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Resolution Estimates for Simple One Dimensional Flames

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Abstract

The accurate resolution of flame structure is critically important to the Direct Numerical Simulation (DNS) of reacting flows. While grid resolution estimates are readily available for cold flows, premixed flames appear to have received relatively little attention. In this paper, a premixed flame characterised by single step chemistry at moderate to high Zeldovitch numbers (β) is analysed, and its structure is used to provide estimates for sufficient grid resolution. It is found that the critical region of the flame exhibits a weak inverse Zeldovitch number dependence, and that heuristic methods of resolution estimation based on flame thickness grow relatively less meaningful as $\beta \rightarrow \infty$. Resolution estimates for second and fourth order finite difference schemes are provided.

Keywords: Combustion, Direct Numerical Simulation, asymptotics, Finite Differences, Numerical Methods

1 Introduction

Direct Numerical Simulation (DNS) is recognised as a powerful tool for the analysis of fundamental physical processes in fluid mechanics. In non-reacting flows, DNS has been used in many applications, with examples ranging from homogeneous isotropic turbulence [20] and channel flows [15], through to transition [26] impinging jets [13] and aeroacoustics [37]. For reacting flows, early applications of DNS can be found for both non-premixed [25], and premixed modes of combustion [29]. As techniques and hardware have developed, more recent studies have focussed on—for example—turbulent transport in flames [28], the inclusion of detailed chemistry ([3, 10, 1]), or investigations into flame-wall interactions ([38]).

Confidence in DNS rests on its ability to resolve accurately the smallest length and time scales in a flow which, in turn, set the limits for the required

mesh resolution. Physical considerations lead to scale estimates for the structures found in a particular problem; numerical considerations provide (broadly speaking) the mesh density required to capture these structures. Many papers have considered high order discretisations. for DNS, both for non-reacting and reacting problems. For the latter, spatial schemes range from classical high order explicit methods [7] and compact finite difference schemes [11], to limited applications of spectral methods [28]. Historically, the reacting flow community has pursued very high order explicit schemes (which are easy to implement, fast, and are readily parallelizable) or compact finite differences. However, high order schemes have less intrinsic diffusivity. Furthermore, they are unstable in general [4] and require special constructions to maintain stability even in the relatively simpler case of non-reacting flows [34]. Both the application of boundary conditions [5, 6], or heat release [24] may introduce spurious and potentially unstable oscillations into higher order schemes that require filtering to remove. The interplay between physics, numerical resolving power and stability has received relatively little attention in the computational combustion community, and provides one of the motivations for this paper.

For non-reactive flows, estimates for the smallest flow features are given by the Kolmogorov length scale l . For the purpose of estimating mesh spacing, $l \sim \text{Re}^{-3/4} L$, where Re is the turbulence Reynolds number and L is the integral length scale (typically the domain size of the DNS). Even for the simplest of cases however, specifying a grid resolution $h = l$ should be treated with caution, since the non-linear convection term can lead to aliasing if not properly taken into account [19, 27]. More generally, most commonly used numerical schemes do not perfectly capture the spectral evolution of a turbulent flow. The schemes themselves suffer from a non-trivial frequency response [16], which in turn leads to phase and group velocity effects that may impinge on overall accuracy [36].

A comparable problem occurs with Large Eddy Simulation (LES), where the situation is both better and worse: better because the requirement for absolute precision is relaxed, but worse because of the greater intrinsic complexities of the geometries and the turbulence thereby produced. Notwithstanding this observation, there exists a number best practice guidelines (i.e. [2, 22, 8]) establishing LES resolution requirements for a range of flow configurations.

In non-premixed combustion, the flame structure is governed by the local mixing of fuel with oxidizer and the transport of heat. The turbulence thus has a strong influence on the flame, resulting in a flame structure typically thicker than the smallest length scales: the estimates for cold flow DNS are thus usually sufficient to capture the non-premixed flame structure. The caveat to this is of course that the flame be treated as a single step reacting system: $F + sO \rightarrow (1 + s)P$, where F , O and P refer to fuel, oxidizer and product, respectively and s is the air/fuel ratio. For premixed combustion, the same simplification (single step chemistry with $R \rightarrow P$) leads neither to the same conclusion regarding resolution, nor does it provide a simple alternative estimate. In many practical premixed combustion problems the smallest scales of interest are determined not by the turbulence, but by the chemistry within the reaction zone of the flame. For such problems, the combustion takes place in laminar flamelets [17, 21],

where the flame thickness remains smaller than the Kolmogorov length scale [39]. Clearly in these cases, classical turbulence based resolution requirements are insufficient. In their place, heuristic arguments are typically used, with estimates of 10 – 40 grid points (depending on the choice of numerical scheme) being deemed sufficient to capture the entire flame structure.

In this paper, high activation energy asymptotics are used to characterize the structure of an unstrained premixed laminar flame characterised by a single step reaction mechanism. Higher order derivatives of the asymptotic solution are calculated, and these derivatives are used to estimate the truncation error associated with explicit finite difference schemes. A link between the flame speed error and diffusion flux error is demonstrated and, using the latter, estimates of grid resolution for a prescribed truncation error are derived. The asymptotic methods underpinning the analysis are not limited to simple chemistry; the simplifications chosen for this paper reflect findings in parallel work on the numerical stability of reacting flow discretisations [24], where the heat release itself (well characterised by a single progress variable) is of key importance to stability. The methods used in this paper can be easily extended to more complete analytic flame descriptions (i.e. to multi species treatments for non-premixed flames [32, 31], or premixed flames [18, 9, 40]). In such cases, the rapid variations undergone by minor species, say, can be used in place of the progress variable as the arbiter of accurate resolution.

The problem formulation and a representative solution is presented in section 2. Activation energy asymptotics are reviewed in section 3, which also includes the higher order derivatives required for the spatial schemes reviewed in section 4. Results of the asymptotics are compared to numerical simulations in section 5 and, from these, estimates are derived for the required resolution. Conclusions are drawn in section 6.

2 Formulation of Problem

The physical feature demanding the highest spatial resolution for the problem considered is the reaction zone within the flame sheet. For a one dimensional problem, a flame burning a mixture of ideal gases with negligible radiative heat transfer satisfies [39, 35, 28]

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u}{\partial x} = 0 \quad (1)$$

$$\frac{\partial \rho u}{\partial t} + \frac{\partial \rho u u}{\partial x} = -\frac{\partial p}{\partial x} + \frac{\partial}{\partial x} (\tau_{xx}) \quad (2)$$

$$\frac{\partial \rho E}{\partial t} + \frac{\partial ((\rho E + p) u)}{\partial x} = \frac{\partial}{\partial x} (u \tau_{xx}) + \frac{\partial}{\partial x} \left(\lambda \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial x} \left(h^0 \rho D \frac{\partial c}{\partial x} \right) \quad (3)$$

$$\frac{\partial \rho c}{\partial t} + \frac{\partial \rho u c}{\partial x} = \omega_c + \frac{\partial}{\partial x} \left(\rho D \frac{\partial c}{\partial x} \right) \quad (4)$$

where ρ is the density, u is the x -wise component of the velocity, p is the pressure, E is the stagnation internal energy and c is reaction progress variable

(a normalised product mass fraction). $h^0 = h_P^f - h_R^f$ is the enthalpy of reaction, τ_{xx} is the x -component of the viscous stress tensor, λ and (ρD) are the thermal conductivity and mass diffusivity, respectively. The (constant) specific heats, thermal conductivity and mass diffusivity are linked by assuming constant Lewis number $Le = \lambda/(\rho D c_p) = 1$ throughout the analysis. For the single step chemistry embodied in equation 4, the reaction rate is given by

$$\omega_c = B\rho(1 - c) \exp\left(-\frac{E}{R^0 T}\right) \quad (5)$$

where B is a constant, E is the activation energy and R^0 is the universal gas constant. The equations are closed by the caloric and thermal equations of state.

Figure 1 shows a typical laminar flame solution. Profiles are given for temperature, density, velocity and pressure. The reaction rate has been adjusted to give a laminar flame speed of 30cm/s, a value typical of many hydrocarbon reactions. The mean flow is from left to right, counter to the flame's direction of propagation; by balancing the mean flow speed against the laminar flame speed, the flame is brought to rest relative to the computational domain. This specification gives a simulation Mach number of $O(10^{-3})$ based on the laminar flame speed. The domain size (used throughout the paper) is 1.5 mm, and figure 1 depicts results from a simulation using a mesh of 128 grid points and Zeldovitch number (defined in section 3) $\beta = 6$. Time integration was performed using a 3rd order Runge-Kutta method [41]. The boundary conditions for this calculation use Navier-Stokes Characteristic Boundary Conditions (NSCBC) [23] for the inviscid components, and zero gradients for temperature, species mass fraction and momentum transport terms. The convective component of the solution was calculated using an explicit 4th order differencing scheme with an associated *restricted norm* [34]. The choice of discretisation for the convection terms is fixed throughout this analysis: previous work has demonstrated that higher order schemes developed solely from Taylor series expansions are generally unstable in the presence of heat release [24]. The restricted norm approximation used here reverts to an explicit fourth order scheme in the interior of the domain but is more stable than other commonly used explicit schemes; the subsequent analysis can then concentrate on the accuracy of the resulting flame profile, as opposed to the stability of the numerical scheme.

3 Activation energy asymptotics

In this section, activation energy asymptotics are reviewed and used to describe the structure of the reaction zone. The early part of the analysis essentially mirrors the development provided by Williams [39].

In one dimensional steady flows, the governing equations can be simplified first by assuming a reference frame moving at the laminar flame speed $u = s_l$, whereupon the temporal derivatives drop out and the continuity equation reduces to $\dot{m} = \rho s_l = \text{const.}$ The second simplification comes from the assump-

tion of unit Lewis number, which allows the removal of equation 3 from the subsequent analysis. To demonstrate this, consider the definition of stagnation internal energy used in equation 3:

$$\rho dE = \rho dh - dp = \rho \sum_{\alpha} h_{\alpha}^f dY_{\alpha} + \rho c_v dT + \rho u du. \quad (6)$$

Non-dimensionalising equation 6 with respect to the upstream quantities ρ_0 , $(c_p)_0$, T_0 and s_l reveals that all terms are $O(1)$ apart from the kinetic contribution, which is $O(M^2)$. To leading order in Mach number, the assumption $h = \text{const} + O(M^2)$ through the flame structure is made. Equations 6, 2 and 4 then allow equation 3 to be written in terms of a dimensionless temperature:

$$\rho \frac{d\hat{T}}{dx} = \omega_c + \gamma \frac{\lambda}{c_p} \left(\frac{\partial}{\partial x} \left(\frac{d\hat{T}}{dx} \right) - \left(\frac{\gamma-1}{\gamma} \right) \frac{1}{Le} \frac{\partial}{\partial x} \left(\frac{\partial c}{\partial x} \right) \right) - \gamma \frac{\tau_{xx}}{h_0} \frac{\partial u}{\partial x}, \quad (7)$$

where

$$\hat{T} = \frac{T - T_0}{T_{\infty} - T_0} = \frac{-c_p(T - T_0)}{h_0} = c + O(M^2). \quad (8)$$

Hence for $Le = 1$ and using equation 8, the energy transport equation simplifies to

$$\rho \frac{d\hat{T}}{dx} = \omega_c + \frac{\lambda}{c_p} \left(\frac{\partial}{\partial x} \left(\frac{\partial \hat{T}}{\partial x} \right) \right) + O(M^2) \quad (9)$$

where it has been recognised that the viscous dissipation term $\gamma h_0^{-1} \tau_{xx} (\partial u / \partial x) \sim O(M^2)$. In the limit of zero Mach number and unit Lewis number, the progress variable transport equation and the energy transport equation are thus identical.

Using the progress variable transport equation, the analysis thus begins with

$$\dot{m} \frac{dc}{dx} = \omega_c + \frac{d}{dx} \left(\rho D \frac{dc}{dx} \right), \quad (10)$$

which, by introducing a mass weighted coordinate $\xi = \int \frac{m c_p}{\lambda} dx$, gives

$$\frac{dc}{d\xi} = \frac{\lambda \omega_c}{\dot{m}^2 c_p} + \frac{d^2 c}{d\xi^2}. \quad (11)$$

Introducing the Zeldovitch number $\beta = \frac{E}{R^0 T_{\infty}} \left(\frac{T_{\infty} - T_0}{T_{\infty}} \right)$, the dimensionless temperature $\tilde{T} = (T - T_0) / (T_{\infty} - T_0)$, and the heat release parameters $\tau = (T_{\infty} - T_0) / T_0$, $\alpha = \tau / (\tau + 1)$, equation 5 becomes

$$\omega_c = B^* \rho (1 - c) \exp \left(- \frac{\beta (1 - \tilde{T})}{1 - \alpha (1 - \tilde{T})} \right) \quad (12)$$

where $B^* = B \exp(-E/(R^0 T_{\infty}))$ is one of the free parameters which may be used to obtain a required flame speed. Upstream and downstream conditions

are given the suffices 0 and ∞ , respectively. The unit Lewis number assumption allows the simplification $c = \tilde{T}$ in the absence of acoustics; this, in addition to an assumed thermal conductivity satisfying $\lambda = (\lambda_0/T_0) T = \lambda_0 (1 + \tau c)$ [39] allows equation 11 to be re-written as

$$\frac{d^2 c}{d\xi^2} - \frac{dc}{d\xi} = -\Lambda (1 - c) \exp\left(-\frac{\beta (1 - c)}{1 - \alpha (1 - c)}\right) \quad (13)$$

$$\Lambda = \frac{\lambda \rho B^*}{\dot{m}^2 c_p} = \text{const} \quad (14)$$

where Λ denotes the flame speed eigenvalue

The arguments supporting activation energy asymptotics are well known, but are repeated here for clarity. Analysis of equation 13 reveals the flame structure to comprise two parts: an *outer zone* in which there is negligible reaction, and an *inner zone*, where reaction and diffusion balance. This observation is supported by the nature of the reaction rate: far upstream from the reaction zone, $\omega_c \rightarrow 0$, and equation 13 simplifies to

$$\frac{d^2 c}{d\xi^2} - \frac{dc}{d\xi} = 0. \quad (15)$$

As the reaction zone is approached, the exponential term grows; as $(1 - c) \rightarrow O(\beta^{-1})$ the term can no longer be neglected and new variables $(\eta, y) = (\beta\xi, \beta(1 - c))$ must be introduced. In the reaction zone $y \sim O(1)$, with η chosen to fix the flame location at $\xi = 0$ and allow matching with the outer solution. The inner zone scales as $O(\beta^{-1})$ times the thickness of the outer zone and satisfies

$$-\frac{d^2 y}{d\eta^2} + \frac{1}{\beta} \frac{dy}{d\eta} = -\frac{\Lambda y}{\beta^2} \exp\left(-\frac{y}{1 - \alpha y/\beta}\right). \quad (16)$$

Equation 16 determines the asymptotic structure of the flame speed eigenvalue: as $\beta \rightarrow \infty$, the convective term vanishes and—to balance the diffusion term—the flame speed must satisfy the asymptotic expansion $\Lambda = \beta^2 (\Lambda_0 + \beta^{-1} \Lambda_1 + \dots)$. After introducing the expansion $y = y_0 + \beta^{-1} y_1 + \dots$, the leading order equation for the inner zone is thus

$$\frac{d^2 y_0}{d\eta^2} = \Lambda_0 y_0 \exp(-y_0), \quad (17)$$

and demonstrates the importance of accurately resolving the second derivative to capture the reaction rate and flame speed.

3.1 Flame speed as in indicator of accuracy

The mass flux $\dot{m} = \rho s_l$ is chosen as the principal measure of accuracy. Since $\dot{m} = \int \omega_c dx$ and $\omega_c \geq 0$ it follows that the exact solution satisfies $(\dot{m})_B = \|(\omega_c)_B\|_1 < K \|(\omega_c)_B\|_\infty$ where B denotes benchmark and K is a constant. The convergence behaviour of the mass flux estimate may therefore be inferred

from $\|\omega_c - (\omega_c)_B\|_\infty$, where ω_c is the calculated reaction rate. The reaction rate and the second derivative are closely related in the inner zone; from equation 17, it follows that $\|\omega_c - (\omega_c)_B\|_\infty \sim \|\delta^2 c / \delta x^2 - (d^2 c / dx^2)_B\|_\infty$ where $\delta / \delta x$ is used throughout to denote numerically evaluated derivatives. Thus, the convergence of the second derivative and of the reaction rate should match, and both should capture the convergence of the flame speed. The approximation to the second derivative depends on the grid spacing h , and this provides the link between convergence and a resolution estimate.

3.2 Higher order derivatives

3.2.1 Inner derivatives

Starting from equation 17, it is straightforward to obtain an equation for the first derivative: multiplying equation 17 by $dy_0/d\eta$, integrating from $\eta = \infty$ to $\eta = \eta_0$ gives

$$\frac{dy_0}{d\eta} = -\sqrt{2\Lambda_0(1 - (1 + y_0)\exp(-y_0))} = -\sqrt{\phi}. \quad (18)$$

$\phi \equiv 2\Lambda_0(1 - (1 + y_0)e^{-y_0})$ is introduced to simplify later equations. The negative square root in equation 18 is taken to match gradients between the inner and outer solutions. Higher order derivatives in η -space are more straightforward (albeit algebraically tedious) to evaluate:

$$\begin{aligned} \frac{d^3 y_0}{d\eta^3} &= \Lambda_0 e^{-y_0} (y_0 - 1) \sqrt{\phi} \\ \frac{d^4 y_0}{d\eta^4} &= \Lambda_0 e^{-y_0} (\phi (y_0 - 2) - (y_0 - 1) \Lambda_0 e^{-y_0} y_0) \\ \frac{d^5 y_0}{d\eta^5} &= \Lambda_0 e^{-y_0} \sqrt{\phi} (\phi (y_0 - 3) - \Lambda_0 e^{-y_0} (4y_0^2 - 8y_0 + 1)) \\ \frac{d^6 y_0}{d\eta^6} &= \Lambda_0 e^{-y_0} (\phi^2 (y_0 - 4) - \phi \Lambda_0 e^{-y_0} (11y_0^2 - 33y_0 + 10) \\ &\quad + \Lambda_0^2 e^{-2y_0} y_0 (4y_0^2 - 8y_0 + 1)). \end{aligned}$$

Higher order derivatives can be calculated as required, but are not required for the differencing schemes considered in this paper. From the preceding equations, it is apparent that the location of maximum curvature (and hence, maximum reaction rate) is at $y_0 = y^* = 1$ in inner coordinates, or at $c = c^* = 1 - \beta^{-1}$.

3.2.2 Matching conditions and higher derivatives

In general, the leading order inner and outer solutions agree only up to the first derivative of the progress variable. Discontinuities in the higher derivatives at the matching point—if unbounded—would throw into question the validity of estimates based on the inner solution. It is therefore worthwhile to examine the mismatch between the inner and outer solutions as $\beta \rightarrow \infty$.

In terms of inner coordinates, it is straightforward to show that the difference between the inner and outer solution satisfies

$$\left. \frac{dy}{d\eta} \right|_i - \left. \frac{dy}{d\eta} \right|_o = \left(1 - \frac{y}{\beta} \right) - \sqrt{\phi}.$$

Define the matching point by $y = y^\#$, where $y^\#$ satisfies

$$1 - \frac{y^\#}{\beta} = \sqrt{2\Lambda_0 (1 - (1 + y^\#) \exp(-y^\#))}. \quad (19)$$

Inspection of equation 19 shows that $y^\# \rightarrow \infty$ as $\beta \rightarrow \infty$, but clearly $|y^\#| \leq \beta$ for physically plausible results. To find the limiting behaviour of $y^\#$, both sides of equation 19 are squared to obtain

$$-2\frac{y^\#}{\beta} + \left(\frac{y^\#}{\beta} \right)^2 = -(1 + y^\#) \exp(-y^\#), \quad (20)$$

where the leading order flame speed eigenvalue estimate $\Lambda_0 = \frac{1}{2} + O(\beta^{-1})$ [39] has also been introduced. Since $(y_m/\beta)^2 \ll (y_m/\beta)$ for large activation energies, equation 20 can be approximated as

$$-2\frac{y^\#}{\beta} = -(1 + y^\#) \exp(-y^\#). \quad (21)$$

Now, introduce $\sigma^\# = y^\#/\beta$ as a variable independent of $y^\#$ and re-write equation 21 as the solution to

$$y^\# = -\text{LambertW}(-2\sigma^\# e^{-1}) - 1$$

where $\text{LambertW}(\cdot)$ is taken as the appropriate branch of the Lambert W function. As $\sigma^\# \rightarrow 0$ the asymptotic expansion for $\text{LambertW}(-2\sigma^\# e^{-1})$

$$\begin{aligned} \text{LambertW}(-2\sigma^\# e^{-1}) &\simeq L_1 - L_2 + \frac{L_2}{L_1} + \frac{L_2(-2 + L_2)}{2L_1^2} + \frac{L_2(6 - 9L_2 + 2L_2^2)}{6L_1^3} + \dots \\ L_1 &= \ln(2\sigma^\# e^{-1}) \\ L_2 &= \ln(-\ln(2\sigma^\# e^{-1})), \end{aligned}$$

is dominated by the first (L_1) term, and the implicit equation for $y^\#$ may be

approximated as

$$y^\# \simeq -\ln \frac{y^\#}{\beta} - \ln 2$$

and so

$$y^\# \sim \text{LambertW}(\beta).$$

By the same arguments as used above, this particular branch of the Lambert W function is dominated by $\ln(\beta)$ for large β , yielding

$$y^\# \sim \ln(\beta).$$

Higher derivatives of the outer solution at the matching point satisfy

$$\left. \frac{d^n y_o}{d\eta^n} \right|_{\#} = -\beta^{-n} \sqrt{\phi^\#}.$$

and thus the size of the discontinuity between inner and outer solutions is given by extending the argument to higher derivatives:

$$\begin{aligned} \left. \frac{d^2 y_i}{d\eta^2} \right|_{\#} - \left. \frac{d^2 y_o}{d\eta^2} \right|_{\#} &= \frac{1}{2} y^\# e^{-y^\#} + \beta^{-1} \sqrt{\phi^\#} \\ \left. \frac{d^3 y_i}{d\eta^3} \right|_{\#} - \left. \frac{d^3 y_o}{d\eta^3} \right|_{\#} &= \frac{1}{2} e^{-y^\#} (y^\# - 1) \sqrt{\phi^\#} + \beta^{-2} \sqrt{\phi^\#} \\ \left. \frac{d^4 y_i}{d\eta^4} \right|_{\#} - \left. \frac{d^4 y_o}{d\eta^4} \right|_{\#} &= \frac{1}{2} e^{-y^\#} \left(\phi^\# (y^\# - 2) - (y^\# - 1) \frac{1}{2} e^{-y^\#} y^\# \right) + \beta^{-3} \sqrt{\phi^\#} \\ &\vdots \end{aligned}$$

It is clear from these equations that the difference between the inner and outer

derivative is dominated by contributions from the former. Furthermore, the higher derivatives of the inner solutions may be simplified by observing that $e^{-2y^\#} \ll e^{-y^\#}$ and $\phi^\# \rightarrow 1$ for large $y^\#$. Hence

$$\left. \frac{d^n y_i}{d\eta^n} \right|_{\#} - \left. \frac{d^n y_o}{d\eta^n} \right|_{\#} \sim y^\# \exp(-y^\#)$$

Using the same asymptotic expansions as those used to estimate $y^\#$ yields

$$y^\# \exp(-y^\#) \sim \beta^{-1} \text{LambertW}^2(\beta) \sim \beta^{-1} \ln^2(\beta) \rightarrow 0$$

for large β and thus the mismatch between inner and outer solutions goes to zero as $\sim \beta^{-1} \ln^2(\beta)$. To interpret this result, we observe that the point of maximum curvature occurs at $y = y^* = 1$, and that strong variations in the solution are localised to this region. As β increases, $|y^\# - y^*| \rightarrow \infty$, the solution around $y^\#$ flattens off and consequently, the derivatives there go to zero. The original asymptotic analysis is accurate to $O(\beta^{-1})$; the analysis of the derivatives is accurate to $O(\beta^{-1} \ln^2(\beta))$.

3.2.3 Physical space derivatives

In order to estimate the error associated with the finite difference schemes, it is necessary to map the quantities in (η, y) coordinates to (x, c) coordinates. Algebraic complexity arises from the inclusion of the variable thermal conductivity

used to simplify the asymptotic analysis:

$$\frac{d}{dx} = \frac{\beta \dot{m} c_p}{\lambda_0} \frac{1}{(1 + \tau c)} \frac{d}{d\eta}. \quad (22)$$

Repeated application of this expression leads to a succession of derivatives in η -space:

$$\frac{d^n}{dx^n} = \left(\frac{\beta \dot{m} c_p}{\lambda_0} \right)^n \frac{1}{(1 + \tau c)} \frac{d}{d\eta} \left(\frac{1}{(1 + \tau c)} \frac{d}{d\eta} \left(\cdots \left(\frac{1}{(1 + \tau c)} \frac{d}{d\eta} \right) \right) \right). \quad (23)$$

Very quickly, the resulting expressions become too complex to be of practical use. Given that the original asymptotic analysis is itself approximate, it is appropriate only to keep those terms in the mapping that are $O(\beta^{-1})$ or larger. As an example, the second derivative in x -space can be written as (superscripted Roman numerals are used to denote the order of the analytic derivative).

$$c^{II} = -\beta \left(\frac{\dot{m} c_p}{\lambda_0} \right)^2 \left(\frac{1}{(1 + \tau c)^2} \left(\frac{d^2 y}{d\eta^2} \right) - \frac{\tau}{\beta (1 + \tau c)} \left(\frac{dy}{d\eta} \right)^2 \right),$$

from which, it is apparent that the second term (essentially arising from the gradient of the thermal conduction) can—to leading order—be omitted, yielding

$$c^{II} = -\beta \left(\frac{\dot{m} c_p}{\lambda} \right)^2 \left(\left(\frac{d^2 y}{d\eta^2} \right) + O(\beta^{-1}) \right).$$

Similar arguments can be made for the higher derivatives to obtain

$$c^{(n)} = -\beta^{n-1} \left(\frac{\dot{m} c_p}{\lambda} \right)^n \left(\left(\frac{d^n y}{d\eta^n} \right) + O(\beta^{-1}) \right).$$

The final estimates for the inner zone flame derivatives are therefore

$$\left(\frac{\lambda}{\dot{m} c_p} \right) c^I(x) = \sqrt{\phi}, \quad (24)$$

$$\left(\frac{\lambda}{\dot{m} c_p} \right)^2 c^{II}(x) = -\beta \Lambda_0 y_0 e^{-y_0}, \quad (25)$$

$$\left(\frac{\lambda}{\dot{m} c_p} \right)^3 c^{III}(x) = -\beta^2 \sqrt{\phi} \Lambda_0 e^{-y_0} (y_0 - 1), \quad (26)$$

$$\left(\frac{\lambda}{\dot{m} c_p} \right)^4 c^{IV}(x) = -\beta^3 \Lambda_0 e^{-y_0} (\phi(y_0 - 2) - (y_0 - 1) \Lambda_0 e^{-y_0} y_0), \quad (27)$$

$$\begin{aligned} \left(\frac{\lambda}{\dot{m} c_p} \right)^5 c^V(x) &= \beta^4 \sqrt{\phi} \Lambda_0 e^{-y_0} (-\phi(y_0 - 3) \\ &\quad + \Lambda_0 e^{-y_0} (4y_0^2 - 8y_0 + 1)) \end{aligned} \quad (28)$$

$$\begin{aligned} \left(\frac{\lambda}{\dot{m} c_p} \right)^6 c^{VI}(x) &= \beta^5 \Lambda_0 e^{-y_0} (\phi \Lambda_0 e^{-y_0} (11y_0^2 - 33y_0 + 10) \\ &\quad - \Lambda_0^2 e^{-2y_0} y_0 (4y_0^2 - 8y_0 + 1) - \phi^2 (y_0 - 4)). \end{aligned} \quad (29)$$

Equations 24 to 29 may thus be further simplified by setting $y_0 = y^* = 1$ to obtain critical values at the point of maximum curvature:

$$c^I \simeq 0.7270 \sqrt{\Lambda_0} \left(\frac{\dot{m} c_p}{\lambda^*} \right), \quad (30)$$

$$c^{II} \simeq -0.3679 \Lambda_0 \left(\frac{\dot{m} c_p}{\lambda^*} \right)^2 \beta, \quad (31)$$

$$c^{III} = 0, \quad (32)$$

$$c^{IV} \simeq 0.1944 \Lambda_0^2 \left(\frac{\dot{m} c_p}{\lambda^*} \right)^4 \beta^3, \quad (33)$$

$$c^V \simeq -1.2482 \times 10^{-2} \Lambda_0^{\frac{5}{2}} \left(\frac{\dot{m} c_p}{\lambda^*} \right)^5 \beta^4, \quad (34)$$

$$c^{VI} \simeq -0.40076 \Lambda_0^3 \left(\frac{\dot{m} c_p}{\lambda^*} \right)^6 \beta^5. \quad (35)$$

where $\lambda^* = \lambda(c^*)$, $\dot{m} = (\rho \lambda B^* / \Lambda c_p)^{\frac{1}{2}}$ and Λ_0 is the leading order flame speed defined above.

4 Spatial differencing schemes

4.1 The choice of convective discretisation

The asymptotic analysis underscores the importance of the second derivative in resolving the flame structure. Nevertheless, for the purposes of simulation, approximations are required for both first and second derivatives. The simulations undertaken in this paper were performed using fourth order restricted norm approximations for the convective term [34]; this effectively limits the choice of diffusive schemes considered to be of 4th order or lower. Given the ubiquity of high order compact and explicit differencing schemes in the reacting flow simulation community (for both convection *and* diffusion), this choice appears restrictive. However; (1) the analysis outlined below can in principle be extended in a straightforward manner to any order compact or explicit method; (2) although high order compact schemes have been discussed for combustion applications [16], high order approximations are prone to becoming left half plane unstable when boundary conditions are applied—this is observed both in non-reacting flows [4, 5, 6] and, more recently, in combustion simulations [24]. The instability has been traced to the *convection* approximation and, although schemes with greater than fourth order accuracy are available, their inclusion here would add only algebraic complexity to the analysis without contributing any additional novelty to the method of estimating resolution.

4.2 Explicit schemes for the second derivative

In the interior of the computational domain, the two explicit differencing schemes considered here can be written as [16]

$$\frac{\delta^2 c_i}{\delta x^2} = \sum_{j=1}^2 \frac{a_j}{h^2} (c_{i+j} - 2c_i + c_{i-j}), \quad (36)$$

where $c_i \equiv c(x_i)$; both the stencil itself and the values a_i are allowed to change as the boundary is approached. In the interior, the coefficients take the values

$$\begin{pmatrix} a_1 & a_2 \end{pmatrix}^T = \begin{cases} \begin{pmatrix} 1 & 0 \end{pmatrix}^T & \text{2nd order} \\ \begin{pmatrix} \frac{4}{3} & -\frac{1}{12} \end{pmatrix}^T & \text{4th order} \end{cases}.$$

The respective truncation errors are proportional to $h^2 (d^4 c/dx^4)$ and $h^4 (d^6 c/dx^6)$; it is the appearance of the fourth and sixth order derivatives in the truncation errors that drives the restriction to $d^6 y_0/d\eta^6$ in section 3.2.

4.3 Resolution estimates

Using the Taylor series expansion for the second order derivative (equation 36) leads to the following:

$$\begin{aligned} \frac{\delta^2 c}{\delta x^2} - \frac{d^2 c}{dx^2} &= \frac{h^2}{12} \left(\left(\frac{d^4 c}{dx^4} \right)_{\xi_1} + \left(\frac{d^4 c}{dx^4} \right)_{\xi_2} \right) \quad (\text{second order}) \\ &= \frac{h^4}{360} \left(a_1 \left(\left(\frac{d^6 c}{dx^6} \right)_{\xi_1} + \left(\frac{d^6 c}{dx^6} \right)_{\xi_2} \right) + 2^6 a_2 \left(\left(\frac{d^6 c}{dx^6} \right)_{\xi_3} + \left(\frac{d^6 c}{dx^6} \right)_{\xi_4} \right) \right) \quad (\text{fourth order}) \end{aligned}$$

where in general $\xi_1 \in [x, x+h]$, $\xi_2 \in [x-h, x]$, $\xi_3 \in [x, x+2h]$, and $\xi_4 \in [x-2h, x]$ [30]. For the purposes of obtaining an estimate, $\xi_{1...4}$ are assumed to coincide with x in the expansion, allowing the above to be approximated as

$$\frac{\delta^2 c}{\delta x^2} - \frac{d^2 c}{dx^2} = \frac{h^2}{6} \frac{d^4 c}{dx^4} \quad (\text{second order}) \quad (37)$$

$$= \frac{11h^4}{540} \frac{d^6 c}{dx^6} \quad (\text{fourth order}), \quad (38)$$

Equations 37 and 38 can then be used to define an error ε as

$$\varepsilon = \frac{\left| \left(\frac{\delta^2 c}{\delta x^2} \right)_{x^*} - \left(\frac{d^2 c}{dx^2} \right)_{x^*} \right|}{\left| \frac{d^2 c}{dx^2} \right|_{x^*}},$$

where $x^* = x(c^*)$. Inverting this argument and making use of equations 37, 38, a user specified error tolerance in the second derivative leads to a grid spacing

requirement given by

$$h_2 = \left(\frac{6 |d^2 c/dx^2|_{c^*}}{|d^4 c/dx^4|_{c^*}} \varepsilon \right)^{\frac{1}{2}} \quad (39)$$

$$h_4 = \left(\frac{540 |d^2 c/dx^2|_{c^*}}{11 |d^6 c/dx^6|_{c^*}} \varepsilon \right)^{\frac{1}{4}}, \quad (40)$$

where the subscript denotes the order of the numerical approximation. The values of $d^2 c/dx^2$, $d^4 c/dx^4$ and $d^6 c/dx^6$ can be taken either from a benchmark numerical solution if available or—more generally—from the asymptotic solution. From the arguments presented in section 3.1, ε should also translate to an estimate of the error in laminar flame speed.

5 Results

In the following sections, numerical solutions to equations 1-4 are compared to the asymptotic solutions. Some care is required here, since there is no guarantee that the leading order asymptotic approximation will be sufficient to guarantee exact agreement with the numerical simulation, even as the latter’s resolution increases. Since a sufficiently resolved simulation should incorporate *all* orders of the asymptotic solution, the numerical solution is used initially to benchmark the error measures.

Single step flames are investigated on one dimensional domains of overall size $L = 1.5mm$. The cases considered are for $\beta = 6$ and $\beta = 10$, with resolutions of 32, 64, 128 and 256 grid points; the finest grid yields the benchmark solutions (denoted B) and all other parameters are as described in section 2. Each simulation is terminated at the same computational time to eliminate as far as possible phase errors (arising from incorrect consumption speeds) misleadingly influencing the results.

5.1 Curvature and flame speed errors

Earlier in the paper, the case was made for the choice of $\dot{m} = \dot{m}(\omega_c)$ as an error metric and for the second derivative as a resolution dependent proxy for this quantity. Figure 2 provides a comparison between two error measures, defined as:

$$\varepsilon_m = \frac{\|\omega_c - (\omega_c)_B\|_\infty}{\|(\omega_c)_B\|_\infty} \quad (41)$$

$$\varepsilon_{c''} = \frac{\|\delta^2 c/\delta x^2 - (\delta^2 c/\delta x^2)_B\|_\infty}{\|(\delta^2 c/\delta x^2)_B\|_\infty}. \quad (42)$$

ε_m is a normalised flame consumption speed error, $\varepsilon_{c''}$ measures the normalised error in the second derivative: both are evaluated at $x = x(c^*)$.

In the figure, the results were obtained for a flame with $\beta = 6$ and using fourth order differences for the diffusive flux; the convergence rate can be seen by comparison to the $\sim O(h^{-4})$ curve also included in the figure. There is a strong correspondence between the two sets of results and it is clear that specifying a target value for $\varepsilon_{c''}$ should ensure $\varepsilon_m < \varepsilon_{c''}$; i.e. the mass flux error is typically less than that of the second derivative, and the resolution estimates provided later in sections 5.3.1 and 5.3.2 will thus lead to slightly conservative estimates of the required number of grid points.

5.2 Critical values for the asymptotic and numerical derivatives in the flame structure

At the critical point in the flame structure, the derivatives scale as $\sim \beta^{n-1} (\dot{m} c_p / \lambda)^n$, in which $\dot{m}$ itself arises from the analysis. Consequently, $c^I, c^{II}, c^{III}, \dots$ become increasingly sensitive to errors in the value of $\dot{m}$. To minimise the effect of this error, two approximations to Λ are used: the leading order approximation $\Lambda = \frac{\beta^2}{2}$ is used in the main body of the work, and a second order correction: $\Lambda = \beta^2 \left(\frac{1}{2} + \beta^{-1}(3\alpha - \kappa) \right)$ where $\kappa = 1.3440$ [39] is used in the mass flux estimate. Although heuristic, it can be seen from table 1 that agreement between the revised analytical mass flux and the numerical benchmark simulation is improved (1 and 2 refer to 1st and 2nd order definitions of Λ , respectively).

β	$\dot{m}_1 (kg/s)$	$\dot{m}_2 (kg/s)$	$\dot{m}_s (kg/s)$
6	0.694	0.596	0.610
10	0.416	0.378	0.382

Table 1: Estimates of the laminar flame speed. The suffices refer to leading order, second order and simulation results

Figure 3 compares the values of the derivatives given in equations 30 - 35 at c^* to those evaluated from the benchmark numerical simulation for the case $\beta = 6$. To compare the results, the progress variable profiles obtained from the numerical solutions were projected onto Fourier space and the n^{th} order derivatives were calculated as $\sim (i\Omega)^n \Psi(\Omega)$, where $\Psi(\Omega)$ is the transform of the periodised progress variable. If $c^n(x^*)$ did not coincide with a grid node, interpolation was used to estimate the derivative.

In general, there is very good agreement between the estimates and the numerical derivatives. In the figure, the different symbol used for the 3rd derivative estimate reflects the fact that $c^{III} \sim 0$ using the leading order expression in (x, c) coordinates; the figure reflects an estimate using instead the full expression for the coordinate transform $(\eta, y) \rightarrow (x, c)$ (equation 23 for $n = 3$). Similarly, it may be deduced that the relatively larger error on the fifth derivative stems from the retention of only the leading order mapping term. Similar results (not reported here) were found for $\beta = 10$; as may be expected, the leading order asymptotic expressions become better approximations as the Zeldovitch number increases.

5.3 Resolution estimates

5.3.1 Resolution requirements in terms of domain size

The two preceding subsections established the parity between errors in the second derivative and the laminar flame speed, and also between $(\delta^n c / \delta x^n)_B$ and their analytic estimates. Thus, the exact derivatives appearing in equations 39 and 40 can be replaced with analytic estimates for c^{II} , c^{IV} and c^{VI} , values for which are given in table 2.

β	$ c^{II} $	$ c^{IV} $	$ c^{VI} $
6	3.287×10^7	9.303×10^{15}	1.027×10^{25}
10	1.906×10^7	5.217×10^{15}	5.569×10^{24}

Table 2: Estimates for the even order derivatives used to calculate flame resolution

Figures 4 & 5 depicts the errors associated with second order approximations to the diffusive term for the $\beta = 6$ and $\beta = 10$ flames. The plots use the definitions given by equations 41 and 42, but with the addition of an estimated error obtained from equation 39. For both plots, a user specified normalised error $\varepsilon_{c''} = 1 \times 10^{-2}$ has been used; equation 39 produces a grid spacing requirement $h = 1.456 \times 10^{-2} mm$ for the $\beta = 6$ case, and $1.481 \times 10^{-2} mm$ for $\beta = 10$. For a fixed domain length of $1.5 mm$, the estimates translate into a required resolution of ~ 103 grid points for $\beta = 6$ and ~ 101 grid points for $\beta = 10$. In both of the figures, the resolution estimates lie on the line interpolating the error convergence curves. From this, it may be deduced that equation 39 provides a reasonable approximation for the curvature error.

The relatively weak dependence of the resolution on the Zeldovitch number can be attributed to two causes: (a) using 2nd order differences, the grid spacing changes only as the square root of the arguments and: (b) the curvatures (and higher derivatives) exhibit a weak inverse dependence on β . This appears to be in contrast to the estimates provided via equations 30 - 35. However, in these estimates, the dependence of the flame speed eigenvalue $\dot{m} = \dot{m}(\beta)$ has not been explicitly taken into account; for example, substituting equation 14 into equation 31 and expanding in terms of β^{-k} at the critical point gives

$$c^{II}|_{c^*} \simeq -0.368 \frac{c_p \rho_0 B^*}{\lambda_0 (1 + \tau)^2 \beta} + O\left(\frac{1}{\beta^2}\right).$$

A key observation then is: given the constancy of all other thermochemical variables, lower Zeldovitch numbers lead to higher values of curvature and more stringent resolution requirements.

For the fourth order discretisation, setting $\varepsilon = 10^{-3}$ in equation 40 provides resolution estimates of ~ 75 grid points ($\beta = 6$) and ~ 74 grid points ($\beta = 10$); Figures 6 and 7 again demonstrate the accuracy of the estimate derived from the Taylor series expansion. To achieve the same level of accuracy as the fourth

order scheme, the second order scheme requires 326 grid points ($\beta = 6$) and 321 grid points ($\beta = 10$).

5.3.2 Resolution requirements in terms of flame thickness

Rather than use the overall domain size to guide the number of grid points, it is more usual to express the required resolution in terms of the flame thickness. There are a number of alternative definitions for the flame thickness[12, 33]; in this paper, we use a variant of the *characteristic* thickness $\Delta = \lambda_\infty (\dot{m}c_p)^{-1}$ provided by Jarosinski [14]

$$\delta_m = \frac{S}{\dot{m}} \overline{\left(\frac{\lambda}{c_p} \right)} \quad (43)$$

where $S \simeq 5$ is almost constant, and the overbar is interpreted as the mean value over the temperature range of the flame. Using the asymptotic model behaviour $\lambda T^{-1} = \text{const}$ and the assumption $\tau = 4$ used in the simulations above, equation 43 yields

$$\begin{aligned} \delta_m &= \frac{S\lambda_0\tau}{\dot{m}c_p \ln(1+\tau)} \\ &= \begin{cases} 5.256 \times 10^{-1} \text{mm} & (\beta = 6) \\ 8.434 \times 10^{-1} \text{mm} & (\beta = 10) \end{cases} \end{aligned}$$

Figures 8 and 9 provide profiles for the scaled reaction rate and progress variable for $\beta = 6$ and $\beta = 10$, taken from their respective benchmark solutions. Also shown on the figures are the two alternative definitions for the flame thickness: Δ and δ_m . From these, it is readily seen that δ_m provides a reasonable estimate for the total flame structure (i.e. including the reaction and preheat zones). Using equation 43 as the revised length scale in place of the domain length, equations 39 and 40 provide

β	grid points (second order)	grid points (fourth order)
$\varepsilon_{c''} = 10^{-2}$		
6	38	16
10	59	24
$\varepsilon_{c''} = 10^{-3}$		
6	119	28
10	184	43

Table 3: Number of grid points required in the flame structure to capture second derivative with an error ϵ

It is interesting to observe that in using equation 43 for the flame thickness definition, the number of required grid points increases as β increases. The reason for this stems from the increasingly long diffusive forelimb associated with the reducing laminar flame speed; this preheat layer thickens relative to the reaction zone. Figures 8 and 9 demonstrate the weak β -dependence of the

reaction zone itself while it can also be clearly seen that δ_m increases. Consequently, for the purposes of critically resolving the flame structure, it is not clear what advantage is obtained by using the full flame thickness as a key parameter.

6 Conclusions

An approach has been presented here for resolving the structure of a simplified flame. Using Taylor series expansions and activation energy asymptotics, a pre-specified accuracy in the laminar flame speed can be translated into an estimation of the required grid density. The method has been applied to explicit second and fourth order schemes for the diffusive flux, although there is no reason in principle why the method cannot be extended to other discretisation schemes.

During the course of the analysis, it has become apparent that the mesh density for a higher order scheme exhibits only a relatively weak dependence on the specified error: this reflects the relationship $h \propto \varepsilon^{1/N}$ for a given order of accuracy N . The reaction zone within the flame also exhibits only a weak inverse dependence on the Zeldovitch number—this is surprising, and shows that the most difficult flames to simulate will be those with low β (all other variables remaining fixed). Under the same conditions, an increasing value of β decreases the laminar flame speed, and the relative length of the diffusive forelimb of the flame grows with respect to that of the reaction zone itself. In the light of this observation, the value of basing required resolution on the overall flame thickness becomes unclear.

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Figure 1: Example laminar flame solution for single step chemistry $R \rightarrow P$. The solution is obtained using 4th order differences satisfying a *restricted norm* [34] for the convective term.

Figure 2: Comparison between $\varepsilon_{c''}$ and ε_m for $\beta = 6$.

Figure 3: Asymptotic and numerical estimates for 1st - 6th order derivatives in physical co-ordinates. $\beta = 6$.

Figure 4: Grid resolution estimate using equation 39 for the case $\beta = 6$ using second order central differences.

Figure 5: Grid resolution estimate using equation 39 for the case $\beta = 10$ using second order central differences.

Figure 6: Grid resolution estimate using equation 40 for the case $\beta = 6$ using fourth order central differences.

Figure 7: Grid resolution estimate using equation 40 for the case $\beta = 10$ using fourth order central differences.

Figure 8: Flame structure for $\beta = 6$

Figure 9: Flame structure for $\beta = 10$.