

# Detailed Simulations of Stratified Ignition and Combustion Processes in a Spray-Guided Gasoline Engine using the SparkCIMM/G-Equation Modeling Framework

Rainer N. Dahms  
Sandia National Laboratories

Michael C. Drake, Ronald O. Grover, Jr., Arun S. Solomon and Todd D. Fansler  
General Motors Company

## ABSTRACT

Recently, high-speed optical imaging data for a single operating point of a spray-guided gasoline engine has, along with the flamelet model and the G-equation theory, enabled the development of the new spark-ignition model SparkCIMM. Within its framework, detailed chemistry flamelet models capture the experimental feature of multiple localized ignition events along the excessively stretched and restriking spark channel, as well as the observations of non-spherical highly-corrugated early turbulent flame fronts. The developed flamelet models account for the substantial turbulent fluctuations in equivalence ratio and enthalpy present under spray-guided conditions. A non-unity Lewis number formulation captures the deficient species diffusion into the highly-curved flame reaction zone. Previously, these diffusion processes were shown to have a significant effect on the early flame development in spray-guided engines due to, initially, locally rich and highly-diluted low turbulent Damköhler number mixtures. Localized flame extinction phenomena are captured by corresponding flamelet criteria. In this paper, the theoretical-numerical SparkCIMM/G-equation framework is applied to three different spray-guided engine operating conditions. These conditions vary substantially in engine speed, load, EGR rate, and in injection and spark-ignition timings. Accurate wall temperatures, flow fields and mixture property conditions at ignition timing were obtained by multiple 3D detailed intake simulations. Swirl numbers, trapped masses, pressure traces before spark advance, and the integral heat release were aimed to be in agreement with experimental data. Spray model parameters were optimized by comparison to spray-rig experiments. Providing such a proper setup for each operating point, the simulation results show excellent agreement with local and cylinder-averaged experimental data. The simulation captures the effects of the operating-point-dependent varying mixture pathways of the spark channel and the propagating flame on ignition and combustion. Turbulent mixture property fluctuations in equivalence ratio, enthalpy, flame stretch, and scalar dissipation are successfully reproduced.

**CITATION:** Dahms, R., Drake, M., Grover, Jr., R., Solomon, A. et al., "Detailed Simulations of Stratified Ignition and Combustion Processes in a Spray-Guided Gasoline Engine using the SparkCIMM/G-Equation Modeling Framework," *SAE Int. J. Engines* 5(2):2012, doi:10.4271/2012-01-0132.

## INTRODUCTION

Spray-guided spark-ignition direct-injection (SG-SIDI) gasoline engines hold the promise to provide substantially improved fuel economy in comparison to former spark-ignition engine concepts [1]. In these engines, the centrally located fuel injector sprays along the cylinder axis towards a closely spaced spark plug. This specification allows a wide stratified-charge operating range. However, the closeness of the fuel spray and spark electrodes can cause unfavorable conditions for ignition with high cyclic variabilities [2]. Due to the short time between injection and sparking, substantial

scalar dissipation rates are induced which affect localized ignition events along the spark channel as well as the propagation of the resulting flame kernels. Due to the high flow-velocity field caused by direct fuel injection, the spark can extend to a length of about  $\ell \sim 10$  mm before a re-strike occurs. Locally launched flame kernels propagate into a highly turbulent, stratified, and diluted fuel cloud, which results in complex interactions of the flame with the turbulent mixing field.

Recently, the new physically-based **spark** channel ignition monitoring model SparkCIMM has been introduced

[3,4,5]. It bridges the gap between a detailed spray/evaporation model and a model for fully developed turbulent flame front propagation. Based on the flamelet model and the G-equation theory, both mainly developed by Peters [6,7,8,9], it captures the experimentally observed features of ignition and non-spherical early flame front phenomena. The early flame is strongly influenced by turbulent mixture property fluctuations and finite chemistry rate effects. The significance of the modeling advances have been shown by comparison to detailed experimental data and to simulations applying models of different physical complexity. Many of the presented modeling advances are not included in previous spark-ignition models (AKTIM [10,11,12,13], ISSIM-LES [14], and DPIK [15,16,17,18]). The SparkCIMM/G-equation numerical-theoretical framework can be used in combination with standard submodels for nitric oxide or unburnt hydrocarbon emissions. Physically-based modeling of soot emissions requires considerably more work, which is, however, beyond the scope of this paper.

In this paper, the developed theoretical-numerical SparkCIMM/G-equation framework has been used to analyze turbulent combustion in three different engine operating points of a SG-SIDI gasoline engine. The naturally aspirated engine is equipped with a four-valve pent-roof head, Siamese ports and a contoured piston bowl. A centrally-mounted 8-hole fuel injector (60 degree cone spray) sprays the fuel along a close-coupled spark plug (J-gap extended-electrode spark plug [9 mm spark plug with a 2 mm spacer] pointed towards the fuel injector and electrodes positioned between two fuel spray plumes) with a high-energy long-duration inductive ignition system (120 mJ/pulse, ~ 2 ms spark duration). The generated engine grid includes, along with the intake runner, the geometrical details of the engine topology. The intake flow fields have been calculated using 3D turbulent flow simulations. An enhanced engine swirl number is generated by the deactivation of the left intake valve.

## THE SPARKCIMM/G-EQUATION MODELING FRAMEWORK

The **spark channel ignition monitoring model** SparkCIMM has recently been introduced and a more detailed documentation of this approach can be found in Dahms et al. [3,4,5]. The general modeling concept is motivated by high-speed laser-sheet imaging data from Drake, Fansler, and their co-workers [1, 2, 19], showing complex phenomena for spark and ignition. The model reduces the progress of spark-ignited turbulent flame front propagation to a characteristic three-stage process. First, the spark energy deposition rate establishes a spark channel, which advects and corrugates with the local flow. Flame kernels are initiated along this spark channel wherever local conditions permit it. These conditions are determined by the mixture composition and the rates of energy deposition and scalar dissipation. Extended flamelet equations and a Karlovitz-number criterion are applied to predict these

localized ignition events [4]. Second, the resulting quasi-spherical flame kernels merge and form a non-spherical flame front. Their propagation is computed using the G-equation model and their flame fronts are tracked by Lagrangian marker particles. Laminar burning velocities and flame thicknesses of the curved flame front are obtained using tabulated premixed flamelets, calculated using a validated detailed chemical mechanism for flame propagation [20] to appropriately consider locally rich and highly diluted mixtures, and formulations to consider the strong influence of turbulent diffusivity and fluctuations of enthalpy, non-unity Lewis number laminar stretch rates, and mixture fraction. Third, the early non-spherical flame transitions into a fully-developed turbulent flame front. Its propagation is also computed by the G-equation model, but it is numerically tracked by a level-set approach as soon as the flame kernel shape is resolved by the applied computational grid. The Lagrangian marker particles, used in SparkCIMM to track the flame front, are then removed from the flow field.

## SPARK CHANNEL MODELING

At the start of energizing, a thin spark channel forms between the electrodes of the spark gap. Its thickness ( $d_{sprk} \sim 0.05$  mm) is too thin to be resolved by common computational grids. Therefore, Lagrangian marker particles are used instead. The motion of the stretched and wrinkled spark channel is modeled by a convection equation solved for

the velocity  $\tilde{u}_p$  of each representative marker particle  $p$  [4]: The indices ( $p$ ) and ( $cell$ ) refer to the particle and to the computational

$$\begin{aligned} \tilde{u}_p = & \tilde{u}_{cell} + \nabla \tilde{u}_{cell} \cdot \tilde{\Delta \vec{x}}_{p,cell} \\ & + \left( \sqrt{\frac{2}{3} \left( \tilde{k}_{cell} + \nabla \tilde{k}_{cell} \cdot \tilde{\Delta \vec{x}}_{p,cell} \right) \left( \frac{d_{sprk}}{\ell_{t,p}} \right)^{1/3}} \right) \\ & \cdot \text{sign}(1, \text{rand}(\Delta \tau^*)) \end{aligned} \quad (1)$$

grid cell value, respectively. The rand-operator provides a random number between  $[-1, 1]$ . The integral turbulent

kinetic energy is denoted by  $\tilde{k}$ ,  $\tilde{\Delta \vec{x}}_{p,cell}$  is the local distance vector between the mean particle position and the corresponding grid cell center, and  $d_{sprk}$  is the thickness of the spark channel. The integral length scale at each particle position is denoted by  $\ell_{t,p}$  and  $\tau^*$  represents the stochastic superimposed fluctuation, which scales with the turbulent turnover time of eddies of the spark channel size [4]. Depending on the stretch of the spark channel, additional particles are introduced to maintain a quasi-equidistant discretization of this arc. Combustion-related mixture

properties of the local flow field are interpolated to these particles from the grid cell values.

### MODELING IGNITION PROCESSES ALONG THE SPARK CHANNEL

The gaseous mixture surrounding the wrinkled and stretched spark channel is monitored during the spark duration at each of the tracked channel particle locations for the formation of a localized ignition spot. These formations are determined by auto-ignition processes, triggered by the spark energy deposition rate, and are thus independent from the ability to support the propagation of a flame front at the local mixture conditions. An ignition spot kernel is placed locally at the position of the corresponding spark channel particle  $p$ , if the averaged temperature  $\tilde{T}_p$  exceeds the cross-over temperature  $T^0$  ( $\sim 1400$  K)[4]:

$$\tilde{T}_p = \frac{1}{\Delta Z} \int_{Z_p - \frac{1}{2}\Delta Z}^{Z_p + \frac{1}{2}\Delta Z} \left( \int_0^1 T(t, Z) \tilde{P}(Z; \tilde{Z}, \tilde{Z}'^2) dZ \right) dZ$$

$$\geq c_{T^0} T^0 \quad c_{T^0} = 1.05 \quad [4] \quad (2)$$

Mixture temperatures  $T(t, Z)$  are computed as a function of time  $t$  and mixture fraction  $Z$ , defined below, by the flamelet model derived by Peters [21]. The flamelet equations consider the effect of scalar mixing on combustion, and they were extended by a source term  $\dot{S}_{sprk}$  to consider spark energy deposition rates [4].

$$\rho \frac{\partial Y_i}{\partial t} = \rho \frac{\chi}{2Le_i} \frac{\partial^2 Y_i}{\partial Z^2} + \dot{m}_i$$

$$\rho \frac{\partial T}{\partial t} = \rho \frac{\chi}{2} \frac{\partial^2 T}{\partial Z^2} + \rho \frac{\chi}{2c_p} \left( \sum_{i=1}^n \frac{c_{p,i}}{Le_i} \frac{\partial Y_i}{\partial Z} + \frac{\partial c_p}{\partial Z} \right) \frac{\partial T}{\partial Z}$$

$$+ \frac{1}{c_p} \left( \frac{\partial p}{\partial t} - \sum_{i=1}^n \dot{m}_i h_i \right) + \dot{S}_{sprk} \quad , \quad (3)$$

with  $Y_i$  as the species mass fractions,  $T$  as the mixture temperature, and  $n$  as the number of species contained in the underlying chemical mechanism. The applied mechanism for primary reference fuels includes 82 species and 368 reactions (provided as supplemental material in [4]) and incorporates low, intermediate, and high-temperature oxidation chemistry. All calculations were performed using a PRF87 mixture, which consists of 87 % iso-octane and 13 % n-heptane by

liquid volume. The averaged temperature  $\tilde{T}_p$  of the mixture surrounding the spark channel at each particle position  $p$  is obtained by a beta-pdf integration [22] using its probability density  $\tilde{P}(Z; \tilde{Z}, \tilde{Z}'^2)$  to account for the substantial turbulent

mixture fraction fluctuations. The mixture fraction  $Z$  is defined as

$$Z = \frac{m_1}{m_1 + m_2} \quad (4)$$

with  $m_1$  as the fuel stream mass and  $m_2$  as the oxidizer stream mass, respectively. Using this definition,  $Z = 0$  refers to the composition of the oxidizer stream (fresh air and exhaust gas recirculation) and  $Z = 1$  refers to the corresponding composition of the fuel stream (PRF87). The statistics of the instantaneous mixture fraction fluctuations are considered by solving the mean 3D mixture fraction equation with an additional source term  $\dot{S}$  to include fuel vaporization:

$$\frac{\partial \langle \rho \rangle \tilde{Z}}{\partial t} + \langle \rho \rangle \nabla \tilde{Z} \cdot \tilde{u} = \nabla \cdot \left( \langle \rho \rangle \tilde{D}_t \nabla \tilde{Z} \right) + \dot{S} \quad , \quad (5)$$

with the turbulent diffusivity  $\tilde{D}_t$  defined as

$$\tilde{D}_t = \frac{\tilde{\mu}_t}{Sc_t} = \frac{c_\mu}{Sc_t} \frac{\tilde{k}^2}{\tilde{\epsilon}} \quad , \quad (6)$$

with  $\tilde{\mu}_t$  as the mean turbulent viscosity and with the modeling constants  $Sc_t$  and  $c_\mu$  defined in Table 1. The mean mixture fraction variance equation is introduced as the second moment of the mixture fraction [6]:

$$\frac{\partial \langle \rho \rangle \tilde{Z}'^2}{\partial t} + \langle \rho \rangle \nabla \tilde{Z}'^2 \cdot \tilde{u} = \nabla \cdot \left( \langle \rho \rangle \tilde{D}_t \nabla \tilde{Z}'^2 \right)$$

$$+ 2 \langle \rho \rangle \tilde{D}_t (\nabla \tilde{Z})^2$$

$$- 2 \langle \rho \rangle \frac{\tilde{\epsilon}}{\tilde{k}} \tilde{Z}'^2 \quad , \quad (7)$$

with  $\tilde{D}_t$  defined in Eq. (6). The range of averaging ( $\Delta Z$ ) in Eq. (2) is computed as given in

$$\Delta Z = \nabla_{||} \tilde{Z} \cdot 2 \tilde{r}_{K,0} \quad , \quad (8)$$

with  $\tilde{r}_{K,0}$  as the mean initial flame kernel radius ( $\sim 0.5$  mm [23]), and  $\nabla_{||} \tilde{Z}$  as the local mean 3D mixture fraction gradient tangential to the spark channel.

A re-strike, typically resetting the spark channel to its original position between the electrodes in the spark gap, is applied if the arc exceeds a predefined length ( $\ell_{sprk} \sim 10$  mm) determined by experiments. After a re-strike, new

Langrangian marker particles are introduced to track the motion of the newly formed spark channel and to monitor the surrounding unburnt mixture for the formation of new ignition spots according to Eqs. (1) and (2). The Lagrangian marker particles used for the representation of the extinguished spark channel are removed from the flow field.

### MODELING LOCALIZED FLAME KERNEL FORMATIONS

The formation of a localized ignition spot along the wrinkled and stretched spark channel, predicted by the extended flamelet equations, does not necessarily lead to a successful flame kernel propagation. Temperatures within

**Table 1. Modeling constants of the G-equation flamelet model.**

| Symbol  | Value | Definition                                 |
|---------|-------|--------------------------------------------|
| $b_1$   | 2.0   | Experiments, Bradley [24]                  |
| $b_2$   | 1.78  | Peters [6]                                 |
| $b_3$   | 1.0   | Experiments, Damköhler [25]                |
| $c_s$   | 2.0   | Peters [6, 7]                              |
| $c_\mu$ | 0.09  | Launder [26]                               |
| $Sc_t$  | 0.7   | analog to $Pr_t$ for the enthalpy equation |

formed ignition spots exceed the cross-over temperature (compare Eq. 2), where chain-breaking reactions dominate over chain-branching reactions. This characteristic temperature therefore also represents the kinetic condition for sustainable flame front propagation. However, if the local Kolmogorov eddies are able to perturb the inner reaction layer of the flame front, which begins to propagate from the ignition spot locations into the unburnt mixture, the turbulence induces a critical loss of radicals towards the preheat zone. Then the flame structure cannot be preserved, leading to its localized extinction (the “broken reaction zones” in the regime diagram for premixed turbulent combustion [6]). Therefore, in SparkCIMM, an ignition spot is turned into a small spherical flame kernel ( $\sim 0.5$  mm [23]) according to a local Karlovitz number criterion, determining a successful flame kernel propagation at the local mixture conditions:

$$Ka_\delta = \delta^2 \frac{v_\eta^2}{s_{L,eff}^2} < 1 \quad , \quad (9)$$

with  $v_\eta$  as the local Kolmogorov velocity scale and with  $\delta$  as the ratio of the width of the inner reaction layer  $\ell_\delta$  to the laminar flame thickness  $\ell_f$  [4]. The effective laminar burning velocity reads

$$s_{L,eff} = \tilde{s}_L + s_{plasma} \quad , \quad (10)$$

including the averaged laminar burning velocity  $\tilde{s}_L$  of the curved flame front under local stratified and diluted mixture conditions, discussed below, and a plasma velocity  $s_{plasma}$  due to spark energy deposition [16, 27, 28]. However, as described above, a re-strike might be initiated after a certain time. In that case, the spark energy deposition rate will not further support the early flame kernel development of already launched flame kernels, vanishing their expansion velocity  $s_{plasma}$ . By that time, the local mixture conditions have to support a sustainable flame front propagation to prevent localized extinctions. Such chemistry-related conditions are discussed below.

To enhance the numerical accuracy and efficiency of this modeling approach, a least-squares method and a temporal sub-cycling technique are applied. The former allows higher-order variable reconstructions of mixture property stratifications within one computational grid cell, and the latter enables the application of time-steps small enough to resolve the complex spark channel phenomena without mainly affecting the overall CFD time-step, respectively.

### EARLY NON-SPHERICAL FLAME KERNEL PROPAGATION

Whenever conditions along the spark channel permit it, as expressed by Eqs. (2) and (9), an ignition spot kernel is turned into a quasi-spherical flame kernel ( $\sim 0.5$  mm [23]). Its propagation is modeled by the G-equation. However, the flame kernel size is still too small to be resolved by the computational grid. Therefore, its propagation is tracked by Lagrangian marker particles. The 3D G-equation is then approximated using these Lagrangian marker particles which are homogeneously distributed along the flame kernel surface. As discussed in the following, a quasi-multidimensional G-equation is then solved for each of these particles.

Representative flame kernel advection velocities are obtained from samples  $i$  of the velocity field along the flame front of each kernel. The mean convection velocity  $\tilde{u}_{FK}$  for the center of gravity of flame kernels (FK) reads [4]

$$\tilde{u}_{FK} = \frac{1}{\bar{\rho}N} \sum_{i=1}^N (\bar{\rho}_i \tilde{u}_i) \quad , \quad (11)$$

with  $\bar{\rho}$  as the averaged density and with  $\bar{\rho}_i$  and  $\tilde{u}_i$  as the localized mean density and mean flow velocity along the flame front, respectively. The turbulent fluctuation term is omitted in Eq. (11), since it enters, consistent with the G-equation theory, into the models for the turbulent burning

velocity and the turbulent curvature term, which are discussed below.

During the spark duration, multiple spherical flame kernels are initiated along the stretched spark channel, which all grow at the local burning velocity. The non-spherical early flame front is reconstructed from the enveloping surface of intersecting spherical flame kernels. The radius of each spherical flame kernel is calculated following

$$\tilde{r}_{FK} = \left( \frac{3}{4} \frac{m_{FK}}{\pi \tilde{\rho}_b} \right)^{1/3}, \quad (12)$$

with  $m_{FK}$  as the burnt mass and  $\tilde{\rho}_b$  as the mean burnt gas density. This density is evaluated from the ideal gas law. The mean flame kernel temperature is calculated using the following equation [4]:

$$\begin{aligned} \frac{d}{dt} \tilde{T}_{FK} = & -\frac{\dot{m}_{FK}}{m_{FK}} (\tilde{T}_{FK} - \tilde{T}_b) + \frac{\dot{Q}_{sprk} \eta_{eff}}{m_{FK} \tilde{c}_p} \\ & + \frac{1}{\tilde{\rho}_b \tilde{c}_p} \frac{dp}{dt}, \end{aligned} \quad (13)$$

with the mean adiabatically burnt gas temperature  $\tilde{T}_b$ , the electrical energy deposition rate  $\dot{Q}_{sprk}$ , the efficiency of electrical energy transfer  $\eta_{eff}$  ( $\sim 0.3$  [29]), and the mean specific heat  $\tilde{c}_p$ . Spark channel re-strikes generally lead to spark energy discharge locations apart from already initialized flame kernel positions. In that case, the energy discharge does not further support the development of the flame kernel, vanishing  $\dot{Q}_{sprk}$  in Eq. (13) and  $s_{plasma}$  in Eq. (9).

The mass consumption rate of each spherical flame kernel is calculated using the following equation:

$$\frac{d}{dt} m_{FK} = \dot{m}_{FK} = 4\pi \tilde{r}_{FK}^2 \rho_u \tilde{s}_{T,\tilde{\kappa}}, \quad (14)$$

with  $\rho_u$  as the unburnt gas density and  $\tilde{r}_{FK}$  as the mean turbulent flame kernel radius, defined in Eq. (12). The mean turbulent propagation velocity  $\tilde{s}_{T,\tilde{\kappa}}$  of each spherical flame kernel is obtained as an averaged value from sample points  $i$  along the local non-spherical flame front, defined as the envelope of intersecting spherical flame kernels. It reads, including effects of turbulent mixture fraction fluctuations, considered by a prescribed beta-pdf integration [22],

$$\tilde{s}_{T,\tilde{\kappa}} = \frac{1}{\tilde{\rho}_u N} \sum_{i=1}^N \left[ \int_0^1 \rho_{u,i} \cdot \max [s_{L,i}, s_{T,\tilde{\kappa},i}] \tilde{P}(Z; \tilde{Z}_i, \tilde{Z}_{i,FK}^{\prime 2}) dZ \right], \quad (15)$$

with the following equation for the turbulent propagation velocity  $s_{T,\tilde{\kappa}}$ :

$$s_{T,\tilde{\kappa}} = s_T - \tilde{D}'_t \tilde{\kappa}, \quad (16)$$

along with the equation for the turbulent burning velocity  $s_T$ :

$$\begin{aligned} s_T = & \underbrace{s_L^0(Z, \tilde{H}(Z)) \cdot [1 - \mathcal{M}(Z, \tilde{H}(Z)) \cdot \ell_f^0(Z, \tilde{H}(Z)) \cdot \tilde{\kappa}]}_{s_L} \\ & \cdot [1 + \tilde{\sigma}_t(Z, \tilde{H}(Z), \tilde{\kappa})], \end{aligned} \quad (17)$$

with the laminar burning velocity  $s_L$ , the mixture fraction  $Z$ , the corresponding mean enthalpy  $\tilde{H}(Z)$ , the Markstein number  $M$ , the laminar flame thickness  $\ell$ , the curvature of the mean turbulent flame front  $\tilde{\kappa}$ , the mean turbulent flame surface area ratio  $\tilde{\sigma}_t$ , and the turbulent flame diffusivity  $\tilde{D}'_t$  as discussed below in detail. As shown in Dahms et al. [5], the turbulent burning velocity  $s_T$  cannot be reduced below laminar values  $s_L$  due to turbulent diffusivity effects, considered in Eq. (16). This is appropriately considered by Eq. (15).

The mixture fraction variance  $\tilde{Z}_{i,FK}^{\prime 2}$  at the flame sample point  $i$  in Eq. (15) is obtained within the inertial subrange at the size of the flame kernel [3]. It is derived from the variance of local integral scale values  $(\tilde{Z}_i^{\prime 2})$ , defined in Eq. (7):

$$\tilde{Z}_{i,FK}^{\prime 2} = \tilde{Z}_i^{\prime 2} \cdot \left( \frac{\ell_{FK}}{\ell_{t,i}} \right)^{2/3}; \quad \ell_{FK} \leq \ell_t, \quad (18)$$

with  $\ell_t$  as the integral length scale. The characteristic flame kernel scale  $\ell_{FK}$  is calculated from the mean turbulent flame kernel radius  $\tilde{r}_{FK}$  computed from Eq. (12) as  $\ell_{FK} = 2.0 \cdot \tilde{r}_{FK}$ .

## MODELING CURVED LAMINAR FLAME STRUCTURES IN STRATIFIED AND DILUTED MIXTURES

In order to accurately model the turbulent burning velocity  $s_T$ , the underlying curved laminar flame structure in stratified mixtures must be made available. Therefore, a validated detailed chemical mechanism without low-temperature oxidation chemistry (87 species and 462 reactions) and optimized for predicting flame propagation [20] has been used to compute one-dimensional premixed flames with variations in equivalence ratio ( $0.3 < \phi < 3.5$ ), unburnt gas temperature ( $300 < T_{ub} < 1100$  K), mixture dilution ( $0 < Y_{Dil} < 0.45$ ), and thermodynamic pressure ( $1 < p < 70$  bar) previous to the 3D engine combustion simulations ( $> 100,000$  different flames). The mixture dilution  $Y_{Dil}$  is defined as the mass fraction of inert combustion products recirculated from exhaust gas:

$$Y_{Dil} = Y_{Inert,EGR} - Y_{N_2,Air,EGR} \quad , \quad (19)$$

with  $Y_{N_2,Air,EGR}$  as the mass fraction of nitrogen contained in unconsumed air within the EGR stream. The laminar burning velocities ( $s_L^0$ ) and laminar flame thicknesses ( $\ell_f^0$ ) of these planar flames have been processed from these calculations, along with corresponding detailed chemical mechanism equilibrium solutions of adiabatically burnt gas temperatures ( $T_b$ ) and heat capacities ( $c_p$ ). To make these detailed chemistry computations available to the 3D simulations, this data has been tabulated in a premixed-flamelet library. Efficient hashing functions then provide the required computational performance of look-up computations during 3D engine combustion simulations. These detailed chemistry planar flame structures are then used to calculate the structure of curved and stratified flames during the engine combustion simulation.

Combustion theory [30] provides corrections to the laminar burning velocity due to curvature and strain rate effects. The burning velocity may also change substantially due to thermo-diffusive instabilities, developing along the flame front. These cellular instabilities and self-acceleration of outwardly propagating flames were experimentally shown for, preferably rich, laminar hydrocarbon flame fronts [31]. In Dahms et al. [5], it is shown that under actual spray-guided spark-ignition conditions, the effects of strain rate and thermo-diffusive cellular instabilities can be neglected due to low turbulent Damköhler number mixtures and highly-corrugated early flame fronts. Also, the curvature of the instantaneous flame front can be approximated by the curvature of the mean turbulent flame front. Then, the laminar burning velocity, including first-order corrections only, reads

$$s_L(\tilde{\kappa}) = s_L^0(1 - \mathcal{M}\ell_f^0\tilde{\kappa}) \quad , \quad (20)$$

with  $\tilde{\kappa}$  as the curvature of the mean turbulent flame front. The Markstein number  $\mathcal{M}$  is dependent on the effective Lewis number  $Le_{eff}$  of the mixture and is calculated according to Bechtold and Matalon [32] as

$$\mathcal{M} = \alpha - (\sigma - 1)\frac{\gamma_1}{\sigma} \quad , \quad (21)$$

and as discussed in detail in [5]. The effective Lewis number  $Le_{eff}$  is defined in [32] as

$$Le_{eff} = 1 + \frac{(Le_E - 1) + (Le_D - 1)A}{1 + A} \quad , \quad (22)$$

with  $Le_E$  and  $Le_D$  as the Lewis numbers of the excess and deficient reactants, and  $A = 1 + Ze(\phi^* - 1)$  with  $\phi^*$  as the ratio of mass of excess-to-deficient reactant in the fresh mixture. It is equal to the equivalence ratio  $\phi$  in fuel-rich mixtures and its reciprocal  $1/\phi$  in fuel-lean mixtures.

The instantaneous laminar burning velocity distribution  $s_L^0(Z)$  of planar flames in stratified mixtures is obtained from the flamelet library for different mixture fraction realizations ( $s_L^0 = f(Z, \tilde{T}_{ub}(Z), \tilde{Y}_{Dil}(Z), p)$ ). However, the look-up parameters  $Z$  and  $\tilde{T}_{ub}$  are interrelated in a non-trivial manner. Partially premixed mixtures in direct-injection engines are also characterized by substantial enthalpy variations due to the mixing of cold fuel vapor with the hot ambient air and due to evaporation heat losses. Therefore, by varying the mixture fraction  $Z$  (or equivalence ratio), the unburnt mixture temperature  $\tilde{T}_{ub}$  and mixture enthalpy alters correspondingly. A local enthalpy flamelet approach reconstructs this fundamental relation  $\tilde{T}_{ub} = f(Z)$  as discussed in detail in Dahms et al. [4]. The model introduces two additional 3D transport equations to track the development of the mean unburnt gas temperature  $\tilde{T}_{ub}$  at  $Z = \tilde{Z}$  and the mean oxidizer-stream temperature  $\tilde{T}_{Ox}$  at  $Z = 0$ , respectively. The equations read

$$\frac{\partial \langle \rho \rangle \tilde{T}}{\partial t} + \langle \rho \rangle \nabla \tilde{T} \cdot \tilde{u} = \nabla \cdot \left( \langle \rho \rangle \tilde{D}_t \nabla \tilde{T} \right) + \dot{S}_{\langle T|Z \rangle} \quad , \quad (23)$$

where  $\tilde{T}$  is either  $\tilde{T}_{ub}$  or  $\tilde{T}_{Ox}$  with  $\tilde{D}_t$  defined in Eq. (6). The source term  $\dot{S}_{\langle T|Z \rangle}$  accounts, in the case of the unburnt gas temperature  $\tilde{T}_{ub}$ , for global pressure gradients and local

enthalpy losses due to spray evaporation and wall heat transfer. In the case of the oxidizer-stream temperature  $\tilde{T}_{Ox}$ , it only accounts for global pressure gradients and wall heat losses. It explicitly excludes heat losses due to fuel evaporation. This equation tracks the thermal stratification induced by the intake process and by wall boundary layers.

The corresponding mixture enthalpies  $\tilde{h}_{Ox}(Z=0)$  and  $\tilde{h}_u(Z=\tilde{Z})$  are computed using the well-defined unburnt gas compositions at  $Z=0$  and  $Z=\tilde{Z}$ , respectively:

$$\begin{aligned} Y_F(Z) &= Z \\ Y_{Dil}(Z) &= (1-Z) \frac{\tilde{Y}_{Dil}(\tilde{Z})}{1-\tilde{Z}} \\ Y_{Air}(Z) &= 1 - Y_F(Z) - Y_{Dil}(Z) \end{aligned} \quad , \quad (24)$$

with  $Y_F$ ,  $Y_{Air}$ , and  $Y_{Dil}$  as the mass fractions of fuel, air, and mixture dilution. Then the enthalpy, used in Eq. (15), can be related to the mixture fraction by the following linear coupling relation:

$$\tilde{H}(Z) = \tilde{h}_{Ox} + \frac{\tilde{h}_u - \tilde{h}_{Ox}}{\tilde{Z}} Z \quad . \quad (25)$$

This equation provides the 3D distribution of the enthalpy and, by using corresponding well defined unburnt gas compositions, the unburnt gas temperature  $\tilde{T}_{ub}(Z)$  as a function of the mixture fraction variable. During the PDF-averaging of instantaneous flame front realizations, which differ in mixture fraction, this temperature distribution modifies the planar flame laminar burning velocity  $s_L^0(Z, \tilde{H}(Z))$  and the corresponding curvature flame front correction term according to Eq. (20). This correction term varies substantially due to the implied modifications of the laminar flame thickness  $\ell_f^0(Z, \tilde{H}(Z))$  and the Markstein number  $\mathcal{M}(Z, \tilde{H}(Z))$ . The enthalpy stratification also modifies the turbulent burning velocity distribution  $s_T(Z, \tilde{H}(Z))$  by affecting the mean turbulent flame surface area ratio  $\tilde{\sigma}_t$  as discussed below.

### MODELING TURBULENT PROPAGATION VELOCITIES OF STRATIFIED NON-UNITY LEWIS NUMBER FLAMES

The formerly introduced equations make the underlying laminar flame structure, which is dependent on the instantaneous fluctuations in mixture fraction, enthalpy, and flame stretch due to non-unity Lewis number effects, available to accurately model the turbulence and flame front interactions.

The turbulent burning velocity  $s_T$  is obtained from the laminar burning velocity and the turbulent flame surface area ratio. The mean turbulent flame surface area ratio  $\tilde{\sigma}_t = (\tilde{s}_T - \tilde{s}_L)/\tilde{s}_L$  is defined as the mean increase of the flame surface area caused by turbulence beyond the laminar value. In comparison to the fundamental equation derived by Peters [6], it has been further generalized to account for the wrinkling and corrugation caused by turbulence on a curved flame structure in stratified mixtures [5]. It reads:

$$\begin{aligned} \tilde{\sigma}_t(Z, \tilde{H}(Z), \tilde{\kappa}) &= -\frac{b_3^2}{4b_1} \sqrt{\frac{3c_\mu c_s}{Sc_t} \frac{\ell_{f,t}}{\ell_f^0}} (1 - \mathcal{M} \ell_f^0 \tilde{\kappa}) \left( \frac{\ell_{f,t}}{\ell_{f,t,alg}} \right)^{2/3} + \\ &\sqrt{\frac{b_3^4}{16b_1^2} \frac{3c_\mu c_s}{Sc_t} \left( \frac{\ell_{f,t}}{\ell_f^0} \right)^2 (1 - \mathcal{M} \ell_f^0 \tilde{\kappa})^2 \left( \frac{\ell_{f,t}}{\ell_{f,t,alg}} \right)^{4/3} + \frac{c_s b_3^2}{2s_L^0 \ell_f^0} \ell_{f,t}^2 \frac{\tilde{\epsilon}}{\tilde{k}_{FK}}} \end{aligned} \quad (26)$$

The modeling constants  $b_1$ ,  $b_3$ ,  $c_\mu$ ,  $c_s$ , and  $Sc_t$  are defined in Table 1. The unsteady turbulent flame brush thickness  $\ell_{f,t}$  is obtained by the solution of the variance equation of mean turbulent flame front positions  $\tilde{G}''^2$  as defined below. Its algebraic value  $\ell_{f,t,alg}$  is obtained by neglecting the temporal derivative in the variance equation of mean turbulent flame front positions using a steady-state assumption [4]. The mean turbulent kinetic energy within the inertial subrange at the size of the flame kernel (FK) is denoted by  $\tilde{k}_{FK}$  and obtained from integral scale values  $\tilde{k}$ , compare Eq. (18). The final turbulent propagation velocity  $\tilde{s}_{T,\tilde{\kappa}}$  in Eq. (15) is obtained from the turbulent burning velocity  $s_T = s_L(1 + \tilde{\sigma}_t)$  and the turbulent curvature term. The latter is computed from the curvature of the mean turbulent flame front  $\tilde{\kappa}$  and the turbulent diffusivity  $\tilde{D}'_t$  of the flame. This turbulent flame diffusivity is defined as

$$\tilde{D}'_t = c_{D'_t} \sqrt{\frac{c_s c_\mu}{2Sc_t} \tilde{k}_{FK} \tilde{G}''^2} \quad , \quad (27)$$

with the modeling constants  $c_s$ ,  $c_\mu$ , and  $Sc_t$  defined in Table 1 and  $\tilde{k}_{FK}$  as the mean turbulent kinetic energy within the inertial subrange at the size of the flame kernel (FK) [4]. The constant  $c_{D'_t}$  is obtained by optimizing the simulation results in order to match the experimental data for one engine operating point. This parameter is then held constant for the simulation of the other operating points. In this study, a constant of  $c_{D'_t} = 0.8$  is used.