

An Efficient Level-Set Flame Propagation Model for Hybrid Unstructured Grids Using the G-Equation

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ABSTRACT

Computational fluid dynamics of gas-fueled large-bore spark ignition engines with pre-chamber ignition can speed up the design process of these engines provided that 1) the reliability of the results is not affected by poor meshing and 2) the time cost of the meshing process does not negatively compensate for the advantages of running a computer simulation. In this work a flame propagation model that runs with arbitrary hybrid meshes was developed and coupled with the KIVA4-MHI CFD solver, in order to address these aims. The solver follows the G-Equation level-set method for turbulent flame propagation by Tan and Reitz, and employs improved numerics to handle meshes featuring different cell types such as hexahedra, tetrahedra, square pyramids and triangular prisms.

Detailed reaction kinetics from the SpeedCHEM solver are used to compute the non-equilibrium composition evolution downstream and upstream of the flame surface, where chemical equilibrium is instead assumed. A generalized least-squares gradient reconstruction algorithm is employed to evaluate spatial derivatives with arbitrary node and cell connectivities, instead of the original ENO scheme. Finally, a new, extended version of the “marching cubes” algorithm for iso-surface tracking was developed and implemented for all four employed cell types.

The solver was tested across different cell types and cell resolutions by simulating spherical ignition in a simple cylindrical combustion chamber. Validation was performed against experimental measurements of torch jet ignition with a diaphragm and of prechamber gaseous fuel combustion two-chamber experimental vessel separated by a variable-diameter nozzle, with different grid resolutions.

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INTRODUCTION

The success of advanced, fuel-efficient and environmentally friendly combustion strategies for internal combustion engines is challenged by the need to meet increasingly stringent regulatory emission mandates [1]. Multi-dimensional Computational Fluid Dynamics (CFD) simulations have become a mandatory design tool for the exploration and implementation of high-efficiency, lean combustion regimes also for gas-fueled spark ignition engines, thanks to recent advancements in:

- in-cylinder flow and turbulence modeling, through large-eddy simulations (LES) [2] for capturing most eddy scales and their

- effects on cycle-to-cycle variations; and anisotropic models for Reynolds-Averaged Navier Stokes simulations (RANS) [3,4];
- methods for chemical kinetics modeling of hydrocarbon ignition processes [5,6], and their application to premixed and partially-premixed combustion [7,8];
- sub-grid scale gas jet injection modeling for practical engine grid sizes [9, 10, 11];
- flame propagation and flame-wall interaction modeling for RANS and LES engine simulations [12,13,14,15].

Natural-gas-fueled engines are naturally attractive for heavy duty applications because of the cheap fuel cost and cheaper pollutant control devices allowed by globally lean engine operation; as well as for significantly lower greenhouse-gas emission, which can be as much as 25% smaller than from traditional heavy hydrocarbon fuels. Lean combustion strategies are an effective way to reduce NO_x emissions and to increase the overall thermodynamic efficiency by reducing wall heat losses, but they must be carefully designed to avoid reaching the lower natural gas's ignitability limit.

In order to cope with this issue, among other charge ignition strategies such as with a pilot injection of diesel or of a secondary, high-reactivity fuel [16,17], pre-chamber-type devices have been proposed, and studied in a variety of configurations [18,19,20,21]. By using a pre-chamber, a near-stoichiometric or slightly rich mixture can be formed and ignited upstream of the combustion chamber in an almost-closed volume. The ignited charge then propagates into the combustion chamber by forming torch-shaped jets, that azimuthally cover the whole combustion chamber and ignite its lean air-fuel mixture, as schematically reported in Figure 1.

Computational modeling of such an engine configuration is challenging. The pre-chamber simulation cannot be decoupled from the combustion chamber simulation. In case a block-structured hexahedral grid is used, a unique complex blocking structure must be defined, and the mesh needs to be basically re-made each time a new pre-chamber geometry is to be tested. Second, the time and spatial scales in the pre-chamber do not allow proper resolution of the flame front development and its near-sound-speed travel within the prechamber nozzles. For the purpose of modeling heavy-duty gas-fueled pre-chamber ignition engines, it is necessary to develop a methodology that:

1. incorporates detailed chemical kinetics for the accurate prediction of the flame front advancement at the lean limit, as well as accurate pollutant formation from the combustion products;
3. tracks all relevant flame propagation properties at mesh scales of typical combustor geometries, hence without having to discretize the inner- and near-inner-flame structure.

In this work we present the development of a computationally efficient methodology suitable for the design of pre-chamber ignition heavy-duty gas-fueled engines. The methodology features an enhanced level-set turbulent flame propagation model using the GEquation [12]. A new 'marching cells' algorithm, or an extended isosurface and iso-volume tracking method for hybrid unstructured grids was developed. The methodology was embedded in an Arbitrary Lagrangian-Eulerian finite volume scheme [22]. Consistency and accuracy of the flame propagation scheme were assessed across meshes featuring different cell types, and validated versus experimental optical measurements of torch-jet flame propagation in restricted channels, representative of pre-chamber-like operation.

FLAME PROPAGATION MODEL DESCRIPTION

Flame propagation in spark-ignited premixed and partially-premixed combustion regimes follows time and spatial scales which cannot be typically captured with the finite volume method on devices of industrial scale such as internal combustion engines.

The laminar flame structure is typically represented as three adjacent layers, for an overall thickness l_F which can be estimated as [12]

$$l_F = \frac{\lambda / c_p|_{T=T_0}}{\rho_u S_{L0}} \quad (1)$$

The bulk of the flame thickness is occupied by an inert pre-heating region where temperature rises but no significant reactions occur. An inner reactive-diffusive layer δ (Figure 2) is a thin portion of the whole thickness, where the fuel is consumed and chemical reactions occur in a diffusion-limited process. A final, slightly thicker oxidation layer, ε , relevant to CO production, is reported to be approximately three times larger, $\varepsilon l_F \sim 3 \delta l_F$.

As summarized for example by the flamelet modeling theory of Peters [23] - and using the nomenclature reported in Figure 2 -, turbulent flame propagation in engines happens under either the corrugated flamelet regime, where the whole flame reaction-diffusion region is embedded within eddies at the Kolmogorov scale; or the thin-reaction-zone regime, which assumes that Kolmogorov eddies can enter the inert zone ahead of the reactive-diffusive region, but not the inner flame layer where the chemical reactions take place.

Peters demonstrated that the inner flame structure is either undisturbed by the smallest eddies (corrugated flamelet), or it can be tracked via an augmented displacement speed of reaction

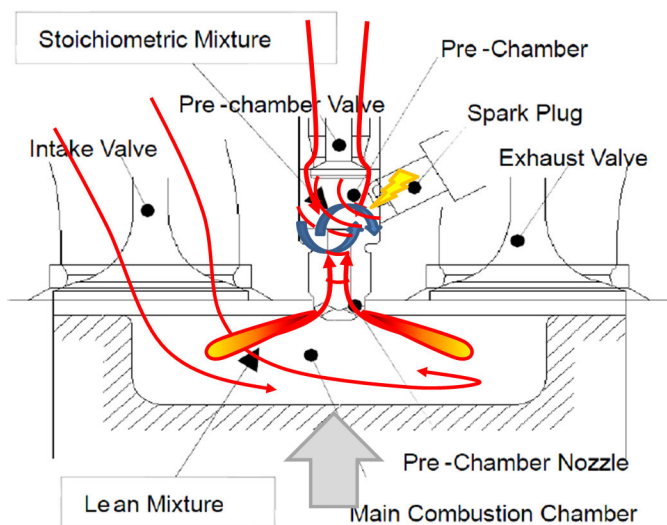


Figure 1. Pre-chamber mixture formation and ignition schematic.

1. features hybrid unstructured body-fitted grids, so that multiple pre-chamber meshes can be generated using automated meshing techniques, without compromising for simulation accuracy near the walls or in narrow regions such as the nozzles;

coefficient (thin-reaction-zone), which incorporate the effects of strain. It is hence possible to describe transport of the flame inner layer using the same equation valid for both regimes.

The inner flame layer is hence modeled as a two-dimensional, faceted interface of infinitesimal thickness, which is ruled by a transport equation.

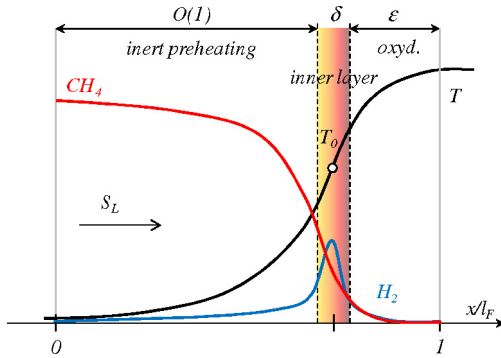


Figure 2. Schematic of asymptotic one-dimensional laminar flamelet structure for a methane-air flame (re-made from [23]) versus normalized flame thickness coordinate x/l_F .

G-Equation Level-Set Flame Formulation

The “G-Equation model” is a flamelet model using the level set method for the solution of the flame front transport equation first proposed by Peters [12]. Level set modeling is a class of tools for handling surface treatment in multi-dimensional models, where the surface is tracked using a level set from a multi-dimensional scalar field (such as the iso-surface $G = 0$) [24]. The current study builds on the G-Equation formulation first developed by Fan and Reitz [25], and later improved by Tan and Reitz [14] and Liang and Reitz [7].

In the G-Equation, a transport equation describing the dynamics of the $G = 0$ flame front is used:

$$\rho \frac{DG}{Dt} = \rho \frac{\partial G}{\partial t} + \rho \mathbf{u} \cdot \nabla G = (\rho S_L^0) \sigma - (\rho D) \kappa \sigma, \quad (2)$$

where σ is a turbulent to laminar flame surface area or flame speed ratio, expressed as:

$$\sigma = \frac{S_T^0}{S_L^0} = 1 + \frac{S_T^0 - S_L^0}{S_L^0} = |\nabla G| + \sigma_T, \quad (3)$$

σ_T being a turbulent contribution term. Within the Reynolds-Averaged Navier Stokes flow representation and k-ε turbulence modeling approach, Equation (2) can be expressed as a Favreaveraged G field (no superscript), plus a variance field (tilde superscript) equation that serves the computation of the σ_T term:

$$\begin{cases} \frac{\partial G}{\partial t} + \mathbf{u} \cdot \nabla G = \frac{\rho_u}{\rho} S_T^0 |\nabla G| - D_T \kappa |\nabla G|, \\ \frac{\partial \tilde{G}}{\partial t} + \mathbf{u} \cdot \nabla \tilde{G} = \nabla_{\parallel} \cdot \left(\frac{\rho_u}{\rho} D_T \nabla_{\parallel} \tilde{G} \right) + 2 D_T (\nabla \tilde{G})^2 - c_s \frac{\tilde{\epsilon}}{\tilde{k}} \tilde{G}, \end{cases} \quad (4)$$

where $\nabla_{\parallel}$ indicates a tangential gradient operator, $\mathbf{u}$ the Favreaveraged fluid velocity, ρ_u and ρ the density of unburnt and burnt flamelet sides, D_T the turbulent diffusivity, c_s a modeling constant, and:

$$\kappa = \nabla \cdot \left(\frac{\nabla G}{|\nabla G|} \right) \quad (5)$$

the Favre-averaged flame front curvature.

Ignition Kernel Modeling

Even with a level set approach a tiny spherical flame front of size less than the mesh during ignition kernel development cannot be resolved by the G-Equation. Hence, the Discrete Particle Ignition Kernel (DPIK) model of Tan and Reitz [14] was implemented and employed.

In this model, the flame front during kernel growth is tracked using Lagrangian particle tracers instead of the G-field solution, and the flame surface density is computed as the number density of particles in each finite volume cell. The ignition kernel is assumed to be perfectly spherical and internally homogeneous (ρk), and a time law for the rate of change of kernel radius is used:

$$\frac{dr_k}{dt} = \frac{\rho_u}{\rho_k} (S_{plasma} + S_T), \quad (6)$$

where the plasma velocity is based on an energy balance of the ignition kernel as a closed thermodynamic system:

$$S_{plasma} = \frac{\eta_{el} \dot{Q}_{el}}{4\pi r_k^2 \left[\rho_u (u_k - h_u) + p \frac{\rho_u}{\rho_k} \right]}. \quad (7)$$

$\dot{Q}_{el}$ represents non-ideal power transfer to the fluid due to the spark discharge, subject to an efficiency $\eta_{el} = 0.3$, p , u and h are pressure, internal energy and enthalpy and the u subscript represents the unburnt region outside of the kernel. The turbulent flame speed term S_T contains a flame stretch factor according to Herweg *et al.* [36]:

$$S_T = S_L^0 \left[1 - \left(\frac{l_F}{15l_I} \right)^{\frac{1}{2}} \left(\frac{u'}{S_L^0} \right)^{\frac{3}{2}} - 2 \frac{l_F}{r_k} \frac{\rho_u}{\rho_k} \right], \quad (8)$$

where l_I is the integral turbulence length scale. The transition from the DPIK model to the G-Equation solver is based on a critical radius criterion:

$$r_k \geq c_{m1} l_I = c_{m1} 0.16 \frac{k^{3/2}}{\epsilon}, \quad (10)$$

where c_{m1} is a model constant usually greater than unity [14].

Currently, transition to the G-Equation solver can only be initiated by the ignition kernel model. Auto-ignition (especially knock-related) phenomena are predicted via the detailed chemistry integration (cf. next paragraph), but are not allowed to initiate a new flame front. Future research will need to focus on incorporating a Borghidiagram-based condition to define when ignition chemistry should switch to flame propagation (for both premixed and non-premixed combustion regimes).

Detailed Chemical Kinetics-Based Combustion Modeling

The availability of detailed chemical kinetic mechanisms for the oxidation of hydrocarbons has had a major impact on the accuracy of internal combustion engine simulations, because of:

1. the ability to characterize ignition delay, combustion development and heat release at a variety of thermodynamic combustion regimes with a same reaction model, which would be unfeasible with simplified ignition schemes;
2. a physics-based pollutant formation description through usage of their direct gas-phase components (NOx, UHC) or precursors (soot);
3. a more accurate description of the local presence of highly-reactive radicals in the multi-dimensional domain, whose transport equations are solved for by the flow solver.

However, its application to multidimensional internal combustion engine simulations is still limited because of the extreme computational burden required to solve the stiff systems of ordinary differential equations (ODEs) associated with reactive networks often featuring hundreds/thousands of species and reactions.

In the present work, detailed combustion kinetics using the SpeedCHEM sparse analytical Jacobian chemistry solver [5,6] were coupled with the G-Equation solver.

Non-Flame Cells

In the model direct chemistry integration is employed to compute the rates of change of species mass fractions due to chemical reactions, treating each computational cell as a homogeneous well-stirred reactor. The reaction mechanism describes a set of n_r reactions among n_s species:

$$\sum_{i=1}^{n_s} \nu'_{k,i} M'_i \leftrightarrow \sum_{i=1}^{n_s} \nu''_{k,i} M''_i, \quad k = 1, \dots, n_r, \quad (11)$$

with ν' and ν'' being stoichiometric reactant/product reaction coefficients, and M the species names. The temporal evolution of the thermodynamic state of the reacting gas-phase mixture with species mass conservation is described by:

$$\frac{dY_i}{dt} = \frac{W_i}{\rho} \sum_{k=1}^{n_r} (\nu''_{k,i} - \nu'_{k,i}) q_k, \quad i = 1, \dots, n_s, \quad (12)$$

with q_k the reaction rate progress variables, W the species molecular weights, and ρ the mixture density. The mass conservation constraint: $\sum Y_i = 1$, or $\sum dY_i/dt = 0$, is automatically verified if the reactions are well-posed, i.e., each one verifies atomic conservation of all chemical elements. In the multi-dimensional domain, the energy conservation resembles a temperature rate of change in an adiabatic constant-volume reactor:

$$\frac{dT}{dt} = -\frac{1}{\bar{c}_v} \sum_{i=1}^{n_s} \left(\frac{U_i}{W_i} \frac{dY_i}{dt} \right), \quad (13)$$

U being molar internal energies, $\bar{c}_v$ the mixture average specific heat at constant volume in mass units.

The code also features libraries for the evaluation of thermodynamic properties of gas-phase mixtures and kinetic laws for various reaction classes (Arrhenius, three-body, reversible/irreversible, mapped pressure-dependent, etc.). All of the equations employ a matrix-based representation that makes use of an object-oriented sparse matrix algebra library, specifically developed for this application. A sparse analytical Jacobian matrix formulation was developed to speed up the most demanding parts of the integration of the ODE system [5].

Coupled with a variety of stiff ODE solvers, the SpeedCHEM package has been demonstrated to achieve up to three orders of magnitude speed up in comparison with the dense CHEMKIN-II library, showing order-of-magnitude speedups also for small reaction mechanisms typically used in large multi-dimensional simulations, as reported in Figure 3. The constant-volume reactor calculation in all non-flame cells also provides a good estimate of whether knock will occur in the end gases [8].

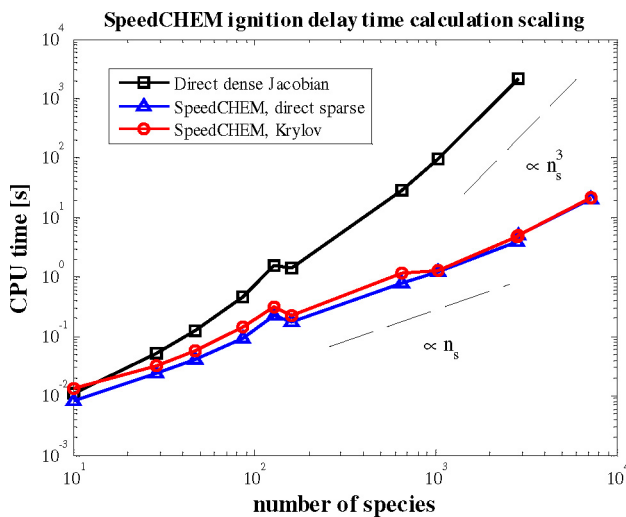


Figure 3. Linear scalability of the SpeedCHEM solver for constant-volume well stirred reactor calculations. (black) dense, (blue) sparse, (red) Krylov linear system solver comparison. Adapted from [6].

Flame Cells

In cells containing the flame front, the method of Liang was applied [7]. Where a flame front is present (with total area A_f), two - not necessarily unique and contiguous - volumes can be geometrically identified within the cell: an unburnt mixture volume V_u and a burnt volume V_b containing combustion products.

The volume containing combustion products, and swept by the flame front, is assumed to be in local equilibrium at the homogeneous cell pressure (deflagration behavior). Its mass fraction composition $Y_{i,b}$ is computed using an equilibrium calculation code [27], which also provides an adiabatic flame temperature that is assumed to be constant across the burnt volume region, $T_{equil} = T_b$. The burnt gas species and mixture densities are given directly from the equation-of-state.

The unburnt species densities can be estimated based on simple mass conservation of the unburnt volume, which is swept by the flame surface. The exact swept volume is evaluated as the difference between the burnt volumes in the cell, computed using the flame triangulation, before (time 'n') and after (phase 'B') the G field advancement. The global rate of species density change can hence be evaluated as:

$$\frac{\partial \rho_i}{\partial t} = (\rho Y_{i,b} - \rho_i) \frac{V_b^B - V_b^n}{V_u}, \quad i = 1, \dots, n_s. \quad (14)$$

No special treatment is applied in case the flame front reaches cells which contain mostly combustion products on its 'unburnt' side. In this unlikely event, when swept by the flame front, they will eventually experience 1) a slow flame speed, because of the extremely low value of $f\phi$; 2) a limited species conversion rate and corresponding heat release, as the 'unburnt' composition ahead of the flame front contains gases which are already close to their corresponding equilibrium composition.

Flame Speed

Laminar flame speed calculations with detailed chemical kinetics require a one-dimensional representation of the laminar flame, which is usually discretized using a finite-difference approach. Fixed point algorithms are needed to solve the coupled nonlinear reaction-diffusion flame equations (also including nonlinear binary diffusion coefficients for each species pair). Even using sparse algebra, this type of calculation requires a CPU time which is of the order of minutes for a single laminar flame configuration, making its adoption practically unfeasible on a large multidimensional domain. While a tabulation approach could be used, it would require to compromise on the species composition on both sides (burnt/unburnt). Also, its accuracy could deteriorate in full-cycle engine calculations where a wide range of pressures is swept. Hence, we decided to adopt mapped laminar flame speed correlations which were verified to be adequate at the pressure ranges experienced by the simulation, and that feature similar input (T , ϕ , p) as a table would have. Still, this remains a challenging topic and potential improvement for future research.

NUMERICAL SOLUTION METHOD

The G-Equation level set representation of the flame front has physical meaning only at the flame front itself, or at the iso-surface defined by $G = 0$. Hence, in our implementation, the G-Equation is solved only at set of flame 'brush' nodes, identified as the ones belonging to cells which contain the flame front; a dummy value of G equal to the signed distance from the flame is instead used far away from the flame.

As the accuracy of the flame equation solution relies on proper calculation of the field gradient and curvature at the flame front, a methodology for iso-surface tracking and handling via a discretized triangulation, and a numerical scheme for spatial derivative evaluation on general unstructured grids are proposed in this study.

A 'Marching Cells' Algorithm for Iso-Surface Triangulation

The 'Marching Cubes' algorithm proposed by Lorensen and Cline [28] is the first of a family of the currently most widely adopted surface-reconstruction methods from three-dimensional data [29,30].

While this algorithm is mainly employed in computer graphics post-processors, it was chosen as a basis for our methodology for the following reasons:

- a non-ambiguous iso-surface triangulation is determined by processing each hexahedron independently (hence the name 'marching cubes'). This makes the algorithm intrinsically fast because it is fully vectorizable;
- all triangulation vertices are uniquely identified at the cell's edges, which makes the methodology 1) easily extensible to hybrid meshes with cells of any kind, and 2) fast as each flame edge, which is shared by several cells, is only processed once;
- the edge piercing point identification principle is based on a multi-linear field interpolation which follows a parameterized representation of the cell. The same parameterization can be exploited to interpolate other useful quantities at the iso-surface or anywhere within the cell.