical enthalpy source-term tables in a CFD code does not differ from the implementation of a regular flamelet solver. The CFD implementation aspects are discussed in e.g. Ref. [4].

3 Results and Discussion

Prior to testing the proposed approach in a CFD calculation, the constant pressure reactor tabulation approach was compared to the transient flamelet tabulation approach. The chemical mechanism used for tabulation and on-line calculations was a skeletal mechanism for n-heptane [5] consisting of 121 species and 973 reactions. Table 1 below lists the conditions for which the test tables were generated. The conditions were chosen such that they are relevant for heavy duty diesel engine part load operating conditions.

Table 1: Conditions for flamelet table testing.

Pressure	8 MPa
Oxidizer	air @ 1060 K
Fuel	n-heptane @ 298 K
Scalar dissipation rates in table	0.1, 1, 10, 100 s ⁻¹

Comparing the transient flamelet ignition process for a scalar dissipation rate at stoichiometric mixture fraction of $\chi_{st} = 0.1$ s⁻¹, the constant pressure reactor table is performing similar to the table generated using the transient flamelet tabulation approach. However, for higher scalar dissipation rates the agreement between the on-line chemistry calculation and the table calculation depends on the choice of tabulation method. The table generated through constant pressure reactor calculations is differing substantially in flamelet auto-ignition prediction behavior at higher scalar dissipation rates. Moreover, it is not correctly reproducing the behavior of the moving reaction front at higher mixture fraction values, since at these high mixture fraction values no auto-ignition is obtained in the constant pressure reactor calculation. This upper mixture fraction auto-ignition limit for constant pressure reactor

calculations, at a relevant time-scale (auto-ignition in less than 10 seconds), depends on the selected oxidizer and fuel enthalpies, and the reactivity of the fuel. On the other hand, the table generated using transient flamelet calculations is able to correctly capture the temperature development during the flamelet ignition process. During the flamelet ignition process, the diffusive term, in the flamelet equation, which includes scalar dissipation rate as a parameter, leads to a transport of species and radicals across mixture fraction isolines which promote reactions at mixture fraction values, which are not auto-igniting in the constant pressure reactor calculation. The diffusive term is also influencing the steady-state flamelet solution, which affects the values at the last table entry point.

Figure 1 shows a comparison between the two different tabulation approaches during the ignition process (0.08 ms, 0.2 ms) and at 2 ms for a flamelet calculation performed for a constant scalar dissipation rate at stoichiometric mixture fraction $\chi_{st} = 10 \text{ s}^{-1}$. Other boundary conditions are the same as in Table 1 above. The calculation using the constant pressure reactor table runs ahead of the flamelet calculation with on-line chemistry, leading to an error in the calculation of the flamelet ignition process. Moreover, the solution after ignition, when using the constant pressure reactor table is approaching the equilibrium solution and not the solution for a quasi-steady burning flamelet. It is possible that this is due to how the last table entry point is defined, and could possibly be remedied by combining the homogeneous reactor auto-ignition table with quasi-steady burning flamelet profiles. This approach was however not investigated due to the findings from an investigation where the auto-igniting flamelets were calculated subjected to decaying scalar dissipation rate.

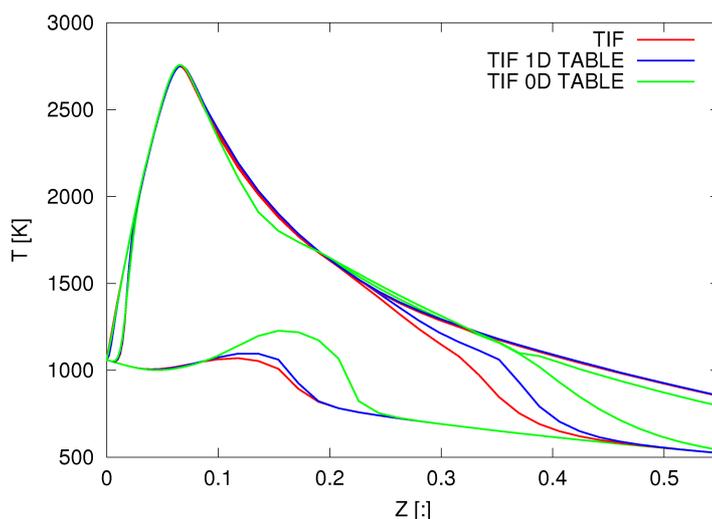


Figure 1. Flamelet temperature at 0.08 ms, 0.2 ms and 2 ms computed with a constant pressure reactor table (green lines) and with a transient flamelet table (blue lines), and with on-line chemistry (red lines) at a pressure of 8 MPa, oxidizer side temperature of 1060 K, fuel side temperature of 298 K, and a scalar dissipation rate at stoichiometric mixture fraction of 10 s^{-1} .

Calculating a flamelet subjected to a decaying scalar dissipation rate with a table calculated using transient flamelet tabulation at constant scalar dissipation rate, reproduces the flamelet ignition process reasonably well while the constant pressure reactor table leads to an under-prediction of flamelet ignition delay time. This is illustrated in Figure 2 below, which depicts the temperature at stoichiometric mixture fraction (Z_{st}), $2 \cdot Z_{st}$ and $Z_{st}/2$ as function of time, for a flamelet ignition process where the scalar dissipation rate at stoichiometric mixture fraction decays as $\chi_{st} = \chi_{st,0} \cdot e^{-kt}$ with $\chi_{st,0} = 100 \text{ s}^{-1}$ and $k=4605.2$. The scalar dissipation rate decays thus to 50 s^{-1} after 0.15 ms, 10 s^{-1} after 0.50 ms and 1 s^{-1} after 1 ms. Furthermore, investigating the ability of the table to reproduce species profiles we find that the tables generated using transient flamelets are performing better than the constant pressure reactor tables.

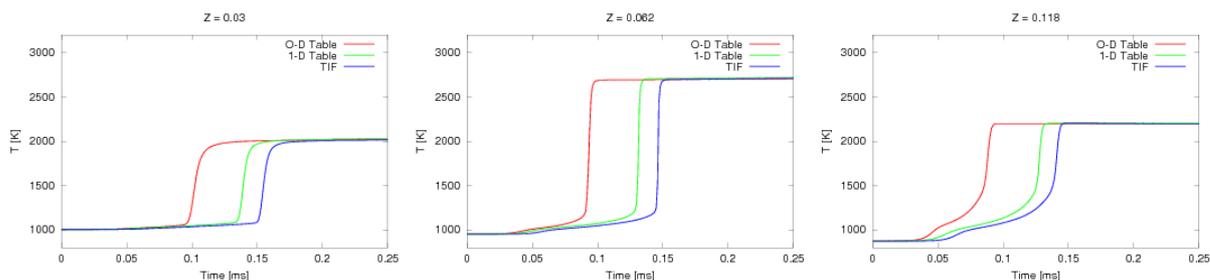


Figure 2. Temperature as function of time for mixture fraction values $Z=0.03$ (left), $Z=0.062$ (middle) and $Z=0.118$ (right) for a flamelet subjected to decaying scalar dissipation rate.

Comparing the computational efficiency, a speed-up factor of 50 is obtained using the tabulated approach for a 2 millisecond flamelet calculation, where the 1D-solver was called once every microsecond (corresponding to a time step size used in CFD simulations) for the chemical mechanism applied here. The main part of the remaining time resides in the table search and retrieve algorithm and a more advanced storage, search and retrieval algorithm as described in Ref. [6] will likely lead to further speed-up.

The table generated using the transient flamelet tabulation approach was tested using STAR-CD version 4.12 [7] in a simplified spray bomb set-up. A 6° slice of a cylinder, with height 80 mm and radius 50 mm was calculated using a grid consisting of one cell layer in azimuthal direction, 80 cells in axial direction and 50 cells in radial direction. The cell size close to the injector nozzle was 0.5 mm and increasing outwards with a constant growth factor. Cyclic boundary conditions were set in azimuthal direction. The initial flow field was quiescent, and the initial composition was air at 1060 K. The initial pressure was set to 8 MPa. The high Reynolds-number $k-\epsilon$ model was selected as turbulence model, and the model selection for thermodynamics followed Ref. [4], i.e. the enthalpy equation was solved in its chemico-thermal (static) formulation, and density calculation was set to follow ideal gas. The injection rate was constant, 0.003 kg/s, during 1.5 ms. The nozzle hole diameter was 0.14 mm. The nozzle was modeled using the built-in effective nozzle model, spray atomization using the built-in Huh model, and breakup using the built-in Reitz model with their default STAR-CD constants [7].

In Figure 3 below section plots for H_2O and CO_2 mass fractions are shown for two different time instances, $t = 0.3$ ms and $t = 1.0$ ms for a calculation using tabulated chemistry and online chemistry. Five transient flamelets were used for the calculation. The differences between the on-line chemistry calculation and the calculation using tabulated chemistry are almost indiscernible.

Comparing a calculation using 50 flamelets with a calculation using 5 flamelets results in visible differences in the temperature field as shown in Figure 4 below. As discussed in Ref. [8] a high number of flamelets is required to correctly capture the lift-off distance when employing the transient flamelet approach. Investigation of lift-off distances is part of future work and not discussed further here.

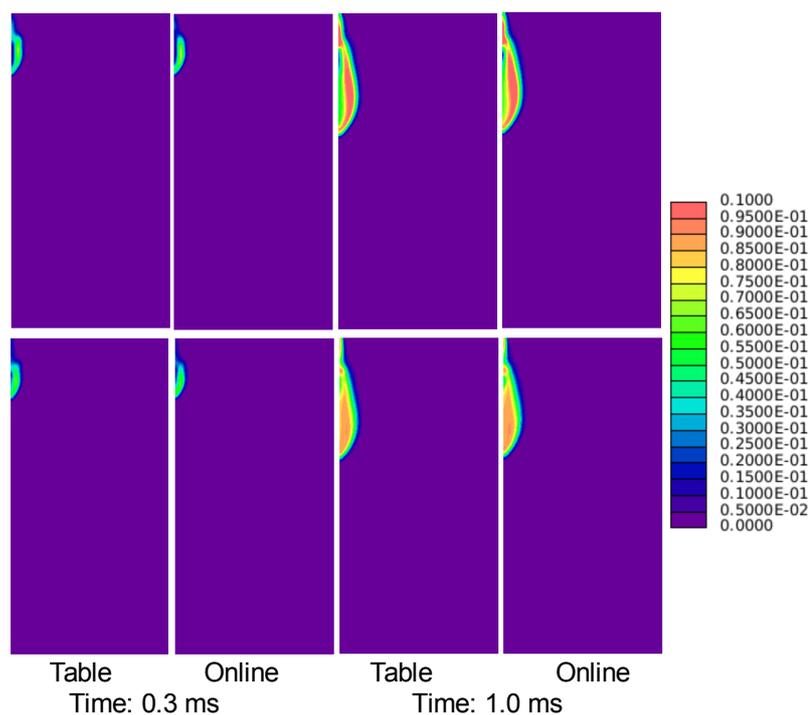


Figure 3. Section plots showing H₂O (upper panels) and CO₂ (lower panels) mass fractions at $t = 0.3$ ms and $t = 1.0$ ms for CFD calculations with 5 flamelets using tabulated chemistry and online chemistry.

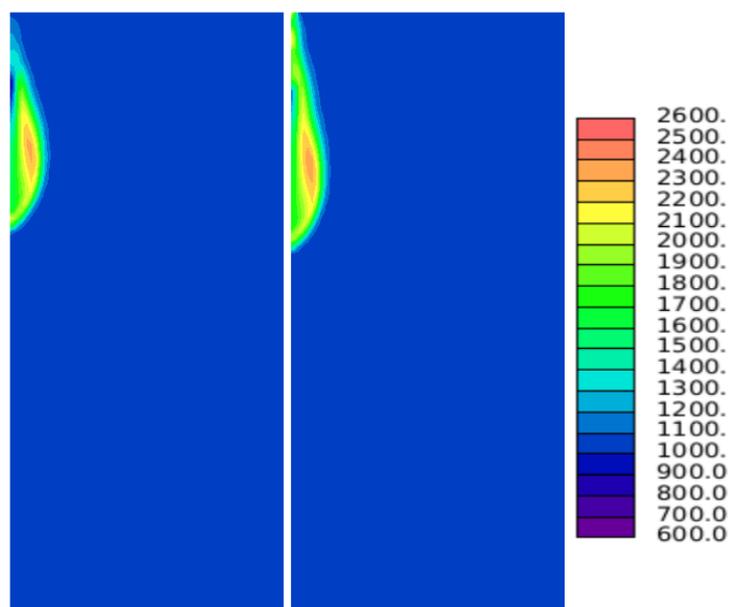


Figure 4. Section plot of temperature at $t = 1.0$ ms for a calculation with 50 transient flamelets (left) and 5 transient flamelets (right). The temperature scale is in Kelvin.

4 Conclusion

A progress variable method based on chemical enthalpy was developed for use in a transient flamelet solver. With the proposed approach the number of scalars transported by the 1D flamelet solver was reduced to only one. Two strategies for table generation were investigated: tabulation based on constant pressure homogeneous reactor calculations, and tabulation of the transient flamelet ignition process using a 1D-solver allowing for considering scalar dissipation rate during the table generation.

Two types of igniting flamelet scenarios were investigated when validating the proposed concept: flamelet ignition at constant scalar dissipation rate; and flamelet ignition at decaying scalar dissipation rate. It was found, comparing temperature and species profiles from calculations using both types of tables, that in order to correctly capture the behavior of an igniting flamelet the latter tabulation strategy is required.

In order to test the applicability of the tabulation method in a reactive flow calculation, a constant volume spray bomb test case was set-up for a CFD code using an interactive flamelet approach. A CFD calculation with the flamelet solver employing the table produced using the transient flamelet tabulation strategy was compared with a CFD calculation where the flamelet solver was calculating chemistry on-line. It was found that the tabulated approach had a very good agreement with the on-line approach.

The main benefit of the proposed model is the decreased amount of computational time required for the flamelet solver, which allows for calculating a large number of transient flamelets at affordable computational cost. This is important in order to capture the lift-off length, and associated processes such as soot formation.

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