DNS of lean hydrogen combustion with flamelet-generated manifolds

By R. J. M. Bastiaans†, A. W. Vreman‡ and H. Pitsch

1. Motivation and objectives

The possible use of hydrogen as an energy carrier is a popular idea in developing scenarios for transitioning from use of fossil fuels to a new sustainable energy. However, combustion of hydrogen is quite different from the burning of traditional fuels, e.g., natural gas, which is extensively used in current combustion equipment. In fact several studies assess the possibility of just adding hydrogen to natural gas up to very high levels. Obviously the burning speed and the density of hydrogen are quite different. More complex phenomena are related to the preferential diffusion effects that are prominently present with hydrogen as a fuel in premixed combustion. In this study we investigate possibilities to reduce hydrogen chemistry, while keeping the fundamental physical behavior. This in order to be able to perform relatively cheap, large-scale DNS studies. The fundamental physical behavior of hydrogen combustion has an important role in subgrid scale modeling in LES simulations. Here flames generate wrinkles without any external hydrodynamic perturbations. In subgrid modeling this has to be taken into account. Thus the DNS studies can guide the advancement of the LES modeling for hydrogen combustion.

2. Instabilities

In the fluid dynamics of exothermal reacting flows, two main types of instabilities are possible. The first one is the Darrieus-Landau instability (Landau 1944, described in Landau & Lifshitz 1987), which is due to the acceleration of the burning gases. Once an initially flat flame surface obtains a small disturbance, the flame front will be wrinkled. Therefore convex and concave regions will be present with respect to the unburnt gases. These gases accelerate normal to the flame front and at convex parts, the streamlines have to diverge toward the flame front and converge after the flame front. The opposite occurs at the concave parts. Because the flow velocity will decrease when approaching the flame and the burning velocity stays approximately constant, the convex parts tend to grow. This describes the so-called hydrodynamic instability. The analysis of Landau, for an infinitely thin flame sheet, gives a positive amplification for all wavenumbers, but it is noted that this only holds for wavenumbers that correspond to wavelengths \( k \delta \ll 1 \). For given \( k \), the growth rate increases with the expansion.

In addition to the hydrodynamic instability, thermo-diffusive effects also alter the stability behavior. These depend on the thermal diffusion of heat, relative to the diffusivity of the fuel, which is expressed by the Lewis number, \( Le \). The thermo-diffusive instability is described extensively in the literature, e.g., Sivashinsky (1983). The conduction of heat

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from the flame front in convex parts will cool the flame and thus the burning velocity will drop. This stabilizes the flame. The diffusion flux of fuel in these parts, however, has a concentrating effect and the flame becomes richer. In lean flames the burning velocity will increase and there is a destabilizing effect. For combustion of hydrogen, in this sense, the lean region is extended up to $\phi = 1.5$ or even slightly higher, since the burning velocity increases up to this equivalence ratio. If the thermal diffusion is larger than mass diffusion of fuel, the Lewis number is larger than unity and the stabilizing effect prevails. For $Le < 1$ there is an additional thermo-diffusive instability. The critical Lewis number, $Le_c$, is not exactly unity. In absence of density differences, Barenblatt et al. (1962) show that the growth rate $\sigma$ of long-wave disturbances is

$$\sigma = D_{th}((1 - Le/\beta - 1) k^2, \quad (2.1)$$

with $D_{th} = \lambda/c_p$ and $\beta = T_a(T_b - T_u)/T_b^2$, including the activation temperature, $T_a = E_a/R$ and the burnt and unburnt temperatures, $T_b$ and $T_u$. Here $\lambda$ is the heat conduction coefficient, $c_p$ the specific heat, $E_a$ the activation energy and $R$ the universal gas constant. Therefore $Le_c = 1 - 2/\beta$, which is lower than 1. Here the theory assumes that combustion can be described with single-step chemistry, specified by an activation temperature. In practice it is not this simple (as will be described in section 3).

Because of the complex behavior of hydrogen combustion, several numerical studies have been performed to study the associated phenomena. An overview of preferential diffusion studies is given in Lipatnikov & Chomiak (2005). Many numerical studies are performed in 2-D, with detailed kinetic mechanisms (e.g., Im & Chen 2002; Bell et al. 2007), whereas 3-D studies are typically performed with simple chemistry, e.g., Chakraborthy & Cant (2005). In the present study we will try to devise a flamelet method for this purpose. If combustion can be described by such a flamelet model, this would form the basis for accurate 3D DNS studies. Moreover, it would enable LES computations to be performed with the possibility of improved chemistry models on the basis of knowledge of subgrid scale flame generated turbulence.

3. Chemistry

In this study we will focus on hydrogen-air flames at an equivalence ratio of $\phi = 0.7$. There are several reasons for taking this value. Stoichiometric to moderately rich conditions are technologically not very relevant because of the high NO$_x$ emissions. Second, at very lean conditions the uncertainty in the burning rate is very high. There is a large difference in measurements that are reported and also within predictions obtained by different kinetic schemes. Below $\phi = 0.5$, the uncertainty in laminar burning velocity can easily become of the order of 100% (see e.g., Ó Conaire et al. 2004). The fundamental instabilities associated with hydrogen combustion obviously contribute quite severely to the large scatter. So at $\phi = 0.7$, both the NO$_x$ peak and the very uncertain region are avoided. Moreover, at this value the change of the laminar burning speed with the equivalence ratio is maximum, resulting in a large amplification of thermo-diffusive instabilities.

At very low equivalence ratios, the flame thickness and its derivative become very large; at $\phi = 0.25$, the flame thickness, $\delta_{th}$, is already about 5 mm. At these very lean flames, the interaction with turbulence is quite interesting because the burning regime is easily changed with small deviations in local conditions. However, the investigation of these phenomena is not in the scope of the present study.

From the previous section the question arises whether single-step chemistry can be a
good approximation to describe the physics of hydrogen combustion. In any case, at least two equations that are relevant to chemistry and heat release have to be solved in order to obtain thermo-diffusive instabilities. From experimenting with a single-step model from Marinov et al. (1996), we found that we cannot obtain the correct burning velocity and flame thickness over a range of equivalence ratios. However, this last property is quite important for flame turbulence interactions. It is also unclear what transport model to use with this single-step scheme. Additionally, the flame should correctly respond to heat losses and stretch. It appeared that this is not possible with a single-step approach. In our tests, an activation temperature of \( T_a = 29716 \) K was found by calculating burner stabilized flames with CHEM1D using the scheme of Ó Conaire et al. (2004). By tuning the pre-exponential factor to the desired burning velocity, \( S_l \), it was found that the derivative of \( S_l \) with the equivalence ratio at \( \phi = 0.7 \) was much too high.

### 3.1. Flamelet approach

An alternative to single-step chemistry is the use of a flamelet approach. This lifts the stiffness and amount of work compared to the application of detailed kinetics. The technique of FGM/FPI (van Oijen & de Goey 2000; Gicquel et al. 2000) might be used for this purpose. In this technique, premixed flames with detailed chemistry are pre-calculated. Then tables are generated, reflecting the solution of these flamelets as a function of one or more control variables. When solving equations for these control variables, we can use the table to retrieve quantities that are not known. In this case, DNS is referred to as a method in which all hydrodynamic scales are resolved, but not necessarily all chemical scales. Having such a look-up table thus requires that the control variables are monotonous functions of the spatial coordinate in the flame solutions.

The Navier-Stokes equations with flamelet chemistry, in which we will use two control variables, hydrogen content and temperature, read:

\[
\begin{align*}
\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_j}{\partial x_j} &= 0, \\
\frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_i u_j}{\partial x_j} &= -\frac{\partial \rho}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} - \rho g_i, \\
\frac{\partial \rho c}{\partial t} + \frac{\partial \rho c u_j}{\partial x_j} &= \frac{\partial}{\partial x_j} \left( \rho D_c \frac{\partial c}{\partial x_j} \right) + \dot{\omega}_c, \\
c p \frac{\partial T}{\partial t} + c_p \frac{\partial T u_j}{\partial x_j} &= \frac{\partial}{\partial x_j} \left( \lambda \frac{\partial T}{\partial x_j} \right) + \Sigma_\alpha c_{p\alpha} \rho D_\alpha \frac{\partial Y_\alpha}{\partial x_j} \frac{\partial T}{\partial x_j} - \Delta Q \dot{\omega}_c,
\end{align*}
\]

where \( c \) is the complement of the scaled mass fraction of hydrogen,

\[
c = \frac{Y_{H_2}^b - Y_{H_2}}{Y_{H_2}^b - Y_{H_2}^l},
\]

\( \alpha \) is an index of species, and \( Y_\alpha = \rho_\alpha / \rho \). The transport of enthalpy by diffusive species fluxes, the second term at the right side of the temperature equation, is explicitly taken into account. The way to handle this in the present FGM context is discussed in section 5. We will neglect buoyancy, Soret, and Dufour effects, although the Soret effect is a small but noticeable phenomenon in hydrogen flames (e.g., Bongers 2005). For the stress and rate of strain we have

\[
\tau_{ij} = 2\mu S_{ij},
\]
With the definition of the Lewis number,

\[ Le_\alpha = \frac{\lambda}{\rho c_p D_\alpha}, \]

we obtain for species and temperature

\[
\frac{\partial \rho c}{\partial t} + \frac{\partial \rho u_j c}{\partial x_j} = \frac{\partial}{\partial x_j} \left( \frac{\lambda}{Le_\alpha c_p} \frac{\partial c}{\partial x_j} \right) + \rho e, \\
\frac{c_p \partial \rho T}{\partial t} + \frac{\partial \rho u_j T}{\partial x_j} = \frac{\partial}{\partial x_j} \left( \frac{\lambda T}{Le_\alpha c_p} \frac{\partial T}{\partial x_j} \right) + \Sigma_\alpha \frac{c_{\text{pa}}}{c_p} \lambda \frac{\partial Y_\alpha}{\partial x_j} \frac{\partial T}{\partial x_j} + \rho \dot{\omega}_T. \tag{3.10}
\]

Because the sum of the species equals unity, the enthalpy transport by diffusive fluxes is zero when all \( c_{\text{pa}} / Le_\alpha \) are equal. Note that the differences in the heat capacity of the different species cannot be assumed to be small. This is the case on a molar base, but not for mass-based values as used in the present equations. Furthermore, the temperature is scaled with its maximum and minimum values, like the progress variable \( c \).

4. Transport

We want to fit the conduction \( \lambda / c_p \) and viscosity \( \mu / c_p \) for the mixture at the globally defined equivalence ratio of \( \phi = 0.7 \) as a function of temperature. This will be evaluated on the basis of laminar computations with the detailed kinetics scheme of Ó Conaire et al. (2004) and detailed transport. From these computations, the Lewis numbers for the main species will also be adopted. The fit (for \( \phi = 0.7, T_0 = 300 \text{ K}, \) and \( p_0 = 101325 \text{ Pa} \)) is given in Fig. 1 and reads

\[
\frac{\lambda}{c_p} = \exp(a_\lambda + b_\lambda \log(T/T_0) + c_\lambda \log(T/T_0)^2), \quad \text{[g cm}^{-1} \text{s}^{-1}] \tag{4.1}
\]

\[
\frac{\mu}{c_p} = \exp(a_\mu + b_\mu \log(T/T_0) + c_\mu \log(T/T_0)^2), \quad \text{[g}^2 \text{J}^{-1} \text{cm}^{-1} \text{s}^{-1}] \tag{4.2}
\]

with

\[
a_\lambda = -7.9796, b_\lambda = 0.6252, c_\lambda = -0.0354; \\
a_\mu = -8.8188, b_\mu = 0.7806, c_\mu = -0.1170.
\]

It can be observed that the fit matches the \( \phi = 0.7 \) line almost exactly. Small deviations are observed in the very beginning of the preheat zone (\( T = 300 - 500 \text{ K} \)), but these are only minor.

With the detailed scheme using complex diffusion, effective Lewis numbers for each species can be calculated. These are found to vary almost linearly with the equivalence ratio and the slopes are very low. Therefore we can use the Lewis numbers around the targeted value of \( \phi = 0.7 \), as given numerically in Table 1.

5. Numerics

We used a straightforward and efficient numerical implementation to solve the equations with parametrized chemistry. The variable density approach involved a Poisson
equation for the pressure, similar to other low-Mach methods as in Pitsch & Steiner (2000); Pierce & Moin (2004).

For the continuity and momentum equations, the standard finite volume method was employed, with second-order central differencing on a staggered Cartesian mesh. The discrete convective terms would conserve kinetic energy if the density were constant. Because of its stability properties, a hybrid time-stepping scheme was used to integrate the momentum equations, Adams-Bashforth for the convective and forward Euler for the viscous terms.

The scalar equation was recast into the equivalent advective formulation. Then the Van Leer third-order accurate MUSCL scheme, which is TVD, was applied to the advective terms. Thus the spatial discretization of the scalar equation introduced numerical diffusion, which was not the case in the momentum equations. However, for the scalar equation, numerical diffusion is hard to avoid if we want to keep the scalars within their physical bounds on coarse grids. The scalar was updated with pure forward Euler, since for an upwind method the hybrid time-stepping scheme has fewer advantages than for central differencing (used in the momentum equation).

Within each time step, the scalar equation was updated first. Then the momentum equations were updated to obtain the uncorrected velocities. Imposing the continuity equation then provided a Poisson equation for the pressure, which was solved using a multi-grid method. Each time step ended with the correction of the velocities using the

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**Table 1.** Effective Lewis numbers for premixed $\phi = 0.7$ hydrogen combustion.

<table>
<thead>
<tr>
<th>Major species</th>
<th>$Le_i$</th>
<th>Minor species</th>
<th>$Le_i$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$H_2$</td>
<td>0.356</td>
<td>$H$</td>
<td>0.217</td>
</tr>
<tr>
<td>$O_2$</td>
<td>1.295</td>
<td>$O$</td>
<td>0.810</td>
</tr>
<tr>
<td>$H_2O$</td>
<td>0.978</td>
<td>$OH$</td>
<td>0.819</td>
</tr>
<tr>
<td>$N_2$</td>
<td>1.341</td>
<td>$HO_2$</td>
<td>1.368</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$H_2O_2$</td>
<td>1.389</td>
</tr>
</tbody>
</table>

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**Figure 1.** Values for $\lambda/c_p$ (left) and $\mu/c_p$ (right) as function of temperature and equivalence ratio for pure hydrogen combustion with complex diffusion and using the detailed chemical scheme of O Conaire et al. (2004). Thin lines, equivalence ratios $\phi = 0.5 - 0.9$ going up with step 0.1 from below. Thick dashed line: present fit for values around $\phi = 0.7$. 

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pressure gradient. See Vreman et al. (2007) for more details about the pressure-correction algorithm.

The equations are solved as described above, but some terms are taken from the manifold. The manifold is constructed by solving the appropriate equations in CHEM1D by using the chemical mechanism of O Conaire et al. (2004). Variables taken from this manifold are the density, the source terms of the hydrogen and temperature equation, as well as the heat capacity, the viscosity, and conductivity. This means that the functionalities for viscosity and conductivity in Section 4 are already used in the calculation of the flamelets.

By constructing the manifold, it must be realized that formally the degrees of freedom of the system are defined by the energy and the element fractions \( Z_H, Z_O \) and \( Z_N \). It would not matter that much what flamelets are used as long as variations of the composition are present. Preferential diffusion effects are responsible for local changes in composition and thus in equivalence ratio. Therefore, we choose to make a sweep in equivalence ratio.

Flamelets are generated for a range of equivalence ratios, \( \phi = 0.4 - 1.0 \). The manifold for the case of constant \( Le_i \) (given by Table 1) is displayed in Fig. 2. In this figure, the lower line corresponds to a flamelet in which \( \phi = 0.4 \) and the upper boundary corresponds to \( \phi = 1.0 \). The upper right boundary corresponds to the end points of relatively rich flames, \( \phi = 0.7 - 1.0 \). If other Lewis numbers are taken, obviously the manifold also changes.

The term for the transport of enthalpy by diffusive species fluxes can, in principle, be represented in FGM. This is because all the species concentrations are known from the manifold. However, this approach will not be taken here, since this would introduce numerical costs that are proportional to the number of reactions in a detailed scheme. Then the computational cost can become of the order of the cost required for using a detailed chemical scheme. However, the stiffness might still be removed.

There are a few alternative options for dealing with this term. First, it might be neglected. If the effect of this term is small, then this might be a good option. A second possibility is to take only the transport by hydrogen into account. Therefore, an assessment is needed to determine whether species other than hydrogen attribute to the transport of heat with species. Third, the entire term can be introduced in the manifold as well. If the term would be of importance, then this is not a very good option. For a turbulent field that applies stretch to the flame zone, the affected flame thickness would change. This is not taken into account if the term is introduced in the manifold being constructed of unstretched flamelets. Therefore, we consider a fourth option, in which a correction term is introduced in the manifold, defined as

\[
\Pi = \Sigma \alpha \frac{c_{\alpha}}{c_p} \frac{L e_{\alpha} \partial Y_{\alpha}}{\partial c/\partial x_j},
\]

so that

\[
\Pi \frac{\partial c}{\partial x_i} \frac{\partial T}{\partial x_i}
\]

is a model for the transport of enthalpy by diffusive fluxes of species. The differences between the second and fourth approximation, with inclusion of heat capacity effects, are shown in Fig. 3. It can be observed that both inclusion of all species as well as inclusion of the heat capacities definitely matter. It can also be seen that the effect is one order of magnitude lower than the chemical source term of the temperature. Therefore it
Figure 2. Manifold for constant Lewis numbers from Table 1. The database includes $\hat{\omega}_c$, $\hat{\omega}_T$, and the values of $\rho$, $c_p$, $\lambda$, and $\mu$ (the last two are not displayed). The dashed line corresponds to $\phi = 0.7$, the lower boundary of the manifold corresponds to $\phi = 0.4$, the upper boundary to $\phi = 1.0$. The scalings of $c$ and $T$ are performed with the values of the $\phi = 0.7$ flamelet. The boundary in the upper right corner is given by fully burnt values.

will still make a noticeable difference. The best choice appears to be the option with the correction term, Eq. 5.1. With this method, the gradient of the temperature is correctly taken into account, as well as a flame representative gradient of the species. Furthermore, it should converge to the laminar value in the case that $c$ and $T$ are perfectly aligned. If the gradients of these quantities are perpendicular, then the total term will be zero, independent of the magnitude of $\Pi$. Therefore, in both limits we have an acceptable behavior of the model.

Note that the construction of the manifold is performed with CHEM1D with a minimal grid size of $1 \cdot 10^{-6}$ m and that the manifold itself is an interpolation of these results on a phase space equidistant $201 \times 201$ grid resolving the thermal thickness $\delta_T \approx 3 \cdot 10^{-4}$ m. Therefore the resolution in the manifold is about $1.5 \cdot 10^{-6}$ m. The manifolds are smooth (as shown in the given figures).

6. Results

6.1. Results for 1-D flame propagation

We have generated and implemented the manifold and the model for the correction term. This was tested in a 1-D propagating mode, where a flame is computed in a 1-D domain using the manifold approach. From the solution, the laminar burning velocity can be measured and compared to the detailed chemistry results. The length of the domain was
Figure 3. Preferential enthalpy diffusion by species terms for unstretched combustion with constant Lewis numbers. Left: contribution associated with the diffusive transport of hydrogen; right: total contribution. Top row: only pure Lewis number effects taken into account; bottom row: complete term with heat capacities.

taken to be 1 cm. Initial profiles of $c$ and $T$ were taken from the detailed calculations and interpolated on the equidistant grid we used. It was performed so that the maximum gradient was located at the center of the domain at 5 mm, $y_0 = 0.5$ cm. Starting from this situation, the flame front starts to propagate toward the lower boundary of the domain. For the evaluation of the laminar burning velocity, there are uncertainties for very early simulation times and when the flame approaches the boundary. This is why the velocity was evaluated in a time interval corresponding to one flame time from the beginning, extending to the position where the middle of the flame is still two flame thicknesses away from the boundary. To that end, a linear fit was used to the position as a function of time, because numerical differentiation of the position produces a noisy signal.

Table 2 provides an overview of the convergence of the burning speed. It can be observed that the flame speed computed using FGM converges toward the true burning velocity. At coarse grids, more acceptable solutions are found for FGM than for detailed calculations. A method involving the tabulation of the entire diffusive enthalpy flux by species as a source term is included to determine whether the extra multiplication of derivatives needed for the correction model would impose additional restrictions on the resolution. This seems not to be the case. It can be noted that there is a small difference between the end values of the detailed code and the FGM methods. This might be due to a small difference in the values of $c_p$ that was observed.

The $\Pi$ term is shown in Fig. 4. The figure gives an impression that this term is most important at the burnt side of the flame. However, the term still has to be multiplied by
Table 2. Convergence of the value of the burning velocity with the grid spacing. Grid spacings are in m, for CHEM1D the minimal value is taken (not equidistant). Burning velocity in cm/s. The "Source" column displays the burning velocity when the entire diffusive enthalpy flux term by species is taken from the manifold as a source term.

<table>
<thead>
<tr>
<th>Grid-size</th>
<th>CHEM1D</th>
<th>Source</th>
<th>II</th>
</tr>
</thead>
<tbody>
<tr>
<td>$8 \cdot 10^{-5}$</td>
<td>-</td>
<td>130.65</td>
<td>133.59</td>
</tr>
<tr>
<td>$4 \cdot 10^{-5}$</td>
<td>138.42</td>
<td>126.61</td>
<td>127.18</td>
</tr>
<tr>
<td>$2 \cdot 10^{-5}$</td>
<td>130.07</td>
<td>128.91</td>
<td>129.02</td>
</tr>
<tr>
<td>$1 \cdot 10^{-5}$</td>
<td>128.69</td>
<td>129.56</td>
<td>129.64</td>
</tr>
<tr>
<td>$5 \cdot 10^{-6}$</td>
<td>128.64</td>
<td>129.69</td>
<td>129.69</td>
</tr>
</tbody>
</table>

Figure 4. Preferential enthalpy diffusion term II for constant Lewis numbers, from Table 1.

the two spatial derivatives of $c$ and $T$. After that the picture of Fig. 3 is obtained again. A scatter plot of realizations in phase space shows that the inclusion of the term describing enthalpy transport by diffusive species fluxes, results in lines that are constantly the same during propagation of the flame. Without the term, especially at the unburnt side, higher values of the temperature are found. This corresponds to a flame that is slightly richer. In this case, the burning velocity is also higher: $S_l = 138.5$ cm/s. Inclusion of the term results in a line that exactly matches the $\phi = 0.7$ line in the manifold. It was observed that at the burnt side, the resulting phase space slightly enters an unphysical domain in which $c$ exceeds 1 (with about 1.5%). This does not seem to depend on the resolution of the computation and thus it does not seem to be an effect of numerical overshoot. More research is needed to fully understand this problem.

6.2. Two-dimensional cellular flames

Two-dimensional simulations were carried out on an equidistant grid of $512 \times 512$ points on a domain of 1 cm$^2$. Spanwise boundary conditions were taken as periodic. Again, the flame was initialized from a detailed computation, positioned at $y_0 = 0.5$ cm. Small velocity perturbations are introduced initially by defining a stream function defined by discrete random numbers. These are windowed with a Gaussian at a mean position $y_0$ and a width of 0.1 cm. Velocities are calculated from the stream function of which the intensity was 5% of the flow velocity at the burnt side ($\approx 6.6$ m/s).
Results of the flame structure at two subsequent times are shown in Fig. 5. It appears that there is a tendency to form cellular flame structures. This is a clear manifestation of preferential diffusion effects. The enthalpy transport by diffusive species fluxes does not influence the appearance of these structures. The term changes the speed at which these structures propagate, which was similarly observed in the 1-D case. The cellular structures have small regions in which the source term approaches zero. Furthermore, small cells are pushed out between larger cells, as can be observed near \( x = 0.65 \text{ cm} \). This behavior is also found by Bell et al. (2007), who used detailed chemistry to simulate a premixed hydrogen flame at an equivalence ratio of \( \phi = 0.37 \). It is striking that the same structures with local extinction appear. They also computed cases for methane and propane in which a local 1-D flame zone stays intact. Their report also refers to experimental observations in which the mentioned phenomenon of cellular structures in premixed hydrogen combustion is observed.

It is remarkable that these kinds of cellular structures can be simulated with FGM. At the extinction points, 1-D flame structures are observed no longer, which is the basic assumption in FGM. In the manifold there are zones in which the source term is very low. Apparently these zones are entered in a more or less correct way. The entries into phase space are depicted in Fig. 6. There is a dense population of trajectories that are on the rich side and a more scattered population at the lean side. This could be explained by a shift in flame structure in the curved regions and the extinction points, respectively.

In order to obtain long time integrations, a stabilization mechanism was incorporated into the numerical code. This was done to keep the mean profile at the same position, and was based on a criterion for the inflow velocity, which can be adjusted. First, the mean spanwise profile of \( c \) was calculated. If the position of this value equal to 0.5 was decreasing, the inflow velocity was adjusted to higher values and vice versa. In this way the flame stays in the middle of the domain and the inflow velocity as a function of time gives the burning speed. In order to get good statistics, a larger spanwise domain size seems to be required; with the present size, the discrete events of pushing out cells are clearly observed in statistics of the burning speed. Nevertheless, it is obvious that the burning speed increases by a factor of about 1.5 as a result of the cellular structures. Due to the low amount of structures within the spanwise direction, it is not known if this is a good measure for the final increase. In this case, it is also observed that, at the low curvature parts of the cusps, the cusps break in two parts. In addition to the simulations...
described so far, 2-D calculations were performed with $\Pi = 0$. This still gives the cusps with local extinction. These simulations resulted in a higher propagation velocity of the entire structure, similar to the 1-D situation excluding the term.

7. Future plans

In the near future, the present parameterization of hydrogen combustion with FGM will be verified by identical calculations using detailed chemistry. The local extinction phenomenon will be studied in greater detail. In 2-D cases, the preferred cell sizes will be investigated. The question is whether this preferred size corresponds to a stationary but propagating situation. Alternatively it could be the case that new cusps are created by the breakup of existing ones and the constantly pushing out of the smaller sized cusps that are created as a consequence of the breakup.

The burning speed as a function of flame stretch will be investigated next. This was previously done (Bastiaans et al. 2007) for lean methane combustion, based on the theory of de Goey & ten Thije Boonkkamp (1999). In lean premixed combustion, the Lewis number of the fuel is (almost) equal to unity and the flames are not unstable. In the case of hydrogen combustion, the fundamental instability is reflected in the Markstein number. This should be taken into account; the (extended) theory will be tested by performing stretch analyses.

Based on DNS, closures for LES have to be derived. Therefore, large-scale 3-D DNS simulations have to be performed.

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