

SYMMETRIES AND AVERAGING OF THE G -EQUATION FOR PREMIXED COMBUSTION

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ABSTRACT

It is demonstrated that the G -equation for premixed combustion admits a diversity of symmetries properties, i.e. invariance characteristics under certain transformations. Included are those of classical mechanics such as Galilean invariance, rotation invariance and others. Also a new generalized scaling symmetry has been established. It is shown that the generalized scaling symmetry precisely defines the physical property of the G -equation. That is to say the value of G at a given flame front is arbitrary. It is also proven that the generalized scaling symmetry precludes the application of classical Reynolds ensemble averaging usually employed in statistical turbulence theory in order to avoid non-unique statistical quantities such as for the mean flame position. Finally a new averaging scheme of the G -field is presented being fully consistent with all symmetries of the G -equation.

INTRODUCTION

Since it was introduced by Williams (1985) in the context of premixed combustion the G -equation (see equation (1) below) has stimulated a broad variety of different analytical, numerical and modelling approaches. Keller and Peters (1994) have shown that there are also a variety of different physical effects which may be included into the formulation such as local flame stretch, curvature, heat loss and unsteady pressure changes.

Since most premixed flames of practical importance are turbulent several analytical and modelling approaches have been developed to deal with the statistical properties of the G -equation (Kerstein *et al.* 1988, Peters 1992,

Peters 1999). Beside the classical averaging of G in the sense of O. Reynolds also the spatial filtering of large-eddy simulation was utilized e.g. by Im *et al.* (1997).

In the present paper both analytical and statistical averaging issues will be discussed employing symmetry group methods. An extensive overview on the application of Lie group methods to all kind of equations in the mathematical sciences can be found in Ibragimov (1995/1996).

SYMMETRY PROPERTIES OF THE G -EQUATION

G -equation formulations

The subsequent analysis is based on the G -equation in its classical form (see e.g. Williams 1985) given by

$$\frac{\partial G}{\partial t} + (\mathbf{u} \cdot \nabla)G = s_L |\nabla G| \quad (1)$$

where s_L denotes the laminar burning velocity. Equation (1) models the propagation of an iso-surface G_0 normal to itself with the velocity s_L . It is derived from the purely kinematic relation

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

between the displacement of the flame front, the local velocity and the burning velocity normal to the flame front.

It is important to note that equation (1) has only a physical meaning at the flame front G_0 . Outside of this iso-surface G is not defined. In addition any level set different from G_0 has no influence on the propagation of the iso-surface of G_0 . For this reason any iso-surface apart

from the flame front can be determined by different equations.

The G -equation has to be complemented by an equation for the velocity vector \mathbf{u} . For the present analysis only constant density flows will be considered explicitly and hence velocity and pressure are determined by the Euler or Navier-Stokes equations

$$\begin{aligned} \nabla \cdot \mathbf{u} &= 0, \\ \frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} &= -\frac{1}{\rho} \nabla p + \nu \Delta \mathbf{u} \end{aligned} \quad (3)$$

where the Euler equation is defined according to the simplification $\nu = 0$.

Symmetries of the G -equation

A symmetry of the equations (1) and (3) is a transformation which maps these equations into itself; i.e. we need to determine the transformations \mathbf{f} and \mathbf{g} which map the original set of variables

$$\mathbf{y} = [t, \mathbf{x}] \quad \text{and} \quad \mathbf{z} = [\mathbf{u}, p, G]. \quad (4)$$

to a new set of variables characterized by an asterisk

$$\begin{aligned} \mathbf{y}^* &= [t^*, \mathbf{x}^*] = \mathbf{f}(\mathbf{y}, \mathbf{z}), \\ \mathbf{z}^* &= [\mathbf{u}^*, p^*, G^*] = \mathbf{g}(\mathbf{y}, \mathbf{z}) \end{aligned} \quad (5)$$

obeying the equivalence

$$\begin{aligned} \mathbf{F}(\mathbf{y}, \mathbf{z}, z_1^*, z_2^*, \dots) &= 0 \Leftrightarrow \\ \mathbf{F}(\mathbf{y}^*, \mathbf{z}^*, z_1^*, z_2^*, \dots) &= 0. \end{aligned} \quad (6)$$

Here \mathbf{F} denotes the differential equations (1) and (3) which do not change its functional form under the transformation (5). z_i indicates the i^{th} derivative order.

In Oberlack *et al.* (2001) all continuous symmetries of (1) and (3) are computed employing Lie group methods leading to

$$\begin{aligned} T_1 : t^* &= t, \quad \mathbf{x}^* = \mathbf{x}, \quad \mathbf{u}^* = \mathbf{u}, \quad p^* = p, \\ G^* &= \Psi^{-1}[a_1 + \Psi(G)], \end{aligned} \quad (7)$$

$$\begin{aligned} T_2 : t^* &= t + a_2, \quad \mathbf{x}^* = \mathbf{x}, \quad \mathbf{u}^* = \mathbf{u}, \\ p^* &= p, \quad G^* = G, \end{aligned} \quad (8)$$

$$\begin{aligned} T_3 : t^* &= e^{a_3 t}, \quad \mathbf{x}^* = e^{a_3 \mathbf{x}}, \quad \mathbf{u}^* = \mathbf{u}, \\ p^* &= p, \quad G^* = G, \end{aligned} \quad (9)$$

$$\begin{aligned} T_{4-6} : t^* &= t, \quad \mathbf{x}^* = \mathbf{a} \cdot \mathbf{x}, \quad \mathbf{u}^* = \mathbf{a} \cdot \mathbf{u}, \\ p^* &= p, \quad G^* = G, \end{aligned} \quad (10)$$

$$\begin{aligned} T_{7-9} : t^* &= t, \quad \mathbf{x}^* = \mathbf{x} + \mathbf{f}(t), \quad \mathbf{u}^* = \mathbf{u} + \frac{d\mathbf{f}}{dt}, \\ p^* &= p - \mathbf{x} \cdot \frac{d^2 \mathbf{f}}{dt^2}, \quad G^* = G, \end{aligned} \quad (11)$$

$$\begin{aligned} T_{10} : t^* &= t, \quad \mathbf{x}^* = \mathbf{x}, \quad \mathbf{u}^* = \mathbf{u}, \\ p^* &= p + \phi(t), \quad G^* = G, \end{aligned} \quad (12)$$

where all a_i are constants, $\mathbf{a} \cdot \mathbf{a}^\top = \mathbf{a}^\top \cdot \mathbf{a} = \mathbf{I}$, $|\mathbf{a}| = 1$, $\mathbf{f}(t)$ and $\phi(t)$ are arbitrary and Ψ is a monotonous function of its argument.

(7) may be reformulated as

$$G^* = \mathcal{F}(G) \quad \text{with} \quad \frac{d\mathcal{F}(G)}{dG} > 0. \quad (13)$$

(7) or rather (13) will subsequently be denoted as *generalized scaling symmetry* or *relabeling symmetry of level sets*.

It is important to note that the Euler equations alone admit an extended set of symmetry transformations comprising two scaling groups (see e.g. Oberlack 1999, 2000a, 2000b, 2001). Only due to the velocity scale given by s_L which is a fixed external velocity which cannot be scaled the system (1) and (3) admits one less scaling symmetry. If in addition in equation (3) $\nu \neq 0$ we find that also the transformation (9) is no longer a scaling symmetry of the system (1) and (3) since additional physical scales enter the equations.

It is interesting to note that the modification of s_L due to curvature, flame stretch or heat release does not break any symmetry except for scaling.

As has been mentioned above it is irrelevant for the generalized scaling symmetry (13) whether the velocity \mathbf{u} is determined by the equations for incompressible flow (3) or if the gas-dynamic equations are employed.

Beside the continuous groups discussed above the system (1) and (3) admits for certain sets of parameter finite groups as is shown in Oberlack *et al.* (2001).

Derivation of the G -equation from its symmetries

In view of averaging and modelling issues below we repeat some results derived in Oberlack *et al.* (2001). That is the fundamental form of the G -equation (1) is solely determined by its symmetries. Presume that the functional form of the G -equation is of the unknown generic form

$$\begin{aligned} \mathcal{H}(t, x_1, x_2, x_3, G, u_1, u_2, u_3, \\ G_t, G_{x_1}, G_{x_2}, G_{x_3}) &= 0 \end{aligned} \quad (14)$$

where the indices of G refer to derivatives with respect to the specified variables.

In Oberlack *et al.* (2001) it is rigorously proven that (1) is uniquely determined from (14) solely employing the symmetries (7)-(12).

STATISTICAL AVERAGING CONCEPTS

Symmetries of Reynolds averaged equations

For the purpose of applying the G -equation approach to statistical quantities in turbulent flows it is necessary to introduce the concept of averaging. For any of the flow quantities, such as velocity or pressure, classical Reynolds averaging leads to equations which have largely the same transformation properties as the instantaneous equations such as rotation symmetry, Galilean invariance and others (see also Oberlack 1999, 2000a, 2000b, 2001). However, employing the generalized scaling symmetry T_1 which is in effect the only non-linear symmetry among (7)-(12) leads to statistical quantities which are non-unique. This will be proven subsequently.

This problem roots in the physical meaning of G itself. In the G -equation an iso-surface G_0 is introduced as a marker for the geometrical flame location. However the chosen numerical value of G_0 is irrelevant for the flame position. This is in effect what is stated by the symmetry T_1 or more conveniently expressed by (13). The symmetry simply states that the value of G can arbitrarily be changed due to the largely arbitrary function \mathcal{F} without changing its physical meaning namely the flame position. From the preceding remarks it is clear that G has obviously quite a different physical meaning compared to any of the other flow quantities such as \mathbf{u} or p . Since in turbulence theory and modelling averaging concepts must be defined this constitutes a major obstacle for modelling the G -equation.

To quantify what has been said above we define the Reynolds ensemble average of any statistical flow quantity Z according to

$$\bar{Z}^{(E)}(\mathbf{x}, t) = \lim_{N \rightarrow \infty} \left(\frac{1}{N} \sum_{n=1}^N Z_n(\mathbf{x}, t) \right). \quad (15)$$

Any fluctuating quantity Z' is defined as

$$Z' = Z - \bar{Z}. \quad (16)$$

Implementing the latter definitions of a mean and fluctuating quantity for the velocity vector and pressure into the Navier-Stokes equations (3) we obtain the classical result

$$\nabla \cdot \bar{\mathbf{u}} = 0, \quad (17)$$

$$\frac{\partial \bar{\mathbf{u}}}{\partial t} + (\bar{\mathbf{u}} \cdot \nabla) \bar{\mathbf{u}} = -\frac{1}{\rho} \nabla \bar{p} + \nu \Delta \bar{\mathbf{u}} - \nabla \cdot (\overline{\mathbf{u}'\mathbf{u}'}). \quad (18)$$

It can readily be shown that any of the symmetries (7)-(12) can be re-written as such that

equation (17) is unaltered by them. As an example we consider the usual Galilean invariance defined by $\mathbf{f} = \mathbf{a}t$.

There are two choices of finding Galilean invariance of (17). Either group analysis is applied to (17) or we deduce the statistical form of Galilean invariance from (11) directly. In the following we will only work out the latter approach.

Applying the ensemble operator (15) to \mathbf{u} and p in equation (11) we obtain

$$\begin{aligned} \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{n=1}^N \mathbf{u}_n^* &= \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{n=1}^N (\mathbf{u}_n + \mathbf{a}), \\ \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{n=1}^N p_n^* &= \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{n=1}^N p_n. \end{aligned} \quad (18)$$

Since \mathbf{a} is not a statistical quantity it may be taken out of the sum and hence (18) may be re-written as

$$\bar{\mathbf{u}}^* = \bar{\mathbf{u}} + \mathbf{a}, \quad \bar{p}^* = \bar{p} \quad (19)$$

furnished by the transformation properties of the independent variables. From the latter we deduce together with the definition of the fluctuating quantities (16) that the \mathbf{u}' and p' transform under the Galilean invariance as

$$\mathbf{u}'^* = \mathbf{u}', \quad p'^* = p'. \quad (20)$$

It is a short exercise to show that (17) is invariant under (19) and (20) extended by the transformations for the independent variables.

Using the same procedure as for the Galilean invariance above we can transform any of the symmetries (8)-(12) *excluding* G to mean and fluctuating variables.

Averaging of the G -equation

In contrast the application of the Reynolds averaging operator to G leads to a contradiction. Suppose we define a mean \bar{G} -field in the usual way corresponding to

$$\bar{G} = \lim_{N \rightarrow \infty} \left(\frac{1}{N} \sum_{n=1}^N G_n \right). \quad (21)$$

Using this definition and applying it to the generalized scaling symmetry (13) we obtain

$$\bar{G}^* = \lim_{N \rightarrow \infty} \left(\frac{1}{N} \sum_{n=1}^N \mathcal{F}(G_n) \right). \quad (22)$$

Since \mathcal{F} may be any non-linear function of its argument with the only restriction having positive slope it is impossible to uniquely define a mean G quantity.

To interpret things from an application point of view we suppose to conduct a computation employing the usual G -equation using an arbitrary initial G -field. In addition we denote the initial flame front at $t = 0$ by G_0 . Letting the computation evolve the flame front defined by G_0 is uniquely determined for all $t > 0$ by its initial position in space. Due to the symmetry $G^* = \mathcal{F}(G)$ with $\frac{d\mathcal{F}}{dG} > 0$ we may think of a second computation with a new initial G^* field defined by $G^* = \exp(G)$ where G is given by the initial G field of the first computation. Of course, also the iso-surface G_0 defining the initial flame front changes to an iso-surface given by the value $G_0^* = \exp(G_0)$. The key property of the generalized scaling symmetry as with any other symmetry is that it generates a new solution for the G -equation. However, the spatial position of the flame front given by G_0 of the first computation and of G_0^* of the second computation are exactly the same for all t . Hence, we find that the generalized scaling symmetry has no influence on the actual flame position in space.

However, defining a mean G -field employing the Reynolds ensemble averaging for the first computation we get \bar{G} defined by (21). In contrast, the mean G field of the second computation \bar{G}^* is defined by

$$\bar{G}^* = \lim_{N \rightarrow \infty} \left(\frac{1}{N} \sum_{n=1}^N \exp(G_n) \right). \quad (23)$$

It is clear from the stochastic behavior of G that

$$\bar{G}^* \neq \exp(\bar{G}). \quad (24)$$

As a result we can immediately conclude that the two mean positions of the flame fronts are different. This result is in striking contrast to the fact that each instantaneous position of the flames determined by G_0 and G_0^* have occupied exactly the same position in space for all $t \geq 0$. If we would have taken any other monotonously increasing function instead of \exp again another mean flame position would have been obtained.

We have to conclude that the classical Reynolds averaging concept does not lead to a unique result for the mean G -field. This is also clear from a physical point of view. The absolute value of the field quantity G itself has no physical meaning. Instead only iso-surfaces of G are the physically relevant quantities which need to be investigated as will be shown subsequently.

Stochastic pdf-based averaging of flame surfaces

For mathematical convenience we introduce the explicit formulation of iso-surfaces $\mathbf{x}_f(\lambda, \mu, t)$ where λ and μ denote a surface attached coordinate system. Employing this formalism equation (2) may be re-written as

$$\frac{d\mathbf{x}_f}{dt} = \mathbf{u}(\mathbf{x}_f, t) + s_L \frac{\frac{\partial \mathbf{x}_f}{\partial \lambda} \times \frac{\partial \mathbf{x}_f}{\partial \mu}}{\left| \frac{\partial \mathbf{x}_f}{\partial \lambda} \times \frac{\partial \mathbf{x}_f}{\partial \mu} \right|}. \quad (25)$$

The quantity required to obtain a complete statistical description of \mathbf{x}_f is the probability density function (*pdf*) P . The *pdf* depends on \mathbf{x}_f as sample space variable while the coordinates λ and μ are ‘‘parameters’’. Hence the *pdf* for arbitrary turbulent flames is represented by $P[\mathbf{x}_f(\lambda, \mu, t)]$, where the brackets denote P being a functional of \mathbf{x}_f .

The derivation of the transport equation for P is in complete resemblance to the Fokker-Planck formalism for stochastic ordinary differential equations. The derivation of the functional differential equation for P is given in Oberlack *et al.* (2001).

Since solutions for functional differential equations are usually very difficult to obtain they are often referred to as unclosed. For the present purpose a moment approach is introduced to obtain the leading order correlations of \mathbf{x}_f .

As an immediate consequence the mean flame position $\hat{\mathbf{x}}(\lambda, \mu, t)$ is defined as

$$\hat{\mathbf{x}}(\lambda, \mu, t) = \iiint_{-\infty}^{\infty} \mathbf{x}_f P[\mathbf{x}_f] d^3 \mathbf{x}_f. \quad (26)$$

All statistical quantities such as $\hat{\mathbf{x}}$ are denoted by a hat and the index f is omitted. Accordingly we may generalize the definition of the flame brush thickness introduced by Peters (2000) corresponding to

$$\ell^2(\lambda, \mu, t) = \iiint_{-\infty}^{\infty} (\mathbf{x}_f - \hat{\mathbf{x}})^2 P[\mathbf{x}_f] d^3 \mathbf{x}_f. \quad (27)$$

Apparently ℓ^2 is not a space filling quantity but designates a scalar quantity assigned to every point on the surface $\hat{\mathbf{x}}(\lambda, \mu, t)$.

Formally an equation for $\hat{\mathbf{x}}(\lambda, \mu, t)$ may be derived by application of the averaging operation (26) to equation (25). We obtain

$$\frac{d\hat{\mathbf{x}}_f}{dt} = \hat{\mathbf{u}} + \widehat{s_L \mathbf{n}}, \quad (28)$$

where $\hat{\mathbf{u}}$ and $\widehat{s_L \mathbf{n}}$ are defined according to

$$\hat{\mathbf{u}} = \iiint_{-\infty}^{\infty} \mathbf{u}(\mathbf{x}_f) P[\mathbf{x}_f] d^3 \mathbf{x}_f \quad \text{and}$$

$$\widehat{s_L \mathbf{n}} = \iiint_{-\infty}^{\infty} s_L \frac{\frac{\partial \mathbf{x}_f}{\partial \lambda} \times \frac{\partial \mathbf{x}_f}{\partial \mu}}{\left| \frac{\partial \mathbf{x}_f}{\partial \lambda} \times \frac{\partial \mathbf{x}_f}{\partial \mu} \right|} P[\mathbf{x}_f] d^3 \mathbf{x}_f. \quad (29)$$

Introducing

$$\check{G}(\mathbf{x}, t) = \check{G}_0 \quad (30)$$

as an implicit representation of the mean flame front position $\hat{\mathbf{x}}$ we may take the time derivative of (30) to obtain

$$\frac{\partial \check{G}}{\partial t} + \nabla \check{G} \cdot \frac{d\hat{\mathbf{x}}}{dt} = 0. \quad (31)$$

It is important to distinguish between the “ $\hat{\cdot}$ ” and the “ $\check{\cdot}$ ” quantities particularly in view of the normal vector to be shown below.

Implementing (28) into (31) we finally find

$$\frac{\partial \check{G}}{\partial t} + \hat{\mathbf{u}} \cdot \nabla \check{G} = -\nabla \check{G} \cdot \widehat{s_L \mathbf{n}}. \quad (32)$$

It should be pointed out that despite the fact that \check{G} appears to be a field quantity as G for the instantaneous fields equation (32) is only physically relevant at the mean flame front \check{G}_0 .

Though the latter equation is unclosed and appropriate models have to be introduced it is apparent that (32) is invariant under the generalized scaling symmetry (13) if G is replaced by \check{G} , i.e.

$$\check{G}^* = \check{F}(\check{G}) \quad \text{with} \quad \frac{d\check{F}}{d\check{G}} > 0. \quad (33)$$

This has in fact important modelling implications. The result mentioned above that the G -equation may be derived from its symmetries may serve as a guideline to model $\widehat{s_L \mathbf{n}}$. The argument is based on the fact that (32) admits all symmetries (7)-(12) written in the mean variables. Invoking the derivation of the G -equation solely from its symmetries we find that the vector $\widehat{s_L \mathbf{n}}$ can only be proportional to $\check{\mathbf{n}}$ or in other words we find the unique model

$$\widehat{s_L \mathbf{n}} = s_T \check{\mathbf{n}} \quad \text{with} \quad \check{\mathbf{n}} = -\frac{\nabla \check{G}}{|\nabla \check{G}|}, \quad (34)$$

which recognizes all symmetries of (32). s_T is the turbulent burning velocity.

At this point it becomes apparent that if s_L is a constant we have to clearly distinguish

between $\hat{\mathbf{n}}$ and $\check{\mathbf{n}}$. The former is the mean of the normal vector of the instantaneous flame fronts while the latter is the normal vector of the mean flame front.

Apart from the latter argument we may also give a geometric interpretation of the necessity to write $\widehat{s_L \mathbf{n}}$ in terms of $\check{\mathbf{n}}$. The vectors $\widehat{s_L \mathbf{n}}$ and $s_T \check{\mathbf{n}}$ need not, in general, be parallel. However, an interface is invariant to tangential components in the movement of any point on it, and so it is completely general to define s_T as the inner product, $s_T = \widehat{s_L \mathbf{n}} \cdot \check{\mathbf{n}}$. In the final step one can then replace $\widehat{s_L \mathbf{n}}$ with $s_T \check{\mathbf{n}}$.

In this context it is important to recognize that the derivation in section is based on the fact that only first order derivatives of G and no derivatives of \mathbf{u} have been employed. From this we may conclude for the modelling of $\widehat{s_L \mathbf{n}}$ that if higher order derivatives of \check{G} are employed more general forms of (34) may be derived.

Extending (34) by including higher order derivatives of \check{G} and the mean velocity there are only a few basic rules to be obeyed in order to propose a proper invariant model with respect to the symmetries (7)-(12) written in the mean variables:

- \check{G} may only appear in $\check{\mathbf{n}}$ according to (34). This ensures obeying the generalized scaling symmetry.
- There may only appear the spatial gradient of the mean velocity based on *grad*, *div* or *rot* in order to recognize Galilean invariance.
- Using proper tensor notation such as dyadic products, tensor invariants e.g. traces, etc. ensures observing the rotation groups.
- The rotation groups are also observed if higher order gradients based on *grad*, *div* or *rot* are applied to $\check{\mathbf{n}}$, the mean velocity gradient or any tensor product of the former two.

It is shown in Oberlack *et al.* (2001) that similar to equation (28) for $\hat{\mathbf{x}}$ we may also give an equation for the square of the flame brush thickness ℓ^2 and related equations.

Also it is shown that certain averaging approaches published in the literature such as the one for plane flames by Kerstein *et al.* 1988 and Wenzel and Peters (1999) or the flame surface density approach by Marble and Broadwell (1977), Pope (1988) and Candel and Poinso

(1990) are consistent with all known symmetries of the G -equation.

In contrast certain SGS models for LES such as those by Im *et al.* (1997) or Weller *et al.* (1998) do not uniquely define G for $t > 0$ by its initial position of G_0 alone. This is in striking contrast to the original property of the G -equation.

SUMMARY

It is demonstrated that the G -equation for premixed combustion admits a very broad variety of symmetry properties including those from classical mechanics. Particularly a new generalized scaling symmetry is obtained which is of considerable importance for a variety of different purposes.

It is proven that the generalized scaling symmetry is an important ingredient to uniquely define the basic functional form of the G -equation. This in fact served as a motivation to show that the generalized scaling symmetry cannot under any circumstances be neglected to derive statistical quantities for turbulent combustion.

It has particularly be shown that usual Reynolds ensemble averaging does not uniquely define mean properties of the G -equation such as the mean flame position. The underlying physical reason being the fact that the value for G is irrelevant and can arbitrarily be changed without altering the actual position of the flame front.

A *pdf* based statistical approach has been introduced which properly recognizes the important generalized scaling symmetry. A new equation for the geometrical location of the mean flame front has been derived. Modelling implications of the generalized scaling symmetry for the unclosed terms have been discussed. A variety of approaches for premixed turbulent combustion published in the literature have been investigated whether they comply with the generalized scaling symmetry or not.

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