Three-dimensional Instationary Numerical Simulation of Spherical Flame Structures

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Abstract

We present numerical simulation of the transient behaviour of freely propagating spherical flame structures in three dimensions. The parameters correspond to a lean H_2–air system with low Lewis number. The governing partial differential equations are solved by means of a parallelized Fourier–pseudospectral code. The algorithm is applied to compute the evolution of thermo–diffusive flames, whereby the influence of the Lewis number, the initial flame radius and the radiation are investigated. The results exhibit different events of flame balls as found in experimental studies under microgravity conditions, i.e. the splitting due to cellular instabilities and extinction.

Introduction

Combustion of mixtures at near extinction conditions have a wide range of applications, e.g. for the improvement of energy conversion engines or fire safety. For many reactive systems there is little knowledge about the behaviour and stability of very lean flames.

Microgravity (μg) conditions provide a suitable environment to study the interaction of scalar transport, chemical reaction and radiation in a reliable way, because the significance of earth-generated buoyancy is excluded. Many μg-experiments are being carried out to investigate the extinction and flammability limits of premixed lean gas mixtures at small Lewis numbers, e.g. in the space shuttle [7]. These studies show different scenarios: local extinction, cellular instabilities, and stationary flame structures, i.e. flame balls.

The aim of the present study is the investigation of the instationary behaviour of flame balls in three space dimensions by means of direct numerical simulation of the governing partial differential equations. The code was implemented and optimized on a massively parallel computer (IBM RS/6000 SP with 256 processors, Rechenzentrum Karlsruhe) so that large scale problems using high resolutions can be solved. Particular interest is dedicted to the influence of the initial radius and the radiative heat loss on the evolution of spherical freely propagating flame structures.

Numerical Method

As governing model we employ the thermo-diffusive equations in their dimensionless form with single-step Arrhenius kinetics and a Stefan–Boltzmann type radiation term

$$\partial_t T - \nabla^2 T = \omega - s \,, \tag{1}$$

$$\partial_t Y - \frac{1}{Le}\nabla^2 Y = -\omega \,, \tag{2}$$

$$\omega = \frac{\beta^2}{2\,Le} Y \exp\left(\frac{\beta(T-1)}{1+\alpha(T-1)}\right) \,, \tag{3}$$

$$s = c\,\frac{\bar{T}^4 - \bar{T}_u^4}{(\bar{T}_b - \bar{T}_u)^4} \,, \tag{4}$$

where $T = (\bar{T} - \bar{T}_u)/(\bar{T}_b - \bar{T}_u)$ denotes the dimensionless reduced temperature and $Y = \bar{Y}/\bar{Y}_u$ the nondimensionalized species concentration. The overbar specifies dimensional quantities, the indices u and b refer to the unburnt and burnt state, respectively, without heat loss. The space and time dimensions are nondimensionalized with the flame thickness and the flame velocity. Further parameters are the Lewis number Le, the Zeldovich number β, the temperature ratio $\alpha = (\bar{T}_b - \bar{T}_u)/\bar{T}_b$, and a radiation constant c, depending on the Stefan–Boltzmann constant and the Planck length. The above model equations exclude convection and assume the density and other thermodynamic properties of the gas to be constant. This is justified as discussed in [6]. The involved physical mechanisms are shown in fig. 1, schematically.

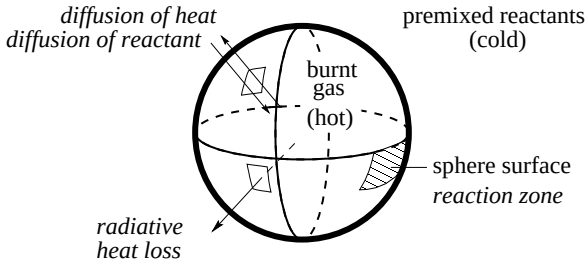

Figure 1: Schematic view of a three-dimensional flame ball

The employed values of the parameters and the initial conditions are given below.

For the numerical solution of the system (1)–(4) we first discretize the equations in time using exact time integration of the linear terms and a second order Adams–Bashforth extrapolation for the non-linear terms. The spatial discretization is done by a classical Fourier-pseudospectral approach [5]. The equations are transformed into Fourier space using a parallel version of the Temperton Fast Fourier Transform (FFT). The non-linear reaction and radiation terms are calculated by collocation in physical space.

The main computational cost is caused by multidimensional FFT's between physical and coefficient space. To achieve high resolution without increasing computing time, the code was implemented on an IBM RS/6000 SP using the message passing interface (MPI) [3].

Results and Discussion

Because flame balls live far from any boundary, periodic boundary conditions can be employed. As initial condition we take the asymptotic solution of the three-dimensional flame balls proportional to $1/r$ [4] with an additional exponential smoothing for large radii to remove even the tiniest discontinuity at the boundaries. In all the following computations, the thermodynamic parameters were $\beta = 10$, $\alpha = 0.64$, $T_b = 830\,\mathrm{K}$, $T_u = 300\,\mathrm{K}$, and $Le = 0.3$, corresponding to a 6.5 % H_2–air flame. The sidelength of the computational box was $L = 80$, and the time step was $\Delta t = 5 \cdot 10^{-4}$. The presented simulations were computed on 64 processors with a spatial resolution of 256^3. This discretization was checked to be sufficient to resolve the narrow chemical reaction zone.

To study the influence of the different parameters, we carried out several simulations varying c and r_0, being the initial flame radius. The evolution of the flame ball is quantified by the integral reaction rate $R(t) = \int_V \omega \mathrm{d}V$.

Figure 2 summarizes the evolution of R for parameter sets together with typical two-dimensional cuts through the reaction rate corresponding to the indicated points in the diagram. Configuration (**a**) with $r_0 = 2, c = 0.1$ exhibits a gradual splitting of the flame into more and more cells (cf. Fig. 2**A**). The evolution of a flame kernel with radius $r_0 = 4$, which is not shown here, also starts with separating into cells, but later the flame is extinguished because of increasing heat loss with growing radius. Larger initial radii, e.g. $r_0 = 6$ in case (**b**), lead to direct extinction without splitting of the flame due to dominating radiation effects (Fig. 2**B**).

A weaker radiation of $c = 0.05$ in (**c**) causes less cooling of the flame ball centre. In this case, even for the large initial radius of $r_0 = 5$, the flame front shows local quenching and instabilities, but at $t = 5$ the front is more wrinkled and not yet separated into isolated cells (Fig. 2**C**). Later, at $t = 10$ (Fig. 2**C'**) the flame ball with $c = 0.05$ has divided up into more cells than in the simulations with $c = 0.1$. Increasing the radiation (**d**) results in a fast cooling of the flame core even for small radii of e.g. $r_0 = 2$ and thus

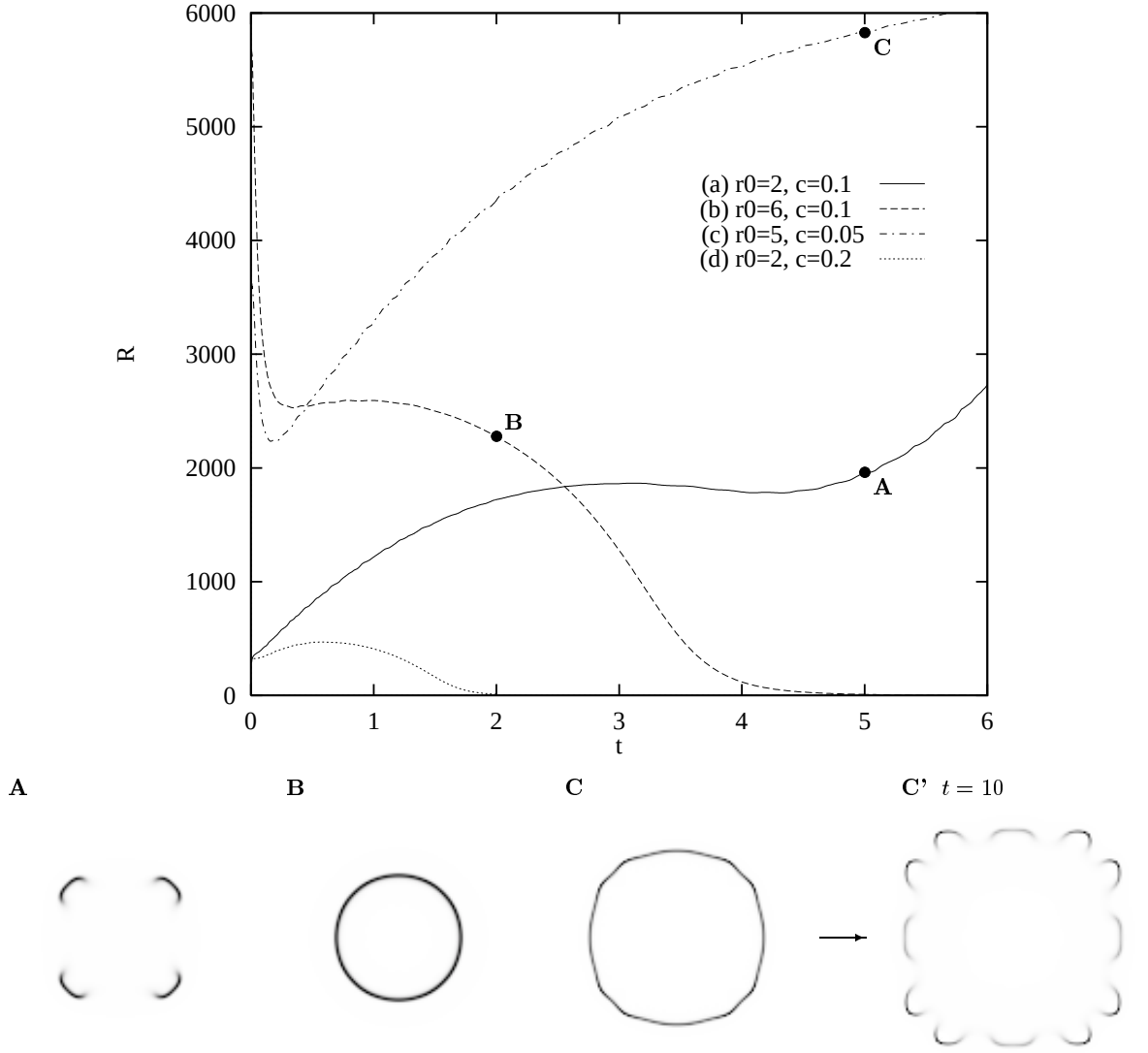

Figure 2: LEFT: Evolution of the integral reaction rate R for different simulations (**a**),(**b**),(**c**), and (**d**); RIGHT: Zoom of horizontal cuts of the reaction rate at the points **A**, **B**, **C** and at a later time, respectively.

the flame ball with $c = 0.2$ shows extinction at early times. Hence, the volumetric heat loss impact implies that systems with high radiation can only exist for small diameters. This qualitatively agrees with the experiments where the influence of radiation can be studied e.g. by adding CF_3Br to the fuel mixture [7] and with the asymptotic analysis of [4].

The patterns created during the splitting are generic with the orientation depending on the perturbation of the flame, which, for example, can be introduced by local stretching of the initial condition. Additionally, the spatial discretization also introduces a slight perturbation, which naturally determines the pattern's orientation in the absence of other disturbances, i.e. for the spherical case.

As an example for an initially stretched flame, we used a rotated ellipsoid with axis' ratios of $r_A : r_B : r_C = 1 : 1 : 2$. The radiation constant was $c = 0.1$. The evolution of the temperature isosurface ($T = 0.5$) and the reaction rate isosurface ($\omega = 1$) are depicted in Fig. 3 at times 0, 5, and 10. To illustrate the orientation of the ellipsoid, the planes perpendicular to the axes of the initial ellipsoid are superimposed, transparently.

Analogous to two-dimensional simulations [2], the structure first breaks up in the directions with the highest perturbation so that it devides into two cells along the longer axis (see Fig. 3, centre). The two cells then degenerate to spherical structures without preferred direction. Hence, we obtain a subsequent splitting into a more complex pattern, now influenced by the spatial discretization. This can be assessed by comparing with an analogous computation with a non–rotated ellipsoid. Comparing the evolution of the total reaction rates for both cases proves that the physical perturbation triggers the splitting until

the separation into two cells has finished [1].

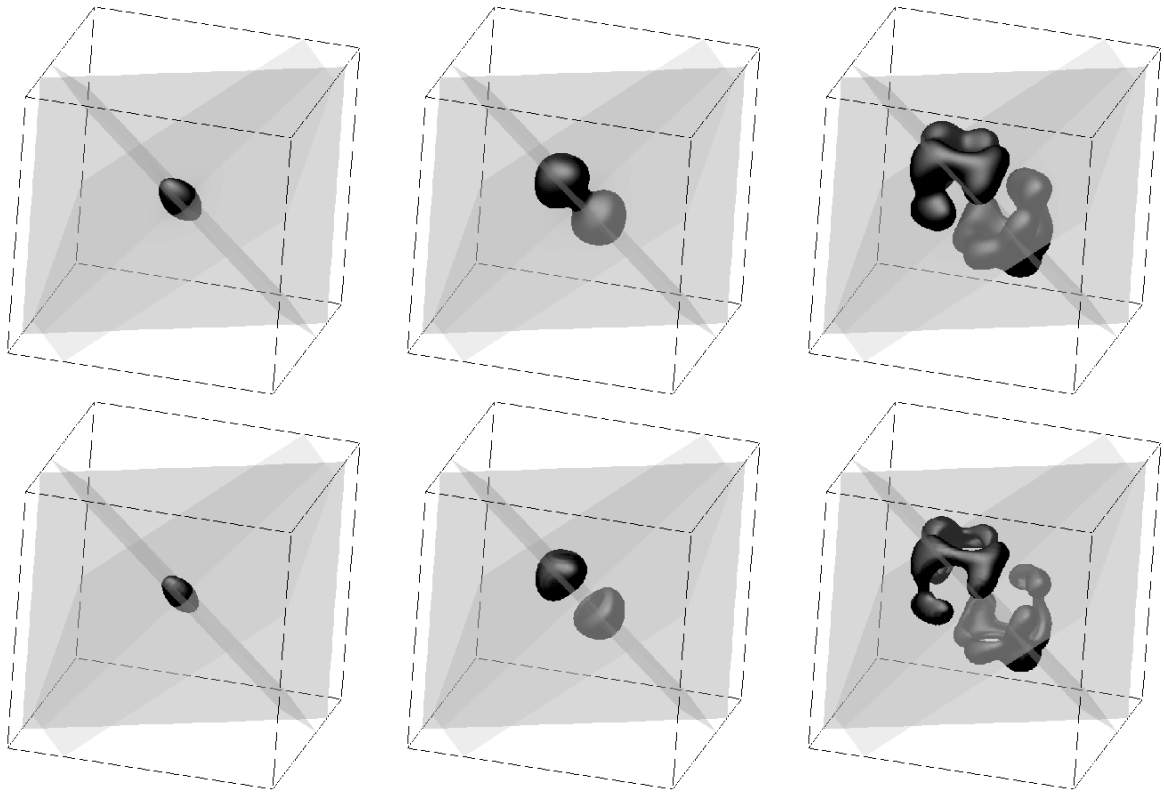

Figure 3: Flame structure with $Le = 0.3$, $c = 0.1$ and rotated elliptic initial condition with $r_A = 1.5$, $r_B = 1.5$, $r_C = 3.0$. The pictures show the isosurfaces of the zoomed fields with box length 40 of the temperature at $T = 0.5$ (top) and the reaction rate at $\omega = 1$ (bottom) for $t = 0$, 5, and 10.

References

[1] Bockhorn H., Fröhlich J., Gerlinger W., Schneider K. (1998) Numerical investigations on the stability of flame balls. ECCOMAS98, John Wiley & Sons, 990.

[2] Bockhorn H., Fröhlich J., Schneider K. (1999) An adaptive two–dimensional wavelet–vaguelette algorithm for the computation of flame balls. *Combustion, Theory and Modelling* **3**, 177.

[3] Bockhorn H., Fröhlich J., Gerlinger W., Schneider K. (1999) Direct numerical simulation of flame balls. *International Workshop SCCE II*, Springer, to appear.

[4] Buckmaster J. (1993) The structure and stability of laminar flames. *Annu. Rev. Fluid Mech.*, **25**, 21.

[5] Canuto C., Hussaini M.Y., Quaternioni A., Zang T.A. (1988) *Spectral Methods in Fluid Dynamics*, Springer, Berlin.

[6] Kagan L., Sivashinski G. (1997) Self-fragmentation of nonadiabatic cellular flames. *Combust. Flame*, **108**, 220.

[7] Ronney P.D., Wu M.-S., Pearlman H.G., Weiland K.J. (1998) Experimental study of flame balls in space: Preliminary results from STS-83. *AIAA Journal*, **36**, No. 8, 1361.