A toy model for detonations and flames

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1 Introduction

In the late 1970's Fickett and Majda introduced qualitative models for supersonic combustion, in an attempt to produce simple equations describing reactive shocks [1, 2]. The rationale was to strip the compressible reactive Euler/Navier-Stokes equations of their non-essential difficulties, in order to gain a deeper mathematical (as well as physical) understanding of the dynamics of shock waves propagating in a reactive medium. Not surprisingly, both Fickett and Majda chose as the starting point Burgers' equation (already known to represent the generic behavior of weakly non-linear hyperbolic waves), and modified it in order to account for the energy released by a chemical reaction. A few years later, Rosales and Majda [3] showed that the Burgers-like "toy" models invented in the late 1970's were closely related to a rational asymptotic approximation, starting from the full reactive Navier-Stokes equations, of weak heat release gaseous detonations. The weak heat release limit was also exploited in the late 1970's by Matkowsky and Sivashinsky to derive reaction-diffusion models for flame propagation [4], which represents in many ways the flame counterpart of reactive Burgers models for detonations.

The models mentioned above can be viewed as canonical mathematical approximations of the reactive Navier-Stokes equations, under the weak heat release assumption, for either slow ($\mathcal{M} \ll 1$), or nearly-supersonic ($\mathcal{M} = 1 + \mathcal{O}(\epsilon)$) waves. Thus, since both approximations come from the same system of equations in the same limit (i.e. weak heat release, large activation energy), an interesting question is whether or not it is possible to produce a "uniform" asymptotic expansion which encompasses both limits. The purpose of this paper is not to pursue such asymptotic derivation, which is likely to be extremely challenging due to the very different spacial and temporal scales involved, but to introduce instead a *toy-model* with the desired properties. As shown in the next section, the toy-model —though not asymptotic— is closely tied to a weakly nonlinear asymptotic theory, and reduces to the classical reaction-diffusion equations for $\mathcal{M} \ll 1$, and to a reactive Burgers' equations for waves with $\mathcal{M} = \mathcal{O}(1)$.

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2 The toy model

In order to motivate the toy model, we begin by briefly reviewing the asymptotic theories of weak-heat release flames and detonations. Let us consider the one-dimensional Navier-Stokes equations in dimensionless form:

$$\rho_t + u\rho_x + \rho u_x = 0, \tag{1}$$

$$\rho\left(u_t + uu_x\right) + \frac{p_x}{\gamma} = \frac{4}{3}\delta \operatorname{Pr} u_{xx}, \tag{2}$$

$$\rho\left(T_t + uT_x\right) - \frac{\gamma-1}{\gamma}\left(p_t + up_x\right) = \delta T_{xx} + q\omega + \frac{4}{3}\delta \operatorname{Pr}\left(\gamma-1\right)^2 u_x^2, \tag{3}$$

$$\rho\left(\lambda_t + u\lambda_x\right) = \rho\omega + \frac{\delta}{\mathrm{Le}}(\rho\lambda_x)_x, \tag{4}$$

$$p = \rho T. \tag{5}$$

Velocities have been rescaled using the ambient sound speed c_a; density, temperature, pressure using the upstream state (ρ_a, T_a, p_a); the spatial scale x_0 was chosen to be the half-reaction length of a ZND detonation, and $\delta \sim 1/\mathrm{Re}$, where $\mathrm{Re} = \rho_a c_a x_0/\tilde{\mu}$ is an "acoustic" Reynolds number. We assume that the heat release is weak: $Q = \mathcal{O}(\epsilon^2)$, with $\epsilon \ll 1$. In our non-dimensionalization $\omega = \mathcal{O}(1)$. From now on we reuse the same symbols, but the variables ρ, u, T, p and λ represent their leading order corrections to the quiescent state ahead of the wave.

When $\mathcal{M} \ll 1$ the flow is nearly isobaric, and the temperature and species equations decouple from the rest, yielding as a leading order approximation

$$T_t = \delta T_{xx} + q\omega, \quad \lambda_t = \frac{\delta}{\mathrm{Le}}\lambda_{xx} + w. \tag{6}$$

This is a classical reaction diffusion system, and depending on the relative size of various terms, different types of traveling waves can be found.

Now the other possible approximation, which stretches the governing equations in a different way, is that of weakly nonlinear wave where compressibility becomes important. This gives

$$u_\tau + uu_\chi = qw, \quad -\lambda_\chi = w, \quad T = u + q\lambda, \tag{7}$$

where $\chi = x - t$, $\tau = \epsilon t$. Each expansion performs reasonably well in its limit of validity. Expansion (7), for example, has been shown to contain both stable and unstable detonation waves, as well as cellular structures when extended to two dimensions, and chaotic solutions [5, 6]. But clearly equation (7) does not support diffusion-dominated waves, and equation (6) does not contain the advective nonlinearity needed to create wave steepening and shock formation. In order to bridge the gap between these theories we included in previous work transport effects in the weakly nonlinear derivation [7]. Including dissipation, the leading order perturbations can then be shown to satisfy:

$$u_\tau + uu_\chi = -\frac{1}{2}T_\chi + \frac{4\delta}{3\epsilon}\operatorname{Pr} u_{\chi\chi}, \tag{8}$$

$$-T_\chi + u_\chi = q\omega + \delta T_{\chi\chi}, \tag{9}$$

$$-\lambda_\chi = \omega + \frac{\delta}{\mathrm{Le}}\lambda_{\chi\chi} \tag{10}$$

It should be clear that setting $\delta = 0$ we recover (7). Interestingly, these equations already contain both supersonic and subsonic traveling waves [8], but all traveling waves within that theory are assumed to be nearly sonic (see Figure 1a). Thus the deflagration waves observed are not the classical flames, but very fast deflagrations similar to those obtained in [9].

As we shall see next, the inability of (8–10) to model diffusion-dominated waves is closely related to the fact that in the weakly nonlinear asymptotic derivation, time derivatives transform as $\partial_t \to \epsilon\partial_\tau - \partial_\chi$, and as $\epsilon \to 0$ the time dependence drops out of the entropy and backward acoustic waves. This simplification should be avoided if we are to include waves which move at $\mathcal{M} \ll 1$, since then χ is no longer the appropriate variable and time-dependence should be retained. Undoing the acoustic transformation of (8–10), and retaining the $\epsilon\partial_\tau = \partial_t$ term in equations (9–10) gives

$$\begin{aligned} u_t + u_x + \epsilon\, u\, u_x &= -\epsilon\,\frac{1}{2}\,T_x + \frac{4\delta}{3\epsilon}\,\mathrm{Pr}\,u_{xx}, &(11)\\ T_t - u_t &= q\,\omega + \delta\,T_{xx}, &(12)\\ \lambda_t &= \omega + \frac{\delta}{\mathrm{Le}}\,\lambda_{xx}. &(13)\end{aligned}$$

This system constitutes the proposed "toy-model". We note that (11–13) is more complex than either (6) or (7), but this is necessary if it is to contain both approximations. Finally, though not "simple", these equations are still much simpler than (1–5). A rational asymptotic derivation of these equations is a current research direction being pursued by the authors.

3 Properties of the model

We now proceed to show that the proposed model indeed contains both diffusion flames and detonations. Consider first waves moving at a nearly acoustic speed. Then, in terms of $\chi = x - t$ and $\tau = \epsilon\, t$, (11–13) becomes

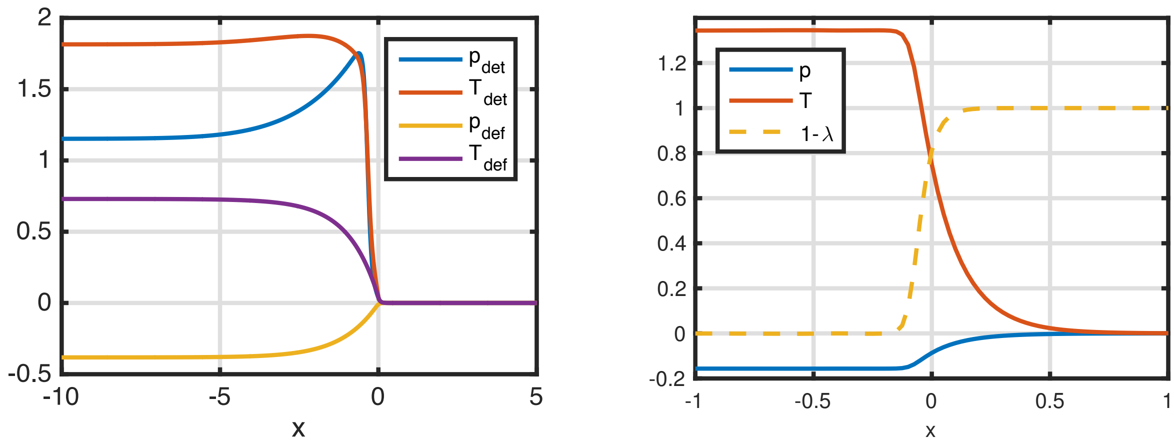
$$\begin{aligned} u_\tau + u\,u_\chi &= -\frac{1}{2}\,T_\chi + \frac{4}{3}\delta\,\mathrm{Pr}\,u_{\chi\chi}, &(14)\\ \epsilon\,T_\tau - T_\chi - \epsilon\,u_\tau + u_\chi, &= q\,\omega + \delta\,T_{\chi\chi}, &(15)\\ \epsilon\,\lambda_\tau - \lambda_\chi &= \omega + \frac{\delta}{\mathrm{Le}}\,\lambda_{\chi\chi}. &(16)\end{aligned}$$

Dropping all the terms with a small coefficient, and using (16) to integrate (15), yields (7). Next we consider a slow moving wave for (11–13). For this purpose, rescale $X = x/\sqrt{\delta}$ to obtain

$$\begin{aligned} \sqrt{\delta}\,u_t + u_X + \epsilon u\,u_X &= -\epsilon\,\frac{1}{2}\,T_X + \epsilon\,\frac{\mu}{\sqrt{\kappa}}\,u_{XX}, &(17)\\ T_t &= q\,\omega + T_{XX} + u_t, &(18)\\ \lambda_t &= \omega + \frac{1}{\mathrm{Pr}}\,\lambda_{XX}. &(19)\end{aligned}$$

Now we observe that (17) is consistent with $u = O(\epsilon)$. Using this, the leading order in (18–19) reduces to (6), thus recovering the reaction-diffusion limit of slow flames.

An important observation, regarding the scalings above, is this: For the near acoustic regime u is taken as $O(1)$ in (11–13). From the motivation of this system given earlier, starting with (8–10), this corresponds to $O(\epsilon)$ pressure perturbations in the reacting Navier-Stokes equations. On the other hand, for slow waves,



(a) Supersonic and subsonic traveling wave solutions of (8–10) with $\mathcal{M} \approx 1$. The dominant balance is between advection and reaction.

(b) Traveling wave solution of (11–13) with $\mathcal{M} \ll 1$. Diffusion plays an important role, and the pressure drops across the wave.

Figure 1: Traveling wave solutions of models (8)–(10) and (11–13) showing detonation- and flame-like structures.

the analysis above yields $O(\epsilon^2)$ pressure perturbations. This precisely matches the behavior of the Navier-Stokes equations in the weak heat release limit considered, where it can be shown that

$$p - 1 = O(\epsilon) \;\text{ for }\; \mathcal{M} \approx 1 \quad\text{and}\quad p - 1 = o(\epsilon) \;\text{ for }\; \mathcal{M} \ll 1. \tag{20}$$

The discussion above shows that (11–13) contains both the limiting cases of flames and weakly nonlinear detonations. For any finite ϵ, however, the system retains compressibility and transport terms.

Unlike the model in [5, 7], classical advection-diffusion flames are present in (11–13), as can be seen in Figure 1b. Because of the finiteness of ϵ, the temperature-pressure feedback is retained. The theory should therefore capture the interaction between flames and the acoustic field, which could be generated externally [10] or by the flame itself. For example, traveling wave solutions admitted by (6) exhibit pulsating instabilities if Le is larger than a critical value depending on the activation energy [11] and cellular instabilities if Le is below a critical value [12]; these instabilities lead to changes in flame area and therefore drive acoustic noise. The acoustic oscillations driven by an unsteady flame can affect the flame by modifying the incoming flow field [13] or mixture composition [14], or by directly interacting with the flame, causing a two-way flame-acoustic coupling [15, 16]. We are currently investigating whether (11–13) captures such coupling dynamics.

Since many of the interesting phenomena in combustion happen in two or three spatial dimensions, it is of course of interest to study the multidimensional counterpart of (11–13). Fortunately, incorporating multidimensional effects in flames and detonations is relatively straightforward in the weak heat release limit [17]. The two-dimensional equations are only slightly more complicated than (11–13), and certainly much simpler than the two-dimensional compressible Navier-Stokes equation for a reacting fluid.

4 Conclusion

We have proposed a new toy-model for combustion which includes, when restricted to the corresponding limits, both diffusion flames and weakly nonlinear detonations. The equations, although simpler than the Navier-Stokes system, still pose an interesting challenge. For a fixed set of physical parameters, exact traveling wave solutions can be found which resemble either a diffusion flame, with pressure decreasing across the wave, or a detonation. Two questions are currently being investigated: (a) can a systematic asymptotic derivation be performed yielding a system similar to (11–13), and (b) what is the behavior of the proposed toy model in the unsteady regime. We hope that numerical simulations will help elucidate the latter in order to determine whether or not the toy-model can be used to better understand flames, detonations, and their possible interactions.

References

[1] W. Fickett, "Detonation in miniature," *Am. J. Phys.*, vol. 47, no. 12, pp. 1050–1059, 1979.

[2] A. J. Majda, "A qualitative model for dynamic combustion," *SIAM J. on Appl. Math.*, vol. 41, no. 1, pp. 70–93, 1981.

[3] R. R. Rosales and A. J. Majda, "Weakly nonlinear detonation waves," *SIAM J. on Appl. Math.*, vol. 43, no. 5, pp. 1086–1118, 1983.

[4] B. J. Matkowsky and G. I. Sivashinsky, "An asymptotic derivation of two models in flame theory associated with the constant density approximation," *SIAM J. on Appl. Math.*, vol. 37, no. 3, pp. 686–699, 1979.

[5] L. M. Faria, *Qualitative and Asymptotic Theory of Detonations*. PhD thesis, King Abdullah University of Science and Technology, 2014.

[6] L. M. Faria, A. R. Kasimov, and R. R. Rosales, "Theory of weakly nonlinear self-sustained detonations," *J. Fluid Mech.*, vol. 784, pp. 163–198, 2015.

[7] L. M. Faria, A. R. Kasimov, and R. R. Rosales, "Weakly nonlinear dissipative detonations," in *25th International Colloquium on the Dynamics of Explosions and Reactive Systems (ICDERS)*, (Leeds, UK), 2015.

[8] L. M. Faria, A. R. Kasimov, and R. R. Rosales, "Dissipative effects in weakly nonlinear detonations." In preparation, 2017.

[9] A. K. Kapila, B. J. Matkowsky, and A. Van Harten, "An asymptotic theory of deflagrations and detonations i. the steady solutions," *SIAM J. on Appl. Math.*, vol. 43, no. 3, pp. 491–519, 1983.

[10] A. Van Harten, A. K. Kapila, and B. J. Matkowsky, "Acoustic coupling of flames," *SIAM J. on Appl. Math.*, vol. 44, no. 5, pp. 982–995, 1984.

[11] B. J. Matkowsky and D. O. Olagunju, "Propagation of a pulsating flame front in a gaseous combustible mixture," *SIAM J. on Appl. Math.*, vol. 39, no. 2, pp. 290–300, 1980.

[12] G. I. Sivashinsky, "Diffusional-thermal theory of cellular flames," *Combust. Sci. Technol.*, vol. 15, no. 3-4, pp. 137–145, 1977.

[13] T. J. Poinsot, A. C. Trouve, D. P. Veynante, S. M. Candel, and E. J. Esposito, "Vortex-driven acoustically coupled combustion instabilities," *J. Fluid Mech.*, vol. 177, pp. 265–292, 1987.

[14] T. Lieuwen and B. T. Zinn, "The role of equivalence ratio oscillations in driving combustion instabilities in low nox gas turbines," *Symp. (International) on Combust.*, vol. 27, no. 2, pp. 1809 – 1816, 1998.

[15] P. Clavin, P. Pelcé, and L. He, "One-dimensional vibratory instability of planar flames propagating in tubes," *J. Fluid Mech.*, vol. 216, pp. 299–322, 1990.

[16] X. Wu, M. Wang, P. Moin, and N. Peters, "Combustion instability due to the nonlinear interaction between sound and flame," *J. Fluid Mech.*, vol. 497, pp. 23–53, 2003.

[17] L. M. Faria, A. R. Kasimov, and R. R. Rosales, "Study of a model equation in detonation theory: multidimensional effects," *SIAM J. on Appl. Math.*, vol. 76, no. 3, pp. 887–909, 2016.