Geometrical Characterization of the Reaction Front in Gaseous Detonations using Fractal Theory

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1 Introduction

A detonation consists of transverse waves sweeping across the detonation front and the structure depends generally on the mixture sensitivity, boundary and initial conditions [1]. In general, the detonation cellular pattern is loosely classified by visual examination as stable, weakly unstable, or highly unstable. For stable mixtures, the cellular pattern is regular and piece-wise laminar and can be described by the ZND model; While for more unstable mixtures, i.e., with highly irregular cellular pattern, the instability strongly manifests inside the reaction zone structure leading to a highly turbulent flow within.

Theoretically, many attempts were made to define a stability parameter for such classification. Linear stability theory [2-4] shows that by increasing the global activation energy E_a of the explosive mixture, the number of instability modes increases; both experimental observation and numerical simulation show that the detonation front becomes more irregular [5, 6]. Recently an alternative stability parameter is also defined taking into account the structure of the reaction zone and the description agrees well with experimental observations for many hydrocarbon mixtures [7]. Although these parameters describe correctly the instability trend, the descriptions remain on a qualitative basis when compared with experimental results.

Applications of fractal theory in fluid dynamics and turbulence statistics are widely studied [8-9]. It has also been used for analyzing turbulent flames. In principle, the fractal dimension is a measure of the roughness of the object. For fractal curve lying in a plane, the fractal dimension is bounded by $1 < D < 2$. The closer the fractal dimension is to its upper limit, i.e., the dimension of space in which it is embedded, the more rough or space-filling the fractal image is. For smooth interface boundary, the fractal dimension D reduces to one. The fractal dimension can thus be thought to provide a geometrical characterization of the degree of complexity, and hence, instability of a frontal interface.

Using PLIF and Schlieren imaging methods, Pintgen and Shepherd [10] looked into detail the detonation front and the reaction zone structure. They had indeed carried out a fractal analysis to determine an average dimension as a geometrical quantity to define the regularity of the fronts. Note that their analyses were performed on the experimental results, which are subjected to the limitation of the experimental techniques (i.e. illumination and imaging system qualities) and image interpretation.

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The precision of their dimension estimate is therefore limited. Nevertheless, this study found that for $\theta = E_a/RT_s \leq 6$, the spread of the fractal dimension is small, varied from 1.05 up to 1.15; For weakly unstable mixtures with intermediate θ, the dimensions lie between 1.05 and 1.4; and, for the highest value of $\theta = 12.4$ in their mixture conditions considered, the maximum dimension found to be 1.5.

Recent advances in scientific computing now allow the detonation front to be simulated numerically with well-resolved qualitative features comparable to experimental observations. CFD contour images are generally used to illustrate visually the structure of the detonation front. In the same spirit as in the work of Pintgen and Shepherd [10], we use here the fractal theory to analyze quantitatively the numerical simulation results of cellular detonation structures. The numerical results were obtained using a multi-component model with an one-step chemistry [11]. The model is formulated by the TCFC approach to avoid artificial pressure fluctuation at the material interface [12]. By varying the activation energy, the cellular pattern becomes more irregular and the objective is to measure the fractal dimension variation and use it as a parameter to quantify the degree of instability of the reaction zone structure. Attempts can be made to link the fractal dimension of the highly unstable case with other results for fractal dimension measurement of scalar interfaces in classical shear and fully developed turbulent flow (e,g, axisymmetric jet and shear mixing layer, etc.).

2 Numerical Simulation and Analysis

The governing equations for the detonation simulation were based on a multi-gas model formulated using a TCFC (thermodynamically consistent and fully conservative) method [11, 12, 13]. This allows artificial pressure fluctuations at the material interface to be eliminated. By considering a flow in which all component are ideal gases, properties are parameterized by the values of γ, the ratio of specific heat capacities, and M, the molecular weight. For detonation simulation, the TCFC model supplements the system of Euler equations with two conservation equations of two alternative variables $\rho\xi/M$ and ρ/M where $\xi=\gamma/(\gamma-1)$:

$$\frac{\partial}{\partial t}\left(\frac{\rho\xi}{M}\right)+\nabla\cdot\left(\frac{\rho\xi}{M}V\right)=\rho\left[\frac{\xi_{reac}}{M_{reac}}-\frac{\xi_{prod}}{M_{prod}}\right]\dot{\omega}=\Delta\left(\xi M^{-1}\right)\dot{\omega}$$

$$\frac{\partial}{\partial t}\left(\frac{\rho}{M}\right)+\nabla\cdot\left(\frac{\rho}{M}V\right)=\rho\left[\frac{1}{M_{reac}}-\frac{1}{M_{prod}}\right]\dot{\omega}=\rho\Delta M^{-1}\dot{\omega}$$

The system of governing equations can be written in conservative form with source terms, and hence its solution can be approximated using any conservative finite volume scheme. Here, the numerical results are obtained using a numerical algorithm based on an operating splitting scheme using the slope limiter centred (SLIC) method as the hyperbolic solver [14] and standard finite differences for the reaction terms. The solver is also incorporated into an adaptive mesh refinement framework for high resolution simulations to be performed [15]. Details of the numerical simulations and some results are previously reported in [11]. The numerical calculations are performed with an effective resolution of 24 grid points per half reaction zone length and the CFL number is taken as 0.8. The initial and mixture conditions are given in Table 1. Three types of mixtures were considered, which roughly mimics the stable, weakly unstable and unstable structure of detonation waves. To detect the reaction front, the mole fraction of the reactant is plotted using a grey-scale colour map and taken for subsequent image processing.

Mixture	P_o (atm)	T_o (K)	γ_{react}	M_{react}	γ_{prod}	M_{prod}	Q *(MJ/kg)*	δ (mm)	E_a/R *(K)*	A *($x10^6\ s^{-1}$)*
$H_2 + O_2$	1	295	1.404	12.01	1.22	14.474	8.27	0.043	11284	900
$H_2 + O_2 + 50\%Ar$	1	295	1.509	25.977	1.2	29.001	4.264	0.040	9486	280
H_2+Air	1	295	1.405	20.911	1.17	23.904	5.306	0.188	15497	3500

Table 1. Mixture properties used in the numerical simulations [11]

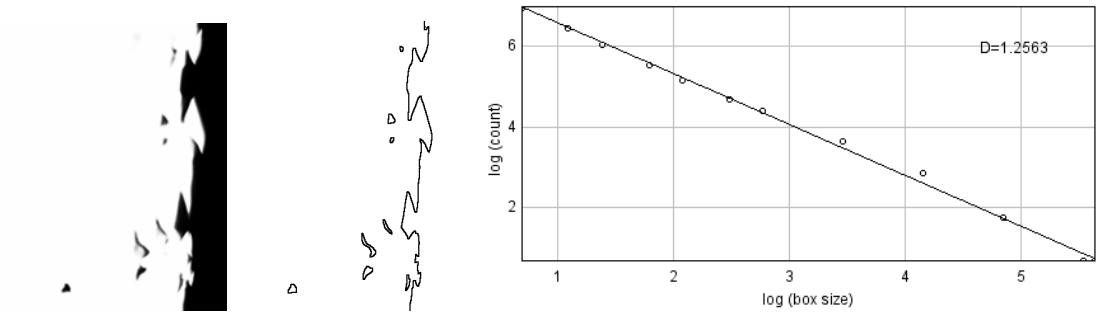

Figure 1. A sequence of image processing procedure and the estimation of fractal dimension

To study the fractal nature of the reaction front, the CFD images from the numerical simulations were analyzed using the software *ImageJ* [16]. To analyze the reaction front structure, the CFD image is first processed into a binary (black/white) image (Fig.1). The binary conversion of the images was performed using a built-in automatic thresholding criterion in *ImageJ* based on an averaging process. Using the binary image, the interface is subsequently tracked using the Sobel edge detection algorithm in the software. To estimate the fractal dimension of the reaction front curve, the box-counting method is employed. The box-counting technique is known as an efficient method in measuring the fractal curve of digital image and is widely used for turbulence interface. The procedure is to systematically lay a series of squares or boxes of decreasing side ε over an image *S* and count the number of boxes $N_\varepsilon(S)$ that overlaps the set for various small ε. (Here, the box sizes used are 2,3,4,6,8,12,16,32,64, 128,256 pixels). The dimension is the logarithmic rate at which $N_\varepsilon(S)$ increases as $\varepsilon \to 0$, which can be estimated by the slope of the regression line of the plot log $N_\varepsilon(S)$ against log ε, i.e.:

$$D(S) = -\lim_{\varepsilon \to 0} \frac{\log(N_\varepsilon(S))}{\log(\varepsilon)}$$

3 Results and Discussion

Figure 2, displaying snapshots of Schlieren-type density gradient and reactant mass fraction plots, describes in detail the flow field behind the detonation front. For the argon diluted case (θ = 4.687), the flow structure is very regular with essential constant spacing between transverse waves. After applying the image processing described in previous section, the edge detected for the reaction front structure from the reactant mass fraction displays a rather regular interface. The fractal analysis gives a dimension of these curves D = 1.181, 1.131, 1.120, 1.121 and 1.146 with an average $\overline{D}$ = 1.139.

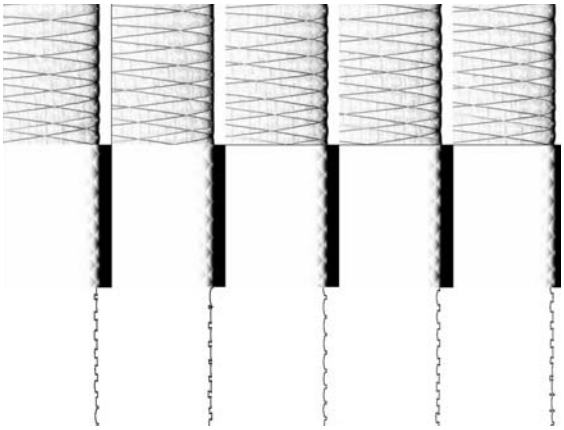

Figure 2. top) Schlieren plot; middle) Reactant mass fraction; and bottom) edge-detected reaction front for the stable detonation with θ = 4.687.

Figure 3 shows similar plots but for a weakly unstable detonation front with θ = 6.386. For the undiluted case, the flow structure becomes less regular with more flow disturbances inside the structure. The edge detected for the reaction front structure from the reactant mass fraction also shows a more irregular curve shape indicating an increase of corrugation of the front. Using the box-counting method, the average fractal dimension is found to be $\overline{D}$ = 1.24.

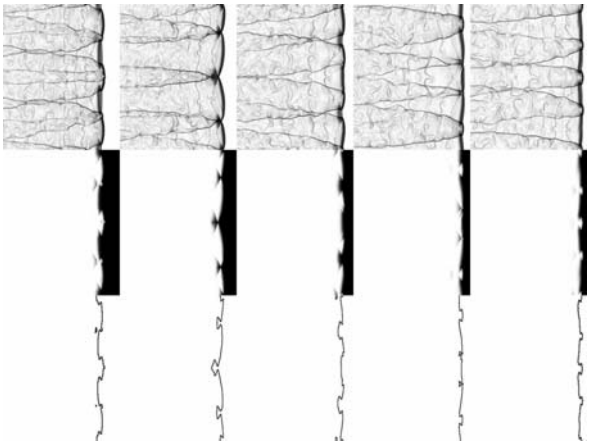

Figure 3. top) Schlieren plot; middle) Reactant mass fraction; and bottom) edge-detected reaction front for the weakly unstable detonation with θ = 6.386.

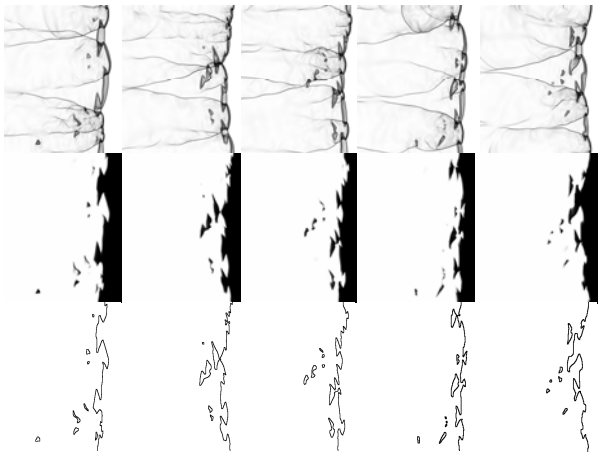

Figure 4. top) Schlieren plot; middle) Reactant mass fraction; and bottom) edge-detected reaction front for the unstable detonation with θ = 10.122.

Further increase in activation energy θ = 10.122 leads to a highly unstable detonation front structure. For the undiluted H_2-air case, the appearance of unburned pockets of reactants and the compressible turbulent nature of the flow are quite apparent (see Fig. 4). The edge-detected reaction front is highly irregular with a fractal dimension close to $\overline{D}$ ~ 1.30.

Figure 5 shows the average fractal dimension of the reaction interface boundary D for each activation energy considered in this study so far giving a detonation front from stable (laminar ZND) to the highly unstable (turbulent) cases. Simulations at higher activation energies θ with finer numerical resolutions are currently in progress and results will be reported. In Fig. 5, the error bars indicate the minimum and maximum fractal dimension obtained from a sequence of images at different times for each activation energy value. The results are statistically bounded away from an

integer. It is found that the fractal dimension of the interfaces increases from an initial value about 1.1 (θ = 4.687) approaching to a value of 1.3 (θ = 10.122). These values agree approximately with previous studies by Pintgen and Shepherd [10] who analyzed the experimental results from their PLIF measurements on the detonation front. For the highly unstable detonation with further increase in the activation energy, the logarithmic trendline indicates that the fractal dimension approaches to that experimentally measured for fully developed turbulence, i.e. $D \sim 1.38$, in axi-symmetric jet, turbulent shear flow or turbulence induced by Richtmeyer-Meshkov instability [17-19]. Such agreement may thus suggest the self-similarity of the turbulence or chaotic flow structure of the reaction zone behind the detonation front.

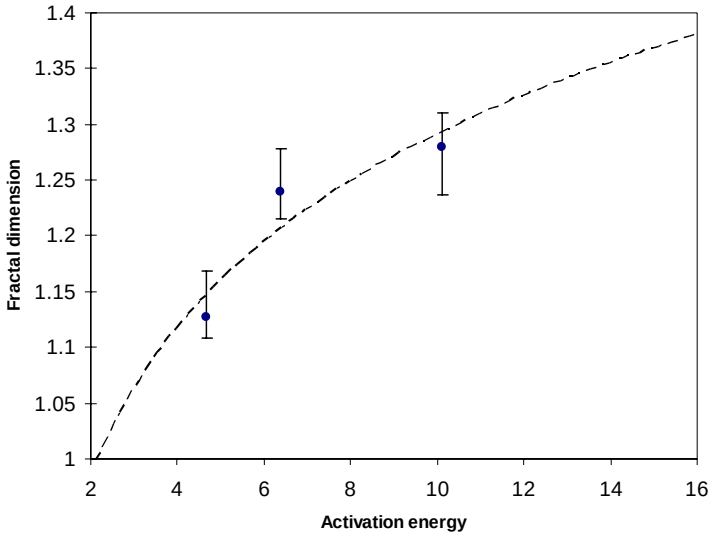

Figure 5. Fractal dimension of the edge-detected reaction front of the detonation estimated using box-counting method as a function of activation energy.

4 Concluding Remarks

In this study, we analyze the CFD simulation results of cellular detonation structures obtained by solving a multi-component model with single-step kinetics formulated based on the TCFC approach. Using the numerical results of cellular detonation propagation in H_2–air and H_2–O_2–Ar mixtures, the model simulates all the salient feature of unstable cellular detonation structure observed in experiments. The model prevents spurious waves at material interfaces, which have a particular detrimental effect for reactive flow simulation. By increasing the activation energy θ, the flow field transits from a laminar one to a compressible turbulent structure.

Unlike experimental images, the high resolution of corresponding digital CFD images can meet the requirement of image processing and fractal dimension measurement using the box-counting method. The fractal dimension of the reaction front of a stable detonation (with low activation energy) is about 1.10 and that of the more irregular cellular detonation will increase with the activation energy values. The growth of fractal dimension tends to approach to a maximum value of ~1.38, close to that reported in Pintgen and Shepherd's study and in a number of other studies for the fractal dimension of scalar level-set interfaces in fully-developed turbulent flows and the similar Richtmeyer-Meskhov instability experiment.

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