

Modeling Non-Premixed Combustion Using Tabulated Kinetics and Different Flame Structure Assumptions

Tommaso Lucchini, Gianluca D'Errico, Angelo Onorati,
 Alessio Frassoldati, and Alessandro Stagni
 Politecnico di Milano

Gilles Hardy
 FPT Motorenforschung AG

ABSTRACT

Nowadays, detailed kinetics is necessary for a proper estimation of both flame structure and pollutant formation in compression ignition engines. However, large mechanisms and the need to include turbulence/chemistry interaction introduce significant computational overheads. For this reason, tabulated kinetics is employed as a possible solution to reduce the CPU time even if table discretization is generally limited by memory occupation. In this work the authors applied tabulated homogeneous reactors (HR) in combination with different turbulent-chemistry interaction approaches to model non-premixed turbulent combustion. The proposed methodologies represent good compromises between accuracy, required memory and computational time. The experimental validation was carried out by considering both constant-volume vessel and Diesel engine experiments. First, the ECN Spray A configuration was simulated at different operating conditions and results from different flame structures are compared with experimental data of ignition delay, flame lift-off, heat release rates, radicals and soot distributions. Afterwards, engine simulations were carried out and computed data are validated by cylinder pressure and heat release rate profiles.

CITATION: Lucchini, T., D'Errico, G., Onorati, A., Frassoldati, A. et al., "Modeling Non-Premixed Combustion Using Tabulated Kinetics and Different Flame Structure Assumptions," *SAE Int. J. Engines* 10(2):2017, doi:10.4271/2017-01-0556.

INTRODUCTION

High power-to-weight ratio and thermal efficiencies close to 45% have made compression-ignition engines among the most widely used prime movers for many industrial and road transportation applications. However, recent changes in emission legislations and the need to continuously reduce the fuel consumption require further improvements to the combustion system. In particular, an optimal combination of combustion chamber design, compression ratio and injection strategy has the potential to increase thermal efficiency and, at the same time, ensure acceptable levels of pollutant emissions [1, 2].

To speed-up the engine development process and identify the most promising configurations in the shortest amount of time, multi-dimensional numerical models are widely employed to predict Diesel combustion, although such topic represents a very challenging task for computational fluid dynamics due to the need to accurately describe the evolution of a turbulent, compressible, reacting and multiphase flow [3, 4]. Since not only engine performances but emissions as well need to be estimated with a good level of accuracy must be estimated with a good level of accuracy, combustion models have to incorporate detailed chemistry and also the effects of its interaction with turbulence [5, 6, 7, 8]. Different combustion approaches are available handling chemical

kinetics in two different ways: direct integration and tabulation. In the first case, reaction-diffusion equations are solved on-line during the simulation for any species included in the chemical mechanism. Computation of reaction rates requires the use of ODE stiff solvers since chemical time-scales are smaller than the flow ones, with a consequent increase of the required computational time. Despite the use of parallel computing and the enhancements of processor performances, the use of very detailed schemes is still prohibitive and maximum number of species which can be employed for practical simulations is generally less than 100. This aspect represents an important limitation related to the capability to predict the main soot precursor species or ignition delays under advanced combustion modes where high levels of charge dilution are generally used [9, 10]. To reduce the computational time, different techniques were developed in the past: among them we can mention on-line tabulation or cell clustering: when applied in combination with the well-mixed model they offer acceptable speed-up factors in case relatively small mechanisms (up to 50 species) are employed [11, 12, 13, 14]. Inclusion of turbulence-chemistry interaction adds significant overheads related to the need to consider the effects of sub-grid mixing either by integrating a presumed PDF or solving additional equations for the different expected flow realizations [5, 15]. This explains the reason why the most widely used approaches are the well-mixed and the Representative Interactive Flamelet.

(RIF) ones. The first one accounts for local flow conditions but cannot include turbulence-chemistry interaction, the second one solves reaction-diffusion equations in the mixture fraction (Z) space having a limited number of nodes and then computes the chemical composition in each cell by presuming a β -PDF distribution for the chemical species which is function of Z and its variance Z''^2 . When a single flamelet is used, flame stabilization cannot be predicted and extension to multiple flamelets is computationally demanding. More sophisticated approaches exist, like Conditional Moment Closure or Transported PDF, but their application so far is still limited to advanced research studies.

The need to account properly for turbulence-chemistry interaction and to achieve results within an acceptable amount of time suggests the use of tabulated kinetics: chemical species reaction rates are stored in a table according to a specified mechanism and flame structure; then they are retrieved as function of the state of the system. Different approaches were presented in the past: the first ones used a rigorous mathematical time-scale analysis to identify the relevant species in the mechanism and use them as independent variables for the tabulation [16]. Afterwards, the attention was mainly focused on the capability to reproduce both auto-ignition and diffusive flame structure and for this reason tabulations based on auto-igniting homogeneous reactors [17, 18] or diffusive flamelets [19, 20, 21] were presented and successfully applied to model Diesel combustion. Approximated diffusion flamelets (ADF) represents an interesting compromise between these approaches since they tabulate diffusion flamelets computed with source terms taken from tables generated using homogeneous reactor calculations [22, 23]. To be used in engine simulations, tabulated kinetics must fulfill the following prerequisites:

1. Acceptable table size to avoid excessive memory occupation during the simulation;
2. Consistency of the results with the ones performed using direct integration and the same flame structure assumption;
3. Minimum number of transport equations to be solved in the CFD domain.

Objective of this work is the development of combustion models based on tabulated homogeneous reactors (HR). Different flame structures are considered: well-mixed, presumed PDF and diffusive flamelets. For all of them, related transport equations are solved on-line with reaction rates retrieved from the table. This makes possible to minimize the size of the table and to account in different ways for turbulence-chemistry interaction. Tabulated quantities are stored as function of state variables of the system (temperature, mixture fraction, pressure) and the combustion progress variable. The table includes data of progress variable reaction rate and chemical composition which is represented by a *virtual* set of seven species preserving the most important thermodynamic properties of the full set used in the mechanism. It is also possible to store mass fractions of additional species which can be employed in sub-models for the computation of pollutant emissions (soot and NO_x).

The proposed approach for combustion modeling based on tabulated kinetics was implemented in the Lib-ICE code which is based on the OpenFOAM® technology [24, 25]. Experiments carried out in the context of the Engine Combustion Network (ECN) using n-dodecane as fuel at constant-volume conditions were used for a complete assessment of the proposed combustion models. Computed results are compared with experimental data but also with the ones available from the same models employing direct-integration. The comparison was performed in terms of vessel pressure, heat release rate, ignition delay time, flame lift-off and soot distribution. Afterwards, preliminary results of combustion simulations in a medium-duty Diesel engine are reported.

COMPUTATIONAL MODEL

This section describes the way tabulated kinetics is handled and how it is incorporated in three different combustion models: well-mixed, presumed PDF and representative interactive flamelets. The following acronyms will be used to easily identify them:

- **TWM** : tabulated well-mixed model;
- **TPPDF** : tabulated presumed PDF model;
- **TRIF** : tabulated representative interactive flamelet.

Results of approaches based on direct integration will be also presented in this paper for model assessment and they will be named as:

- **DIWM** : well mixed model;
- **DIRIF** : representative interactive flamelet model.

Chemistry table

Figure 1 summarizes the way chemistry is tabulated in the proposed approach. The user specifies a chemical mechanism and a range of initial conditions for homogeneous constant pressure reactor calculations in terms of:

- Mixture fraction Z ;
- Ambient pressure p ;
- Initial reactor temperature T_u ;
- Residual gas fraction EGR ;

On the basis of such quantities, initial chemical composition is computed and reactor calculation is started. T_u can be initialized in two ways:

1. Temperature is independent from Z ;
2. Reactor temperature varies from values specified at $Z = 0$ and $Z = 1$ including, eventually, fuel evaporation:

$$h(Z) = (1-Z) \cdot h(T_{Z=0}) + Z \cdot h(T_{Z=1}) - Z \cdot h_l(T_{Z=1}) \quad (1)$$

$$T_u(Z) = T(h(Z));$$

Both approaches are equivalent and provides the same results, since in both cases all possible expected thermochemical states of the system are covered. Option 2 is probably more suitable for table discretization in diffusion combustion problems because the user provides well known values of expected oxidizer temperatures ($T_{Z=0}$), fuel temperature and its heat of evaporation.

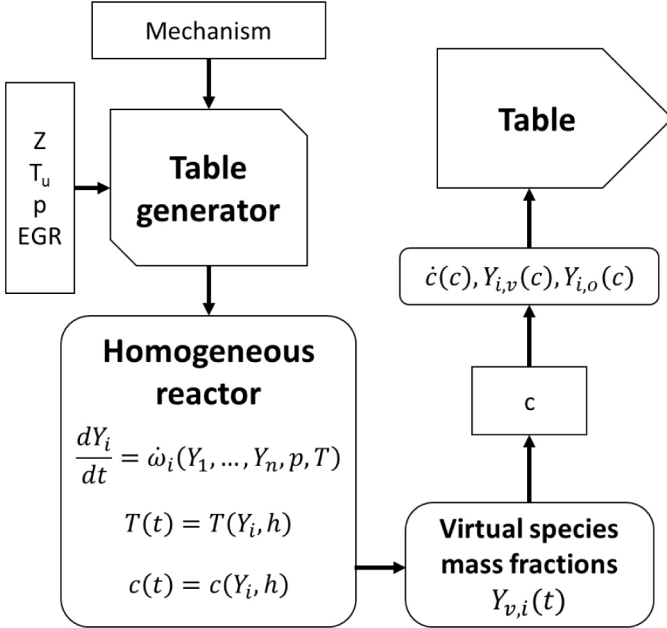


Figure 1. Generation of the chemistry table based on the homogeneous reactor assumption.

For any specified condition, chemical species equations are solved:

$$\frac{dY_i}{dt} = \dot{\omega}_i(T, p, Y_1, \dots, Y_n) \quad (3)$$

with reactor temperature T computed directly from the initial enthalpy value. After every time step two different operations are performed: evaluation of the progress variable C and computation of the chemical composition by means of the *virtual* species approach. Definition of the combustion progress variable is not straightforward and it was widely discussed in past works [19, 26, 20]. This aspect is even more complex in case of large hydrocarbon fuel auto-ignition since it might take place either in one or two stages. In this work, the definition proposed by Lehtiniemi et al. [20] was adopted, with C being equal to the heat released by combustion, computed as the difference between the current and the initial value of the reactor formation enthalpy, also known as h_{298} :

$$C = \sum_{i=1}^{N_s} h_{298,i} \cdot Y_i(t) - \sum_{i=1}^{N_s} h_{298,i} \cdot Y_i(0) \quad (4)$$

where N_s is the total number of chemical species used by the specified mechanism. The adopted definition for C uniquely characterizes each point in the thermochemical state space and is appropriate for a transport equation. At the end of each reactor calculation, progress

variable reaction rates and chemical composition are stored as function of the discrete values of the normalized progress variable c , specified by the user:

$$c = \frac{C - C_{min}}{C_{max} - C_{min}} \quad (5)$$

where C_{min} and C_{max} are minimum and maximum values of the progress variable which are found at initial and after auto-ignition conditions. C_{min} and C_{max} are stored in the table as function of Z, T_u, p . From the values of times at which the specified c_i values were found, the progress variable reaction rate is computed with the forward differencing scheme as follows:

$$\dot{c}_i = \frac{c_{i+1} - c_i}{t_{i+1} - t_i} \quad (6)$$

$\dot{c}$ is then multiplied by the term $C_{max} - C_{min}$ in order to have the proper source term $\dot{C}$ in the progress variable transport equation. For any tabulated value of the progress variable c , the chemical composition is also stored. However, to avoid the storage of the entire set of species and keep an acceptable size of the table, only seven ones named *virtual* species are tabulated and their mass fractions are computed in order to preserve the main thermochemical properties of the full set used in the detailed mechanism. Virtual species used in this work are N_2 , O_2 , *fuel*, CO_2 , CO , H_2O , H_2 and their composition is computed for any c value as follows:

$$\sigma_H = \sum_{i=1}^{N_s} N_{H,i} \cdot x_i = \sum_{k=1}^{N_v} N_{H,k} \cdot x_{v,i} \quad (7)$$

$$\sigma_C = \sum_{i=1}^{N_s} N_{C,i} \cdot x_i = \sum_{k=1}^{N_v} N_{C,k} \cdot x_{v,i} \quad (8)$$

$$\sigma_O = \sum_{i=1}^{N_s} N_{O,i} \cdot x_i = \sum_{k=1}^{N_v} N_{O,k} \cdot x_{v,i} \quad (9)$$

$$\sigma_N = \sum_{i=1}^{N_s} N_{N,i} \cdot x_i = \sum_{k=1}^{N_v} N_{N,k} \cdot x_{v,i} \quad (10)$$

$$h = \sum_{i=1}^{N_s} Y_i \cdot h_i(T) = \sum_{k=1}^{N_v} Y_{i,v} \cdot h_i(T) \quad (11)$$

$$c_p = \sum_{i=1}^{N_s} Y_i \cdot c_{p,i}(T) = \sum_{k=1}^{N_v} Y_{i,v} \cdot c_{p,k}(T) \quad (12)$$

$$\sum_{k=1}^{N_v} Y_{i,v} = 1.0 \quad (13)$$

In Eqs. 7, 8, 9, 10, 11, 12, σ is the total number of elements (C, H, O and N) in the reactor; N_s is the total number of species used by the chemical mechanism; N_v is the total number of virtual species; N is the total number of elements (C, H, O and N) in each chemical species; x refers to mole fractions; Y refers to mass fractions; h is the mass specific enthalpy; c_p is the mass specific heat. The virtual species approach was presented and validated by the authors in a previous work [24]. Constant-volume and constant pressure reactor calculations performed in a wide range of conditions made possible to verify that cumulative heat release, reactor temperature and pressure evolutions are consistent with the cases where the full set of species is used. No unphysical results with negative species were found.

The table also includes the mass fractions of chemical species which are of interest for the user (Y_o in Fig. 1), either for post-processing reason or because they are relevant for the formation of the main pollutants and have to be used by the related sub-models.

Tabulated Well Mixed Model (TWM)

The operation of the tabulated well-mixed model is reported in Fig. 2. In the CFD domain, transport equations for mixture fraction, enthalpy, unburned gas temperature and progress variable are solved and then the table is accessed with the local cell values. Interpolation of table values at cell conditions is performed by means of an inverse, distance weighted technique. Mixture fraction equation includes fuel evaporation:

$$\frac{\partial \rho Z}{\partial t} + \nabla(\rho \mathbf{U} Z) - \nabla(\mu_t \nabla Z) = \dot{S}_Z \quad (14)$$

The progress variable source term used in the C transport equation is derived from Eq. 6:

$$\frac{\partial \rho C}{\partial t} + \nabla(\rho \mathbf{U} C) - \nabla\left(\frac{\mu_t}{Sc_t} \nabla C\right) = \rho \dot{C} \quad (15)$$

$$\dot{C} = (C_{max} - C_{min}) \cdot \dot{c} \quad (16)$$

To consistently access the table data, it is necessary to solve an additional equation for the unburned gas enthalpy which is then used to estimate the unburned gas temperature T_u which is one of the independent variables of the table:

$$\frac{\partial \rho h_u}{\partial t} + \nabla(\rho \mathbf{U} h_u) - \nabla(\alpha_t \nabla h_u) = \dot{Q}_s + \frac{\rho}{\rho_u} \cdot \frac{Dp}{Dt} \quad (17)$$

where α_t is the turbulent thermal diffusivity and ρ_u is the density of unburned gases which is computed from cell pressure, chemical composition at $C = 0$ and T_u . $\dot{Q}_s$ is the term related to spray evaporation which assumes different values in case the mixing line is assumed or not in the table generation process.

It is expected that both in case of direct-integration and tabulated kinetics the well mixed model produces similar results. However, it must be pointed out that tabulation introduces significant simplifications since a $N_s + 2$ dimensional problem is then reduced only to four dimensions. This aspect mainly affects the ignition process when C is diffused to rich mixtures ($\phi > 3$) which are characterized by a long ignition delay and a single stage very fast ignition. As a consequence, rich regions will be ignited almost instantaneously and high values of C will be diffused back to lean or stoichiometric mixtures leading to a very anticipated auto-ignition. To avoid this, reaction rates are set to zero in regions where dual-stage ignition does not happen, corresponding approximately to $\phi = 3$. This aspect might have some effects on prediction of soot emissions since inception and surface grow phases take place where the mixture is very rich. In terms of ignition delay, increasing the maximum equivalence ratio value at which reaction rates are computed from 3 to 4 will reduce the ignition delay by a factor of 25%, leading to a significant underestimation of experimental data.

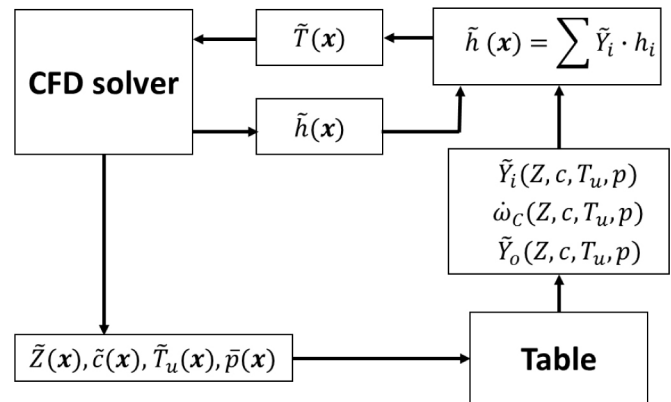


Figure 2. Operation of the tabulated well-mixed combustion model (TWM).

Tabulated Presumed PDF Combustion Model (TPPDF)

This approach was applied in [17, 27] to simulation of compression-ignition engines: turbulence chemistry interaction is incorporated in the computation of the progress variable source term, assuming a probability density function for both progress variable and mixture fraction as follows:

$$\dot{C} = \int_0^1 \int_0^1 \dot{C}(p, T_u, Z, c) p(Z, \widetilde{Z}''^2) p(c, \widetilde{c}''^2) dc dZ \quad (18)$$

since this work is mainly focused on diffusion combustion, a δ -PDF distribution was assumed for the progress variable while a β -PDF function was used for the mixture fraction. This requires to additionally solve the mixture fraction variance $\widetilde{Z}''^2$ equation:

$$\frac{\partial \rho \widetilde{Z''^2}}{\partial t} + \nabla(\rho \mathbf{U} \widetilde{Z''^2}) - \nabla \cdot \left(\mu_t \nabla \widetilde{Z''^2} \right) = 2 \frac{\mu_t}{S_c} |\nabla Z|^2 - \rho \chi \quad (19)$$

The sink term appearing in Eq. 19 is the average scalar dissipation rate, which is function of the turbulent time scale and mixture fraction variance:

$$\chi = C_\chi \frac{\varepsilon}{k} \widetilde{Z''^2} \quad (20)$$

To conveniently apply this model to engine simulations without introducing significant computational overheads, the table based on homogeneous reactor is processed to include the effects of turbulence chemistry interaction as shown in Fig. 3. In particular, the user specifies ranges of mixture fraction and progress variable segregation factors (S_Z and S_c , respectively), defined as the ratio between variance and maximum variance values:

$$S_Z = \frac{\widetilde{Z''^2}}{Z(1-Z)} \quad (21)$$

$$S_c = \frac{\widetilde{c''^2}}{c(1-c)} \quad (22)$$

for any value of Z , S_Z , c and S_c it is possible to compute variances and the coefficients for the probability density function distributions. On the basis of them, integration is performed for all the tabulated quantities f_{HR} and a new table including the effects of mixture fraction and progress variable fluctuations is available for the presumed PDF combustion model.

$$f_{seg} = \int_0^1 \int_0^1 f_{HR}(p, T_u, Z, c) p(Z, \widetilde{Z''^2}) p(c, \widetilde{c''^2}) dc dZ \quad (23)$$

Compared to other widely used combustion models for non-premixed combustion, the TPPDF model does not consider any sub-grid diffusion in the mixture fraction space, while other approaches does either through a suitable mixing model [28] or by means of the scalar dissipation rate term. Turbulence/chemistry interaction with the presumed PDF combustion model is expected to reduce the maximum flame temperatures and to increase the thickness of the flame compared to the well-mixed model.

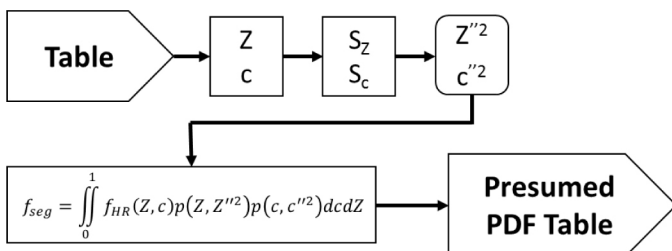


Figure 3. Generation of the chemistry table used for the presumed PDF combustion model (TPPDF).

Tabulated Representative Interactive Flamelet Model (TRIF)

This model is based on the laminar flamelet concept, assuming that the smallest turbulent time and length scales are much larger than the chemical ones and there exists a locally undisturbed sheet where reactions occur [7]. This sheet can be treated as an ensemble of stretched counter-flow diffusion flames, called *flamelets*. The advantage of such treatment is that all reacting scalars only depend on the mixture fraction variable, Z , which is related to the local fuel-to-air ratio for non-premixed combustion. Hence, local chemical composition can be estimated from the Z field in the CFD domain, assuming that its sub-grid distribution can be represented by a β -pdf. In order to properly account for local flow and turbulence effects on the flame structure and predict flame stabilization, a multiple number of flamelets can be used. Each one is representative of a certain portion of the injected fuel mass, and chemical composition in each cell is computed from mixture fraction and flamelet marker distribution as follows:

$$Y_i(\vec{x}) = \sum_{j=1}^{N_f} M_j \int_0^1 Y_{j,i}(\tilde{Z}) P(\tilde{Z}, \widetilde{Z''^2}) dZ \quad (24)$$

For each flamelet marker, the following transport equation is solved:

$$\frac{\partial \rho \tilde{M}_j}{\partial t} + \nabla(\rho \mathbf{U} \tilde{M}_j) - \nabla \cdot \left(\frac{\mu_t}{S_{cZ}} \nabla \tilde{M}_j \right) = \dot{S}_{M_j} \quad (25)$$

where the source term $\dot{S}_{M_j}$ corresponds to $\dot{S}_Z$ only for a specified interval of the injection duration, while it is zero elsewhere. Flamelet markers must also satisfy the following relation:

$$Z = \sum_{j=1}^{N_f} M_j \quad (26)$$

The local flame structure is defined by the flamelet equations that are solved for the progress variable C and enthalpy assuming unity Lewis number [7] in the mixture fraction space:

$$\rho \frac{\partial C}{\partial t} = \rho \frac{\chi_z}{2} \frac{\partial^2 C}{\partial Z^2} + \dot{C} \quad (27)$$

$$\rho \frac{\partial h}{\partial t} = \rho \frac{\chi_z}{2} \frac{\partial^2 h}{\partial Z^2} + \frac{dp}{dt} \quad (28)$$

The chemical composition in the mixture fraction space is retrieved from the chemistry table in the same way as done for the TWM model in the CFD domain. Effects of mixing related to turbulence and flow-field are grouped into the scalar dissipation rate term χ_z which is function of the scalar dissipation rate at stoichiometric mixture fraction conditions $\widetilde{\chi_{st,j}}$ which is computed for each flamelet.