

Implementation and Validation of the G-equation Model Coupled with Flamelet Libraries for Simulating Premixed Combustion in I.C. Engines

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ABSTRACT

The G-equation model was implemented in the commercial code ANSYS CFX and validated against experimental data in order to successfully simulate turbulent premixed combustion in internal combustion engines. The model is based on the level-set approach. Two transport equations are solved respectively for the G-scalar mean value, representing the local distance function from the time-averaged mean flame front, and its variance, correlated to the turbulent flame brush thickness. The model closure for tracking the flame front is based on an algebraic expression for the turbulent burning velocity.

The composition of the reacted mixture is evaluated by coupling the code with flamelet libraries generated with the ANSYS CFX-RIF package by means of a reaction progress variable computed as a function of the G-related quantities. An innovative technique for periodically re-initializing the G-scalar field, in order to enforce geometrical consistency and avoid numerical instabilities, was developed, consisting of a least-square-based interface reconstruction and a minimization of the distance from the discretized flame front.

In order to make the code suitable for spark-ignition engine applications the combustion model was coupled with a spark kernel model that simulates the early stages of the ignition process at sub-grid scales. The robustness and accuracy of the level-set approach with moving structured and unstructured meshes were assessed and the parallel performance of the

combustion model was optimized in order to deal with large meshes in industrial applications.

Validation was carried out by comparing simulations against experimental data for three different test-cases: a steady flame in a slot-burner, a transient spark-ignited premixed combustion in a cylinder with fixed walls and optical access and a spark-ignition research engine with flat head and flat piston.

The results show good numerical properties and other attractive features in terms of geometrical description of the flame front and coupling with sub-models for detailed chemistry and spark-ignition.

INTRODUCTION

The three-dimensional simulation of turbulent reacting flows in Internal Combustion Engines (ICE) still represents one of the most challenging applications of Computational Fluid Dynamics (CFD). In order to optimize engine performance, automotive manufacturers are investing increasing resources in virtual prototyping, thus requiring to CFD developers and software vendors more and more demanding features in terms of modeling capabilities, stability, accuracy and usability.

By restricting our focus to turbulent combustion in Spark-Ignition (SI) engines the complexity of the physics that has to be accounted for has increased impressively over the last decade. One can get a sample of it, just by considering the evolution of the simulation targets in

some ICE modeling areas, for instance ignition and chemistry.

Presently, a proper SI modeling framework should include not only accurate sub-models for the release and the evolution of the spark-kernel, as suggested by Herweg and Maly [1], but also have the flexibility necessary for predicting knock and handling multiple ignition events (e.g. by re-ignition or multi-spark systems). This task has been tackled by many authors like Fan and Reitz [2], Duclos and Colin [3], Bianchi and Falfari [4], who highlighted the need not only for adequate kernel-models but also for a smooth coupling with the main combustion code.

Similarly, simple reaction mechanisms involving less than ten species are not sufficient for properly modeling the complex non-equilibrium effects influencing the pollutant formation and pathological engine behaviors like knock. Many works have been carried out by different authors in order to include detailed kinetic schemes and knock sub-models in their numerical investigations, like for instance by Liang et al. [5] [6], Teraji et al. [7], and D'Errico et al. [8], only in order to cite a few works among the most recent ones.

Nowadays the modeling challenge for ICE cannot be called fully accomplished because of the complexity of the real applications. On the other hand, it is clear that a CFD framework that does offer in the short term robustness, accuracy and a flexible integration between the different modeling areas will have the best chances of success. These requirements are even stricter if one extends the application range of CFD tools to Gasoline Direct Injection (GDI) engines, where the spray dynamics and the regimes of stratified or partially premixed combustion further increase the complexity of a numerical analysis.

The ideal target for a CFD software vendor would be to provide users with a simulation platform able to span over a wide range of SI engines. From Port Fuel Injection (PFI) high performance engines equipping racing vehicles, where the hypothesis of homogeneous mixture and fully premixed combustion can be reasonably assumed, up to GDI engines of passenger cars. Such different applications may be successfully investigated only by choosing a combustion model which provides, besides an accurate description of the flame propagation, also hooks to proper sub-models for multiple-ignition, knocking, detailed kinetics and species prediction for both fully and partially premixed conditions.

The development of CFD techniques for predicting the flame propagation under a wide range of operating conditions was addressed by many authors. For instance, Tan and Reitz [11] presented a universal turbulent combustion model suited for PFI, GDI and Diesel engines as well, by extending the G-equation model, originally proposed by Williams [12] and widely elaborated by Peters [13]. The same level-set approach

was reprised by Liang et al. [5] and integrated with an auto-ignition sub-model and a 22-species 42-reactions iso-octane mechanism in order to investigate knock in SI engines. A modeling framework with similar capabilities was developed by Teraji et al. [7], starting from the Extended Coherent Flame Model (ECFM) proposed by Duclos et al. [14] and Colin et al. [15], by integrating it with an auto-ignition model.

The above-mentioned works are only a few examples of two main streams of CFD investigations focused on modeling combustion in SI engines respectively by means of the ECFM and the G-equation model. Both approaches have been successfully implemented in ANSYS software [16] [17] and are available either in the standard release or as prototype. However, an explicit comparison of the performance of the two models is out of the scope of the present work, which on the contrary addresses features, implementation and results specific to the G-equation model. In fact, while modeling aspects and performance of the ECFM are well known in the automotive community, there is still some lacks of information about the potential of the level-set approach, its main numerical implications and how these can be resolved.

In this paper the authors present the G-equation model implemented in a custom-version of the ANSYS CFX code [17] [18] and based on the formulation by Peters [13]. Many efforts were invested in defining a proper numerical treatment for ensuring accuracy and robustness. An extensive validation was carried out by running three different test-cases dealing with fully premixed combustion in a slot-burner, a closed vessel with fixed walls and a "pancake" engine with flat head and flat piston, respectively. These applications are clearly far from the complexity-level of real GDI engines, where the combustion is partially premixed and strongly influenced by the mixture formation process. However, this work should be considered as a first step towards future industrial applications. Moreover, the choice of simpler test-cases was extremely convenient in order to tackle numerical and modeling issues, which otherwise would have been covered by other uncertainties. Last but not least, as explained in the next sections, the model framework was designed with already in mind the extension to partially premixed flames.

CONTRIBUTION OF THE PRESENT WORK

The implementation of the G-equation model discussed in this paper offers some original features with respect to previous works like the classical formulation reported by Peters [13] and the versions developed by Tan and Reitz [9] or by Duchamp and Pitsch [21].

The re-initialization of the G-scalar field, whose zero-level isosurface represents the position of the mean flame-front, is a critical section of this interface-tracking method, as explained by Sethian [22]. In the present work this task is performed according to a new algorithm

consisting of a linear least-square flame reconstruction. This allows discretizing the interface between fresh and burnt gases as a zero-thickness cloud of scattered points, which are subsequently taken as reference in order to update the distance of the mesh nodes from the actual flame front.

The computation of the chemical species in the burnt gases was performed by coupling the 3D code with diffusive steady flamelet libraries, using as input quantities the reaction progress, the mixture fraction mean value and its variance. The look-up tables were generated by means of the ANSYS CFX-RIF tool [18].

The spark-kernel model available in the standard release of ANSYS CFX [17] was modified in order to take into account the evolution of the G-equation-related quantities during the mixture ignition.

COMBUSTION MODEL

The G-equation model was based on the existing framework shared by other models available in the ANSYS CFX code [17] for computing fully and partially premixed combustion, namely the Burning Velocity Model (BVM), proposed by Zimont [19] [20], and the ECFM.

All three models share two main tasks: the prediction of the flame front propagation and the estimation of the chemical species in the reacted mixture. The latter step is performed exactly in the same way. What really differentiates the models is the way a turbulent flame is propagated in the computational domain.

FLAME FRONT PROPAGATION

In the BVM and the ECFM the numerical tracking of a turbulent premixed flame is accomplished by solving a transport equation for the so-called reaction progress variable, c . This quantity varies in the range between 0 (fresh mixture) and 1 (burnt gases) and may be viewed as the probability of finding combustion products. The difference between the two models may be summarized in the analytical closure for the source term in the Partial Differential Equation (PDE) for c . In the BVM an algebraic relationship is used, based on the turbulent burning velocity s_T . This quantity may be estimated according to various correlations, like the ones suggested by Zimont [19] and Peters [13], respectively. The ECFM, instead, uses a combination of the laminar burning velocity s_L and the flame surface density Σ . The latter quantity is computed by solving an additional transport equation.

In the G-equation model the tracking of the turbulent flame is based on the level-set approach [22]. The fundamental assumption is that any interface separating two regions may be described as the G_0 isosurface of a scalar quantity G , thus leading to the following position:

$$G(\mathbf{x}, t) = G_0 \Leftrightarrow \text{flame} \quad (1)$$

A convenient choice is to set G_0 equal to zero and to have fresh gases for negative values and combustion products for positive ones. For laminar flames the propagating speed of the front may be described by the following kinematic equation:

$$\frac{d\mathbf{x}_f}{dt} = \mathbf{v}_f + \mathbf{n}s_L \quad (2)$$

where $\mathbf{x}_f$ represent the position of the flame, $\mathbf{v}_f$ the velocity of the underlying flow-field, $\mathbf{n}$ the normal to the front surface and s_L the laminar burning velocity. By differentiating Eq. (1) with respect to time and combining with Eq. (2) one gets a transport equation for the G-scalar, the so-called "G-equation":

$$\frac{\partial G}{\partial t} + \mathbf{v}_f \cdot \nabla G = s_L |\nabla G| \quad (3)$$

An extension to turbulent combustion may be derived according to the usual Favre-averaging and to proper closure assumptions, which are extensively explained by Peters [13]. The resulting model is summarized by the following transport equations for the mean value of the G-scalar and its variance.

$$\bar{\rho} \frac{\partial \tilde{G}}{\partial t} + \bar{\rho} \tilde{\mathbf{v}} \cdot \nabla \tilde{G} = (\bar{\rho} s_T^0) |\nabla \tilde{G}| - \bar{\rho} D'_t \tilde{\kappa} |\nabla \tilde{G}| \quad (4)$$

$$\bar{\rho} \frac{\partial \tilde{G}''^2}{\partial t} + \bar{\rho} \tilde{\mathbf{v}} \cdot \nabla \tilde{G}''^2 = \nabla_{||} \cdot (\bar{\rho} D_t \nabla_{||} \tilde{G}''^2) + 2\bar{\rho} D_t (\nabla \tilde{G})^2 - c_s \bar{\rho} \frac{\tilde{\epsilon}}{k} \tilde{G}''^2 \quad (5)$$

The $||$ subscript in the G-variance diffusion term means that only the turbulent diffusion parallel to the mean flame front is accounted for, since the contribution of the diffusion normal to G-isolines is already included in the turbulent burning velocity s_T [13].

Model Closure

The term $s_{T,0}$ in the G-scalar equation (4) represents the turbulent burning velocity of a planar flame and it is modeled by means of an algebraic correlation. In the present work the relationship between s_T and s_L suggested by Ewald [25] was implemented in the ANSYS CFX code:

$$s_T = s_L (1 + \sigma_t) \quad (6)$$

$$\sigma_t = \frac{l_{f,t}}{l_f} \left(-\frac{b_3^2}{4b_1} \sqrt{\frac{3c_\mu c_s}{Sc_t}} l^{*q} + \sqrt{\frac{b_3^4}{16b_1^2} \frac{3c_\mu c_s}{Sc_t} l^{*2q} + \frac{c_s b_3^2}{2} \frac{l_f}{s_L} \frac{\epsilon}{k}} \right) \quad (7)$$

Equation (7) relates the turbulent flame surface area ratio σ_t to the turbulent-to-laminar flame thickness ratio $l_{f,t}/l_f$. The laminar flame thickness l_f is defined as a function of some fluid thermo-chemical properties evaluated on the fresh gas side:

$$l_f = \left(\frac{\lambda / c_p}{\rho s_L} \right)_{unburned} \quad (8)$$

The turbulent flame brush thickness $l_{f,t}$ is defined as the square root of the G-variance normalized by the gradient of the G-scalar and represents the link between the two transported quantities of the G-equation model:

$$l_{f,t} = \frac{\sqrt{\tilde{G}^{\prime 2}}}{|\nabla \tilde{G}|} \quad (9)$$

Ewald's closure for the turbulent burning velocity (7) consists essentially of the same correlation proposed by Peters [13] corrected by the factor $(l^*)^q$ where

$$l^* = \frac{l_{f,t}}{l_{f,t,alg}} \quad (10)$$

is the ratio between the turbulent flame brush thickness $l_{f,t}$ and the algebraic flame brush thickness $l_{f,t,alg}$. The latter is computed according to Equation (9) by using an algebraic solution for the G-variance, obtained by neglecting the spatial and temporal derivatives in Equation (5):

$$2D_t (\nabla \tilde{G})^2 = c_s \tilde{G}_{alg}^{\prime 2} \frac{\epsilon}{k} \quad (11)$$

This corresponds to an equilibrium solution for the G-variance where the turbulent production equals the dissipation. By expressing the turbulent diffusivity D_t as a function of the turbulent Schmidt number Sc_t , the turbulent kinetic energy k and the turbulent eddy dissipation ϵ , the algebraic flame brush thickness can eventually be written as:

$$l_{f,t,alg} = \sqrt{\frac{\tilde{G}_{alg}^{\prime 2}}{|\nabla \tilde{G}|}} = \sqrt{\frac{2c_\mu}{c_s Sc_t} \frac{k^{3/2}}{\epsilon}} \quad (12)$$

The condition $l^*=0$ refers to a laminar flame configuration, while $l^*=1$ to a fully developed one. When the exponent q is set to zero, then expression (7) reverts to original Peters' correlation. In [25] the value $q=0.66$ was assessed to be particularly suitable for ICE simulations.

One of the most attractive features of the G-equation model is its capability to provide with a kinematic and a geometrical description of the flame front. In particular, curvature effects on the flame speed are taken into account by means of the last term in Equation (4). The curvature κ is a function of the interface normal, which, in its turn, is related to ∇G :

$$\kappa = \nabla \cdot \mathbf{n} \quad \mathbf{n} = -\frac{\nabla \tilde{G}}{|\nabla \tilde{G}|} \quad (13)$$

The turbulent diffusivity in the curvature term of Equation (4) is expressed in analogy to a mixing length approach by using the turbulent flame brush thickness as length scale, resulting in:

$$D'_t = \sqrt{\frac{c_\mu c_s}{2Sc_t}} l_{f,t} k^{1/2} \quad (14)$$

Coefficient	Value	Reference/description
b_1	2.0	Experimental Data [26]
b_3	1.0	Experimental Data [27]
c_s	2.0	[28], [29]
q	0.66	[25]
c_μ	0.09	from k - ϵ model
Sc_t	0.70	Turbulent Schmidt Number

Table 1: Coefficients for turbulent burning velocity closure according to Ewald [25]

All simulations described in this work were performed by using Ewald's correlation for s_T . Alternatively, the user could select a different closure among the ones already available in ANSYS CFX. The default values for the coefficients in the expression (7) are summarized in Table 1.

EVALUATION OF CHEMICAL SPECIES

In the premixed combustion models available in ANSYS CFX detailed chemistry may be accounted for by means of look-up tables generated with ANSYS CFX-RIF. This tool solves the steady diffusive flamelet equations [13] for different fuels and reaction mechanisms and returns the Favre-averaged mass fractions of the species in the burnt mixture $Y_{i,b}$ as:

$$\tilde{Y}_{i,b}(\tilde{Z}, \tilde{Z}^{\prime 2}, \chi) = \int_0^1 Y_{i,b}(Z, \chi) \tilde{P}(Z) dZ \quad (15)$$

In (15) the flamelet solution $Y_{i,b}(Z, \chi)$ is integrated over the mixture fraction Z according to the “Presumed Shape PDF Approach” [13], by assuming as Probability Density Function (PDF) for Z a beta distribution, whose parameters are related to the Z -mean and Z -variance.

Two additional transport equations for these quantities are solved in ANSYS CFX. The Z -mean is initialized as a function of the stoichiometric value Z_{st} and the local equivalence ratio ϕ , according to:

$$Z = \frac{Z_{st}\phi}{1 - Z_{st} + Z_{st}\phi} \quad (16)$$

The initial guess for the Z -variance is typically set to a very low number, for instance 10^{-9} .

The Favre-averaged mass fractions in the unburnt mixture $Y_{i,u}$ are zero for all reactive species except for fuel and oxidizer. Those mass fractions may be easily evaluated starting from the initial conditions as linear functions of the local mean mixture fraction, which describes a possible mixing process.

Eventually, at every computational control-volume the mass fraction of the i -th species Y_i is evaluated by weighting the corresponding values on the unburnt and burnt sides, $Y_{i,u}$ and $Y_{i,b}$ respectively, with the reaction progress c :

$$\tilde{Y}_i = (1 - c)\tilde{Y}_{i,u} + c\tilde{Y}_{i,b} \quad (17)$$

The reaction progress is a primitive variable in the BVM and ECFM, meaning that a transport equation is solved for that quantity. In contrast, in the G-equation model it is derived from the G-scalar and G-variance, by assuming that the PDF of G is a Gaussian distribution:

$$c = \int_{G=G_0}^{\infty} \frac{1}{\sqrt{2\pi\tilde{G}''^2}} \exp\left\{-\frac{(G - \tilde{G})^2}{2\tilde{G}''^2}\right\} dG \quad (18)$$

Eventually the temperature T of the reacting mixture may be computed iteratively by finding the roots of the function

$$\tilde{H} = \sum \tilde{Y}_i h_i(T) \quad (19)$$

where Y_i is computed according to (17), h_i are the species enthalpies, tabulated as polynomials of T , and H is the mean value of the mixture enthalpy obtained by solving the energy conservation equation.

The procedure outlined in this section for coupling the G-equation model with the flamelet libraries and the flow-solver is summarized in Figure 1. In case of fully premixed combustion, the workflow is simplified by deactivating the solution of Z -mean and Z -variance,

frozen to their respective initial values, since no further mixing of the reactants is occurring.

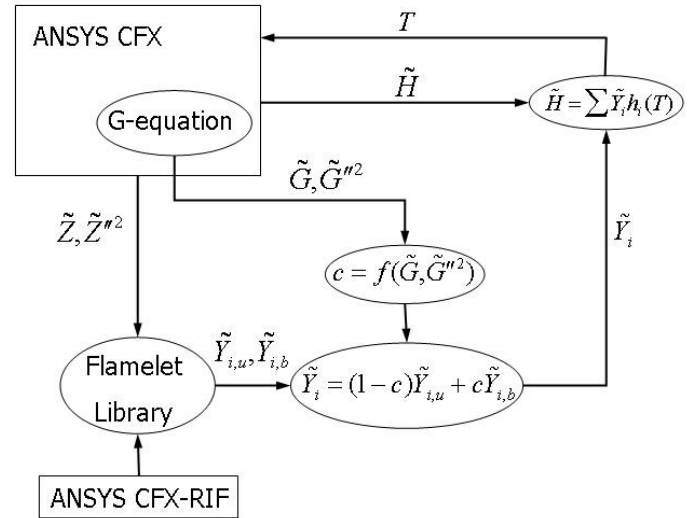


Figure 1: Coupling of the G-equation model in ANSYS CFX with flamelet libraries.

IGNITION MODEL

The spark-kernel model available in ANSYS CFX [17] solves an ordinary differential equation describing the growth rate of the kernel radius as a function of the turbulent burning velocity:

$$\frac{dr_k}{dt} = \frac{\rho_u}{\rho_b} s_{T,k} \quad (20)$$

The density ratio ρ_u/ρ_b and $s_{T,k}$ are evaluated by averaging the corresponding quantities computed by ANSYS CFX over a spherical domain, centered on the initial spark-location and with a constant, user-defined radius, r_T . This region acts like a mask interfacing the 0D model to the 3D flow-solver.

The turbulent burning velocity $s_{T,k}$ is modeled according to the closure correlation chosen by the user and with a modification accounting for high curvature when the kernel is small:

$$s_{T,k} = \max\left(s_L, s_T - \frac{2}{r_k} D_t\right), D_t = \frac{c_\mu}{Sc_t} \frac{k^2}{\varepsilon} \quad (21)$$

Generally speaking, the purpose of an ignition model is to initialize the primary combustion variables and update them during the early stages of the flame propagation, when the kernel-size is too small for the grid resolution and therefore cannot be solved by the 3D code. In ANSYS CFX the quantities mapped back from the spark-model to the flow-solver are either the reaction progress (BVM), the reaction progress and the flame-surface density (ECFM) or the G-scalar and the G-variance (G-

equation). The 0D model is switched off and the control is transferred back to the transport equation for the flame propagation when the kernel radius r_k reaches the prescribed value r_T . In order to ensure a smooth transition, r_T should be sufficiently large such that the mask region can be resolved by the mesh.

In the G-equation model, during the kernel growth ($r_k < r_T$), the G-scalar is computed by simply enforcing a spherical distribution with G_0 located at a distance r_k from the ignition point:

$$G(x, y, z, t) = r_k(t) - \sqrt{x^2 + y^2 + z^2} \quad (22)$$

This is a remarkable feature of the level-set approach, since a new flame front, even in multiple instances like in multi-spark ignition systems or by re-ignition [1] and knock, can be easily initialized, just by feeding a function describing analytically the geometrical shape of the interface.

The implementation hereby described also includes a modification to the G-variance equation suggested by Ewald [25]. In that work the author points out that the spark is affected only by turbulent structures which are smaller in size than the spark itself. In the G-equation model this can be accomplished by down-scaling the turbulent kinetic energy k in the production and dissipation terms of the G-variance equation (5), whenever the diameter of the kernel computed by the 0D model is smaller than a prescribed turbulent length scale l_t . By assuming l_t equal to the algebraic flame brush thickness $l_{f,t,alg}$, one can substitute k with the following k_{spk} value:

$$2r_k < l_t = l_{f,t,alg} : k \rightarrow k_{spk} = k \left(\frac{2r_k}{l_t} \right)^{2/3} \quad (23)$$

Until the kernel-size reaches the transition radius r_T , the G-scalar and the G-variance are updated according to the ignition model. The coupling with the Flamelet library and the flow-solver, as depicted in Figure 1, does not change at all. This leads to a consistent approach for the whole duration of the combustion and ensures a smooth transition in terms of flame front tracking at the deactivation of the spark-kernel model.

NUMERICS AND IMPLEMENTATION

The G-equation model was implemented into ANSYS CFX, a finite volume code with finite-element discretization. The variable arrangement is co-located, i.e. all variables are stored on the mesh nodes. However, the control-volumes are centered on the grid vertices and define a dual mesh for the solution of the conservation equations.

As explained in the previous section, the model itself requires two additional transport equations and a new algebraic closure for the turbulent burning velocity. All those components could be easily introduced into the modular and extensible data structure of ANSYS CFX. However, special numerical treatment was nonetheless necessary in order to cope with some particular aspects of the level-set approach and its parallelization.

LEVEL SET METHOD

The level-set method is a generic front-tracking approach. The description of a propagating interface can be reduced to a scalar advection equation and a constant-value isosurface of the transported quantity. This is accomplished in the G-equation combustion model by means of the equations (1) and (4). However, those relationships are rigorously valid only at the flame front, i.e. at the G_0 isosurface.

The straightforward extension of the G-scalar transport equation to the whole computational domain is a very attractive option in the framework of a general-purpose CFD code. In fact, this allows re-using all existing machinery implemented for solving the usual PDEs for scalar quantities, such as energy, turbulent eddy dissipation, etc., without any further modification.

The main remaining issue concerns with the choice of the most convenient constraint that the level-set scalar has to fulfill far from the front and how this can be numerically enforced.

Figure 2 shows three possible scalar quantities that can be used for identifying the interface centered on the i -th cell of a 1D mesh. The first one is the Heaviside function $c(x)$, a basic step function which varies from 1 to 0 at the interface. This is exactly what happens to the reaction progress variable. The second option is the Volume of Fluid (VOF). In contrast to $c(x)$, $VOF(i)$ is not a continuous distribution rather a discrete quantity, defined on a cell-by-cell basis. At the interface the VOF can assume any value in the range $]0,1[$. Lastly, the front position can be located by means of a function $G(x)$ expressing the signed distance from the interface itself.

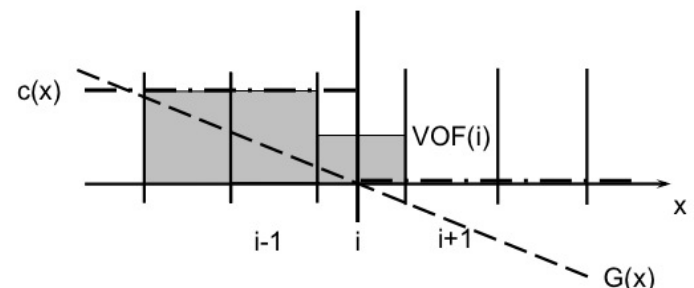


Figure 2: Reaction progress, VOF, G-scalar