Standard Mathematical Model of Detonation and Physical Reality

Khasainov B., Veyssiere B.
Institut PPRIME P' (UPR 3346 CNRS), Département Fluide-Thermique-Combustion
ENSMA, 1 Avenue Clément Ader, BP 40109, 86961 Futuroscope-Chasseneuil, France

1 Introduction

In 1979 Ficket and Davis [1] have introduced "the simplest possible reaction … with the simple first-order Arrhenius form for the reaction rate":

$$da/dt=k(1-a)exp(-E/RT) \tag{1}$$

This reaction rate depends only on the reaction progress variable a, the temperature T and the pre-exponential factor k which "serves only to set the time scale". Later on this simple example coupled with Euler equations was considered as the standard detonation model in numerous works devoted to analysis of structure and stability of 1D and 2D detonations – see for example a recent review [2].

However, eq.(1) is inconsistent with experimental data on detonation cell sizes which show that the detonation cell width λ and hence the induction period are nearly inversely proportional to ambient pressure P_o: $\lambda \sim (P_o)^{-1.1}$ [3,4].

Our purpose is to show that the use of the reaction rate law (1) even with modified but constant $k=k_oP_o$ or $k=k_o\rho_o$ can be misleading in many detonation problems where propagation of transverse waves is important. Particularly, we have compared numerical solutions of 2D Euler equations coupled with (i) the reaction rate law (1) and (ii) with that taking into account the effect of local density changes:

$$da/dt=Z\rho(1-a)exp(-E/RT) \tag{2}$$

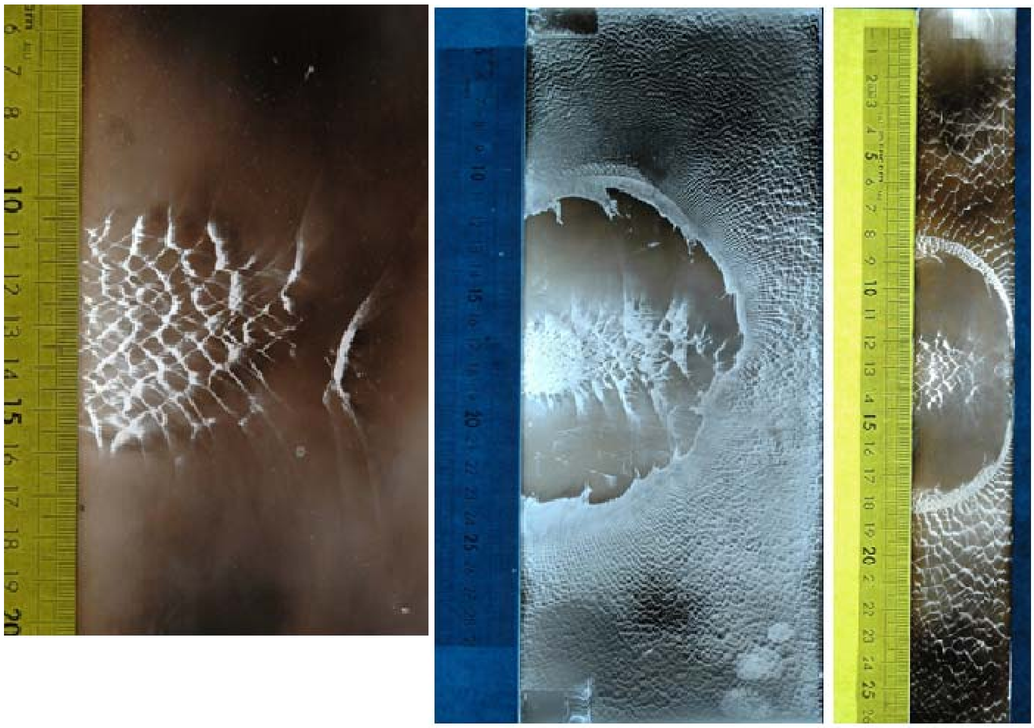
At a first glance it seems natural to neglect the effect of density in comparison with the exponential effect of temperature and to come back to eq.(1). Nevertheless the examples given below show with no ambiguity that the use of eq.(1) can give erroneous results in contrast to reaction rate law (2).

2 Problem Description

The problem considered below is the detonation diffraction from a tube to an open space, hence the critical diameter of detonation transition d_{cr} would scale with the cell size, namely $d_{cr}\approx 13\lambda$ [3,4]. Figure 1 shows typical experimental soot records [5] in the case of a) detonation extinction, b)

Correspondence to: boris.khasainov@ensma.fr

successful detonation transition to an open space and c) transition accelerated due to a presence of a disk in front of the tube exit. In cases when detonation transition occurs, the brightest feature of the flow pattern is the presence of very fine detonation cells left by "super-detonation" propagating transversally in a layer between the shock front and the decoupled front of reaction products.



a) extinction

b) transition to an open space

c) Transition accelerated by a frontal plate

Figure 1. Soot records of detonation transition in C_2H_2/O_2 stoichiometric mixture [5].

The properties of the gaseous mixture are the same as in the standard model [1], namely γ=1.2, the activation energy E=50RT_o, the reaction heat Q=50RT_o, the initial temperature and pressure T_o=293 K and P_o=1.013 bar respectively. Thus, D_{CJ}= 1940 m/s and P_{CJ}=21.8 bar. The constants k and Z in eq.(1) and eq.(2) were chosen to provide the same half-reaction zone length of about 1.5 mm: k=4.37x10^8 1/s and Z=5x10^7 m^3/(s·kg) respectively, as one can see it in Fig.2a. Figure 2b shows that in case of standard reaction (1) the temperature gradient and hence the heat release rate behind the shock front is nearly 2 times larger than with eq.(2), hence the standard reaction mechanism induces twice stiffer kinetics equation. Hence, the detonation cell width corresponding to kinetics (1) should be smaller than with eq.(2) in spite of an equality of the half-reaction zone lengths. Therefore numerical 2D simulations with eq.(2) were performed with Δx=Δr=0.15 mm (10 grid points per half-reaction zone) and with twice better resolution with the standard reaction law (1).

3 Results and Discussion

The 2D Euler equations coupled with eq.(1) or (2) were solved numerically using the FCT technique [6]. The adaptation procedure [7] along longitudinal coordinate was applied till the detonation front arrival to the end of tube. The number of longitudinal cells inside the tube was 2200, while outside the tube the grid was made of uniform cells with 7800 x 8000 grid points. Before comparing the numerical soot traces corresponding to eqs. (1) and (2) it is worth to describe the features of the flow pattern during an escape of detonation products from a tube to a space. Figure 3 shows distributions of pressure profiles during the detonation diffraction from the 4-m long tube to a space in the case of kinetics (2). Calculations were performed assuming cylindrical symmetry of the flow which seems to be a reasonable approximation – see Fig.1. Thus, below the flow pattern at negative values of radial coordinate r is just a mirror image of the calculated flow pattern at $r \geq 0$. One can see in Fig.3 that the amplitude of shock wave decreases with time and triple points practically disappear indicating that the detonation failure occurs at early stage of the diffraction process.

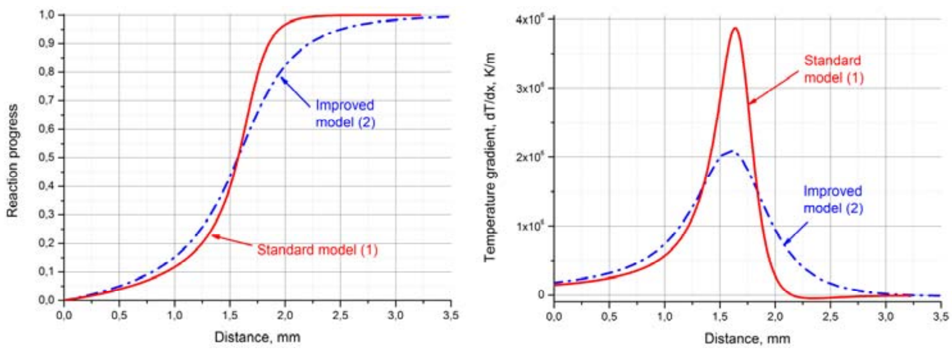


Figure 2. a) Reaction progress behind the shock front of steady detonation (left) and b) evolution of temperature gradient behind the shock front (right).

Figure 4 displays for the same instants the temperature distributions, where one can clearly see that the decoupling between the shock front and front of reaction products becomes more and more important with time and that the thickness of this zone between the smooth shock front and very irregular front of reaction products grows faster in transverse direction. Figure 5 presents for completeness the profiles of gas density and reaction progress, but for brevity only at t=2.147 ms. Thus, just behind the shock front there is a zone where both temperature and density are elevated that could create favorable conditions for transverse wave propagation. Moreover, a gas density jump in this zone amounts to a factor of 10 ($\approx \frac{\gamma+1}{\gamma-1}$) and this increase is ignored by the standard reaction model (1). However, at early stage of detonation diffraction the qualitative picture of the process is the same in both cases.

Figure 6 compares the traces of maximum pressure in the case of reaction laws (1) and (2) for the critical detonation transition cases, i.e. at tube diameters very slightly exceeding the critical detonation transition diameter d_{cr}. Their respective values are $(d_{cr})_1$=60 mm and $(d_{cr})_2$=104.1 mm with eqs. (1) and (2) respectively, and corresponding number $n_{cr} = d_{cr}/\lambda$ of detonation cells over tube diameter is 7-8 and 12-13 respectively. Worth noting that the ratios $(d_{cr})_1/(d_{cr})_2$ and $(n_{cr})_1/(n_{cr})_2$ are inversely proportional to that of the heat release rates (see Fig.2). Apparently the standard reaction law results in slightly worse quantitative agreement with the detonation transition criterion of $d_{cr} \approx 13\lambda$ than the reaction law (2). However, there is a dramatic qualitative difference between the two cases: a) an amplitude of triple points is significantly higher in the case of eq.(2) and b) no traces of super-detonation are seen in case of eq.(1) in contrast to eq.(2) which results in a flow pattern similar to that observed experimentally and displayed in Fig.1b. This critical difference between numerical solutions obtained with reaction models (1) or (2) stems from the fact that detonation transition is due to transverse waves which propagate in a *preshocked* layer behind the incident shock wave while the standard detonation model is insensitive to a local density increase, though both reaction laws are equally sensitive to the temperature.

When a disk is put in front of the tube exit at distances of about 1-2 tube diameters [5], the critical detonation diameter can be decreased by a factor of about 2 - these experimental results are reviewed in [5]. Indeed, shock reflection from the disk could facilitate an ignition of the precompressed and preheated gas behind the leading shock and give rise to a propagation of super-detonation like it is shown in Fig.7 calculated using the eq.(2) and in experimental Fig.1c. Since the standard reaction law is insensitive to the existence of local layers with elevated density, this law fails predicting the effect of frontal obstacle on the formation of transverse super-detonation and on the critical detonation transition diameter – see Fig.8. Hence, the reaction rate law (2) is consistent with experimental observations of the detonation diffraction phenomena in contrast to the solution corresponding to the standard detonation model (1).

The inconsistency of the standard detonation model is supported also by the fact that in numerical studies of the DDT [8] this team has switched in 1999 to the reaction law (2) but with no explications.

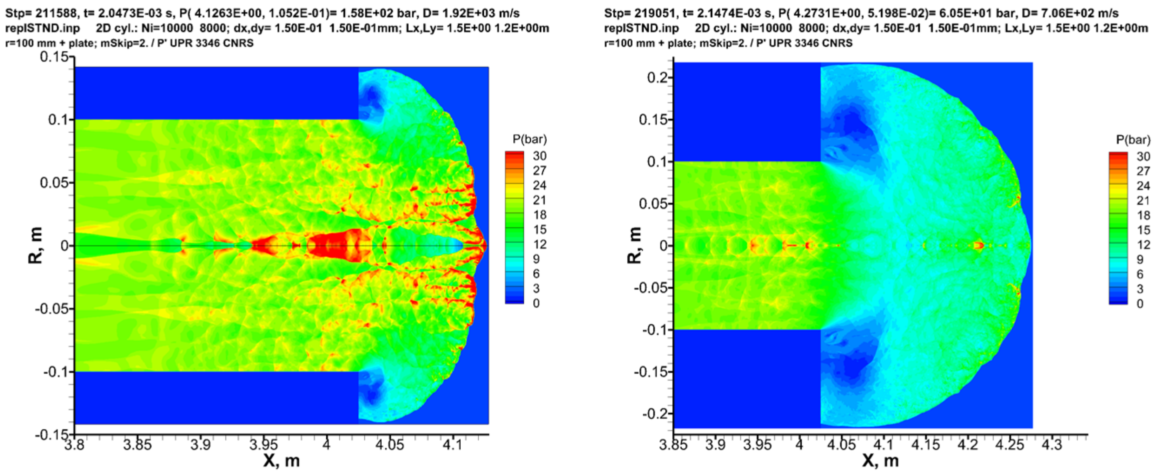


Figure 3. Pressure distributions at t=2.047 (left) and 2.147 ms (right).

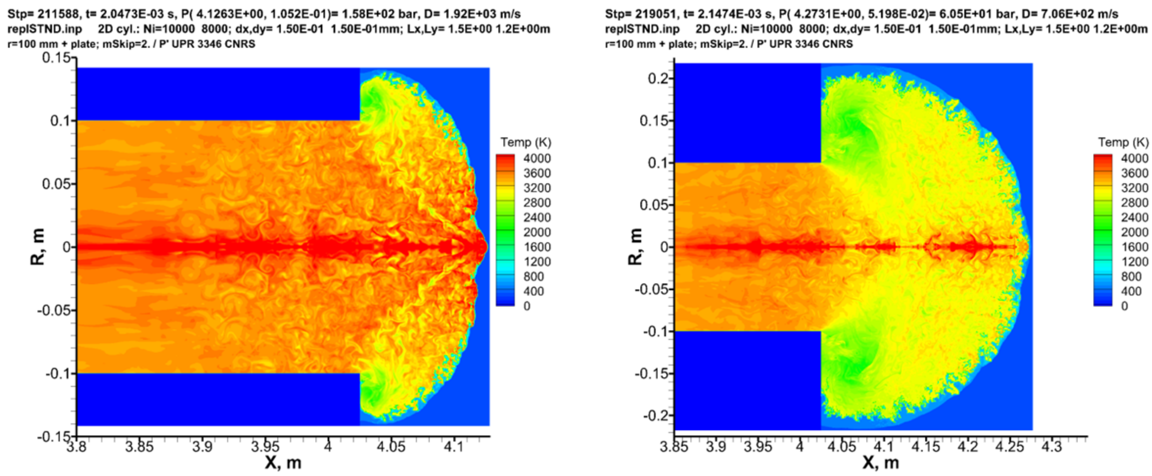


Figure 4. Temperature distributions at t=2.047 (left) and 2.147 ms (right).

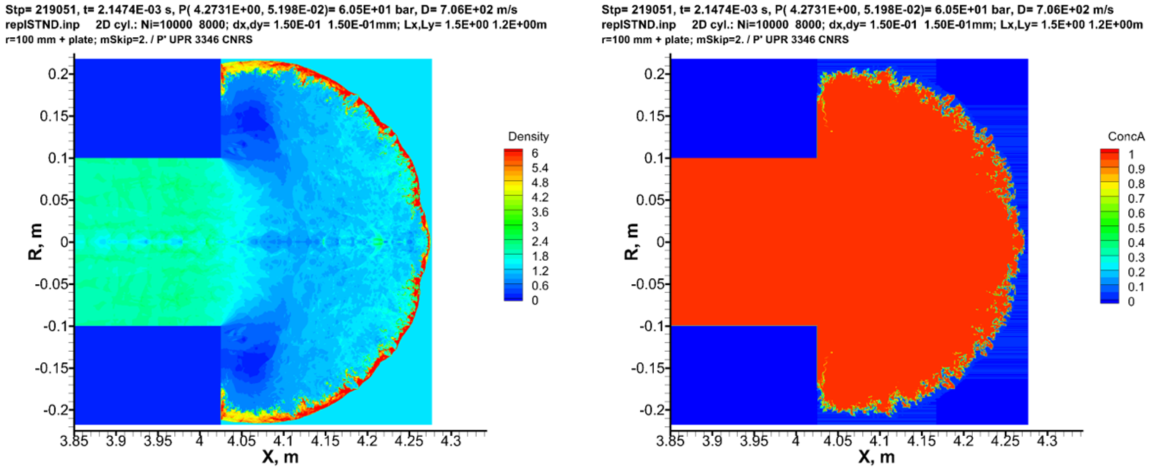


Figure 5. Density (left, kg/m^3) and reaction progress (right) distributions at t=2.147 ms.

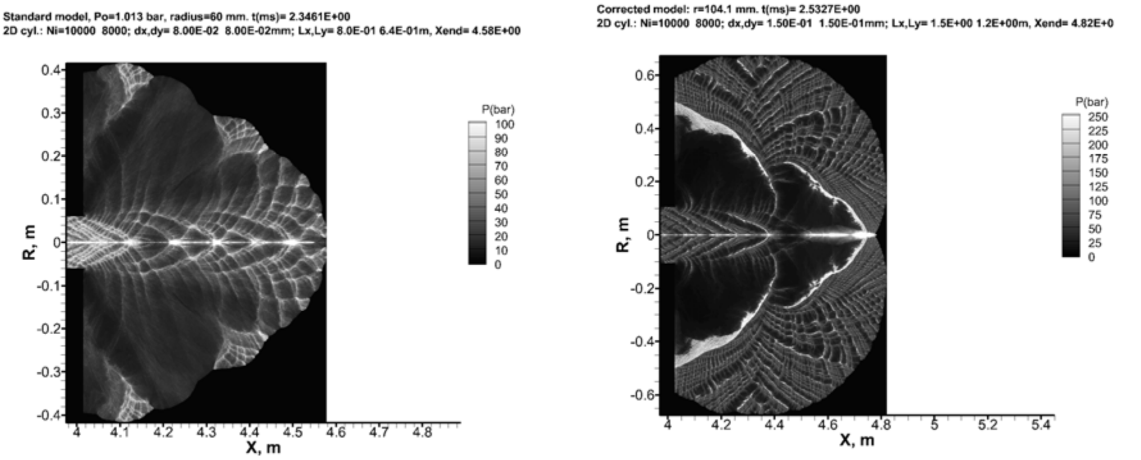


Figure 6. Detonation transition history to an open space in the case of eq.(1) (left) and eq.(2) – right.

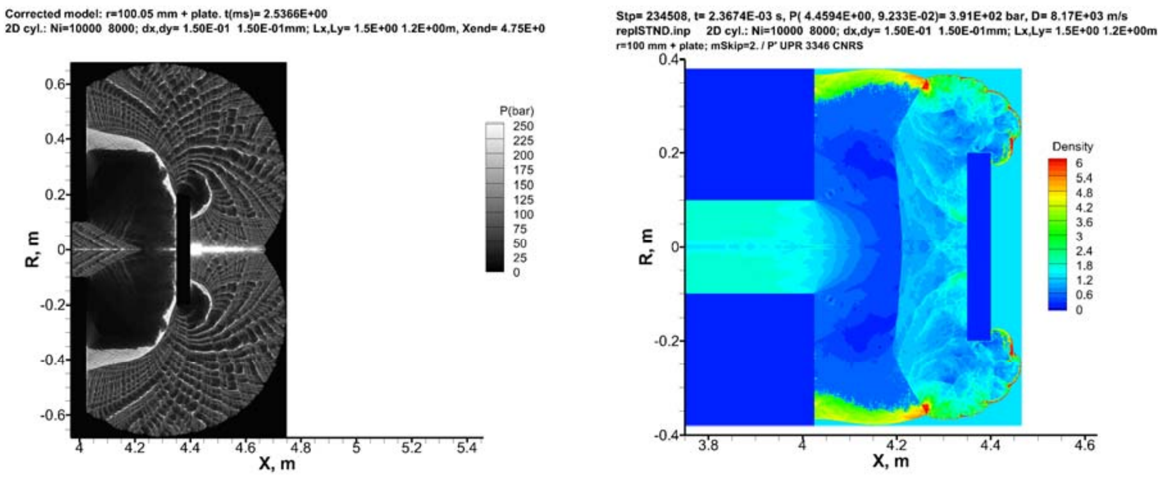


Figure 7. Left: detonation transition history in presence of frontal obstacle. Right: pressure profiles in presence of frontal plate. Both cases correspond to reaction law (2).

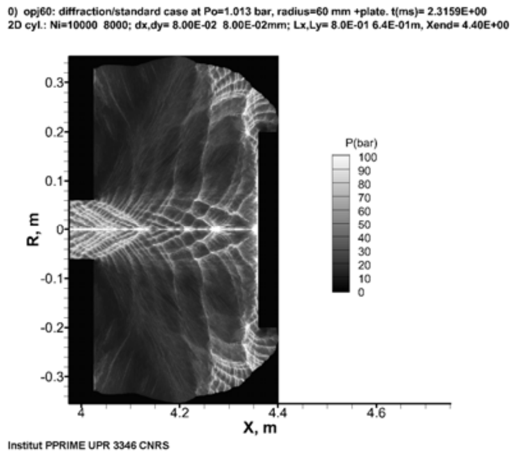


Figure 8. Transition history in presence of frontal obstacle (with standard detonation model).

4 Conclusions

Comparative analysis is performed of 2D numerical solutions of Euler equations coupled with the standard, density independent reaction rate law with that taking into account the effect of local density. It is shown that in the case of detonation diffraction from a tube to a space the predictions based on reaction rate law depending on density reasonably agree with experimental trends. On the contrary, the standard detonation model does not correspond to the physical reality since it implicitly impedes propagation of transverse waves which is crucial in detonation problems. Thus, it is worth to be careful with the conclusions based on the standard detonation model.

References

[1] W. Fickett, W.C. Davis. Detonation. Theory and Experiment. Dover Publications, Inc. Mineola, New York, 1979, p.45.

[2] Hoi Dick Ng and Fan Zhang. Detonation instability. In: Shock Wave Science and Technology Reference Library, Vol. 6. Detonation Dynamics. Springer-Verlag. Berlin Heidelberg. 2012

[3] John H.S. Lee. The detonation phenomenon. Cambridge University Press. 2008.

[4] A.A. Vasilev. Dynamic Parameters of Detonation In: Shock Wave Science and Technology Reference Library, Vol. 6. Detonation Dynamics. Springer-Verlag Berlin Heidelberg 2012.

[5] A. Smoliska, B. Khasainov, F. Virot, D. Desbordes, H.-N.Presles, A.A. Vasil'ev, A.V. Trotsyuk, P.A. Fomin, V.A. Vasil'ev. Detonation Diffraction from Tube to Space via Frontal Obstacle. Proceedings of the ECM 2013, Vienne, 2009.

[6] E.S. Oran, J.P. Boris. Numerical Simulation of Reactive Flow, 2nd edn. Cambridge University Press, Cambridge, 2001.

[7] B. Khasainov, F. Virot, H.-N. Presles, D. Desbordes. Parametric study of double cellular detonation structure. Shock Waves. V 23, No 3, 213-220, 2013.

[8] A.M. Khohlov, E.S. Oran, G.O. Thomas. Numerical simulation of deflagration-to-detonation transition: the role of shock–flame interactions in turbulent flames Original Research. Combustion and Flame, V 117, No 1–2, 323-339, 1999.