# Simulation and Analysis of Accelerating Flames in Tubes

## C. Regis L. Bauwens, Luc Bauwens & Ida Wierzba

University of Calgary, Calgary, Alberta, Canada

Corresponding author: Regis Bauwens (rbauwens@telus.net)

## Introduction

Flame acceleration in tubes is of concern because of the risk of deflagration-to-detonation transition. When a flammable mixture is ignited at the closed end of a tube open at its other end, the flame has been observed to oscillate as it propagates along the tube (Guenoche 1964, Jones & Thomas 1991, Kerampran et al. 2000). These oscillations are due to an interaction between tube acoustics set in motion by the expansion due to ignition at the closed end, and Rayleigh-Taylor instability associated with the periodic acoustic acceleration of the density interface (Kerampran et al. 2001). However, even the one-dimensional acoustic problem is not trivial, because of the presence of the moving density and temperature interface. An analysis of that problem is presented and the surprisingly chaotic results are compared with numerical simulation, which yields similar results.

### Acoustic Theory

The problem is described by the inviscid nonconducting Euler equations. The reaction front is moving at a fixed propagation speed in relation to the unburnt mixture, and the heat release per unit mass of mixture is taken to be constant.

To resolve acoustics, a small Mach number model is required in which space and time are scaled in a ratio of the order of the speed of sound. On such a time scale, the motion of the front is slow, calling for a multiple time scale analysis, with two time scales that differ by a factor of the order of the Mach number. Length is scaled by the tube length, and the slow time  $\tau$ , by the length divided by the front burning velocity into the unburnt mixture. As to the fast time  $\theta$ , initially, it is enough to assume  $\theta = O(\tau)/M$ , in which M is the Mach number based upon the burning velocity and the speed of sound in cold mixture.

This yields a leading order approximation described by the linear acoustics equations, in which the location of the front is in effect frozen. The dispersion relation in a duct with a temperature jump is (Rott 1969):

$$\cos\omega(1-X)\cos\omega X/\sqrt{\alpha} = \sqrt{\alpha}\sin\omega(1-X)\sin\omega X/\sqrt{\alpha} \tag{1}$$

in which  $X(\tau)$  is the location of the front in a tube with unit length and  $\alpha$  is the expansion ratio across the front, hence also the temperature ratio, due to heat release. Finally,  $\omega(\tau)$  is the frequency that is sought for. The evolution of the resonant modes, as X evolves from 0 to 1, is shown on Fig. 1. Somewhat similar results were obtained by Clavin et al. (1990), but for a front moving from open to closed end. In both cases, one readily can check that the various curves exhibit inflection points precisely when the front crosses a velocity node. At these points, the slope also vanishes, so that the mode in question briefly stops growing, which is consistent with the Rayleigh criterion (Kerampran et al. 2001). A complete solution requires the evolution of the amplitudes to be determined as the front moves. Technically, this requires examining the second order correction to the full nonlinear problem. The second order problem has the same linear kernel as the first order acoustic problem, but it includes forcing that depends upon the first order acoustic solution. The forcing includes contributions proportional to the leading order solution and also quadratic terms. The former are secular, and they would lead to amplitudes growing linearly on the fast time scale, which is not acceptable. Setting the amplitude of the secular solution to zero (taking into account forcing due to not only the forcing terms but also at boundaries and at the front) yields a condition that determines the evolution of the amplitudes of the leading order solution. However, first, this requires the fast time to be defined as follows:

$$\theta = \frac{1}{M} \int_0^\tau \omega(s) ds \tag{2}$$

After lengthy algebra, this procedure yields the following condition for each mode (on the unburnt side)

$$\frac{d(\omega^{1/2}U_R)}{dX} = 2\omega X(\alpha - 1) \frac{\tan \omega (1 - X)[\alpha \tan^2 \omega (1 - X) + 1]}{[\alpha \tan^2 \omega (1 - X) + \alpha - X(\alpha - 1)]^2}$$
(3)

in which  $X = \alpha \tau$  and  $U_R(\tau)$  is the amplitude of mode  $\omega(\tau)$  on the burnt side.

Finally, the initial values of the amplitudes  $U_R(0)$  are determined assuming an impulsive start. Initially, until the first acoustic wave reflects at the open end, the front moves away from the open end at a speed  $\alpha$  times the burning velocity. Burnt fluid between the closed end and the front is at rest. Between the front and the acoustic discontinuity traveling rapidly toward the open end, the speed of the unburnt fluid is  $\alpha - 1$  times the burning velocity. Fitting this initial condition to the series solution determines the initial amplitudes. The complete solution, respectively for velocity and pressure, in the unburnt and burnt regions, is then readily constructed.

#### Numerical Simulation

A one-dimensional numerical simulation is performed, based upon the inviscid non-conducting Euler equations, in an ENO-based implementation adapted from a code originally developed by Xu et al. 1997. As in the analysis, the flame is represented as a front propagating at constant speed into the unburnt mixture, accompanied by energy release. Because of the order of magnitude difference between the speed of sound and the speed of the front, a subgrid model is implemented within the computational cell where the front lies. Indeed, in order to properly capture acoustics, an acoustic CFL condition has to be satisfied; in effect the time steps have to be small enough to track acoustics on the spatial grid. But over such a small time step, the motion of the front is smaller in a ratio of the Mach number. Thus the precise location of the front within the cell needs to be tracked. This is dealt with by adding an extra artificial spatial cell on each side of the front, such that the ENO algorithm can handle each partial domain up to the last physical grid point. A second order accurate linear extrapolation is used to populate the arrays in the extra nodes.

#### Results

Results were obtained assuming a ratio burning velocity/speed of sound in the unburnt mixture equal to  $0.01/\sqrt{\gamma}$ ,  $\gamma = 1.4$ , and an expansion ratio  $\alpha = 9$ . Under these conditions, the steady component of the front motion moves at a Mach number of approximately 0.08.

Figure 1 shows the evolution of the lowest resonant modes as a function of the (frozen) front location. Figures 2 and 3 show respectively the velocity at the open end and the pressure at the closed end. In these plots, the series solutions were truncated after 100 modes. Finally, Figures 4 and 5 show similar results from the numerical simulation. Qualitatively, the computational results are similar to those of Bjerketveldt et al. (2002), which were obtained using a first-order accurate random choice method. However, the current solution is higher order accurate, yielding results that are much sharper.

Comparing both sets of results, some differences are clear. The analytical results exhibit noticeable overshoots before significant sharp jumps. The jumps themselves are not as sharp as in the numerical results. Finally, as time proceeds, the differences between the overall shape becomes larger. However, the general behavior is quite similar. Any differences fall well within the approximate nature of the analysis, given that the Mach number taken to be small has an actual value of 0.08 in the case shown. In particular, the comparison does validate the very irregular nature of the results. Flow reversals are predicted even in this simple one-dimensional model, which does not include the destabilizing effect of the acceleration due to acoustics on the flame front. That Rayleigh-Taylor instability has dramatic effects on the front, as shown in experiments (Kerampran et al. 2000, 2001).

## Conclusions

A one-dimensional acoustic theory has been developed, yielding results as close to exact numerical ones as one can reasonably expect from the approximate nature of the low Mach number model. Results show velocity and pressure profiles that are very irregular, not unlike experimental measurements (Kerampran et al. 2000, 2001).

## References

Bjerketveldt, D., Vaagsaether, K., Kristoffersen, K. & Mjaavatten, A., J. Phys. IV France 12 247-251, 2002.
Clavin, P., Pelcé, P., & He, L.T., J. Fluid Mech. 216: 299-322, 1990.
Guénoche, H., in Nonsteady flame propagation, Markstein, Ed., Pergamon Press, 1964.
Jones , S.A.S. & Thomas, G.O., Combust. Flame 87: 21-32, 1991.
Kerampran, S., Desbordes, D. & Veyssière, B., Combust. Sci. Technology, 2000.
Kerampran, Desbordes, Veyssière, Bauwens, Khimicheskaya Fizika 20: 8-16, 2001.

Rott N., ZAMP, 20: 230-250, 1969.

Xu, S.J., Aslam, T. & Stewart D.S.S., Combust. Theory Modelling, 1: 113-142, 1997.



Figure 1: Evolution of the eigenmodes as the front moves along the duct



Figure 2: Open end velocity (analysis)



Figure 4: Open end velocity (simulation)



Figure 3: Closed end pressure (analysis)



Figure 5: Closed end pressure (simulation)