Weakly nonlinear dissipative detonations

Luiz M. Faria, Aslan R. Kasimov
King Abdullah University of Science and Technology
Thuwal, Saudi Arabia
Rodolfo R. Rosales
Massachusetts Institute of Technology
Cambridge, MA USA

1 Introduction

The ZND theory comprises the basis for most of our analytical understanding of detonations, describing them as supersonic combustion waves sustained by chemical reactions that the wave itself triggers. The applicability of the ZND theory, however, depends on a number of assumptions, such as one-dimensionality, steadiness of the traveling wave, and absence of dissipative effects. Several prior works have been devoted to obtaining a simplified asymptotic theory of inviscid detonations which attempt to capture their unsteady multidimensional nature (e.g. [1, 3, 6, 7]). These works represent a step beyond the ZND theory and allow for a deeper theoretical understanding of inviscid detonations. Much less attention has been paid at rationally incorporating dissipative processes in the ZND theory.

While detonations tend to be very fast, and often dissipative effects can be safely ignored, there are circumstances in which this is not the case. For detonations propagating in porous media, for instance, it has been observed that the speed of propagation can be as low as half the Chapman-Jouguet value. In detonations propagating in narrow tubes, the effect of heat/momentum losses to the walls cannot be negligible. In such cases, the theory of ideal detonations, based on the reactive Euler equations as a modeling basis, must be modified to better reflect physical reality.

In this work, we propose a multidimensional weakly nonlinear asymptotic theory of dissipative detonations, wherein a rational and systematic reduction is performed starting from the reactive compressible Navier-Stokes equations. In order to retain all dissipative effects (i.e. heat dissipation, species diffusion, and viscosity), we scale the Reynolds, Prandtl, and Lewis numbers in a way that allows to balance various nonlinearities present in the governing equations. The main ideas of weakly nonlinear detonations, where a high activation energy and weak heat release limit are considered, are similar to those presented in [6]. The further assumption of the Newtonian limit, used in [2] for an inviscid one-dimensional case, is also employed in the current work. The final result is a set of three partial differential equations which describe, in the distinguished limit considered, dissipative detonations.

2 Asymptotic model

We consider, as a starting point, the reactive compressible Navier-Stokes equations. Several modeling approximations regarding the diffusive process are employed. In particular, Fick's law is used for the

Correspondence to: aslan.kasimov@kaust.edu.sa

diffusion of species, and Fourier law is used for the heat dissipation. This, as well as assumptions on the equation of state (ideal polytropic gas) and chemical kinetics (single step irreversible Arrhenius law), significantly reduces the complexity of the governing equations. The governing equations are then given by

$$\frac{\mathrm{D}\rho}{\mathrm{D}t} + \rho\nabla\cdot\mathbf{u} = 0, \tag{1}$$

$$\rho\frac{\mathrm{D}\mathbf{u}}{\mathrm{D}t} = \nabla\cdot\left(-\left(p+\frac{2}{3}\mu\mathrm{div}\left(\mathbf{u}\right)\right)\mathbf{I} + 2\mu\mathbf{D}\right), \tag{2}$$

$$\rho\frac{\mathrm{D}T}{\mathrm{D}t} - \frac{1}{c_p}\frac{\mathrm{D}p}{\mathrm{D}t} = \frac{1}{c_p}\left(\tilde{Q}\rho\tilde{W} - \frac{2}{3}\mu\left(\nabla\cdot\mathbf{u}\right)^2 + \mu\left(\nabla\mathbf{u}:\nabla\mathbf{u}\right) + \mu\left(\nabla\mathbf{u}:\nabla\mathbf{u}^T\right) + \nabla\cdot\left(d\nabla T\right)\right) \tag{3}$$

$$\rho\frac{\mathrm{D}\Lambda}{\mathrm{D}t} = \rho\tilde{W} + \nabla\cdot(\rho d\nabla\Lambda). \tag{4}$$

with $\tilde{W} = \tilde{k}(1-\Lambda)\exp(-\tilde{E}/RT)$ and $c_p = \gamma R/\left(\gamma-1\right)$. Here $\mathrm{D}/\mathrm{D}t = \partial/\partial t + \mathbf{u}\cdot\nabla$ is the material derivative and the other symbols have their standard meaning (i.e. $\mathbf{u}$ is the velocity vector, p is the pressure, $\tilde{E}$ is the activation energy, etc.).

Here, we focus on the two-dimensional case. Consider a localized wave moving into an equilibrium, quiescent state and let ρ_a, p_a, T_a and $u_a = \sqrt{p_a/\rho_a}$ denote, respectively, the density, pressure, temperature and Newtonian sound speed in the fresh mixture ahead of the wave. We rescale the dependent variables with respect to this reference state. The independent variables are rescaled as follows:$x = \left(X - D_0 t\right)/x_0, \quad y = Y/y_0, \quad \tau = t/t_0$, where X and Y are the original spatial variables and D_0 is a typical wave speed, which is to be determined in the process of deriving the asymptotic model by requiring non-triviality of the leading-order corrections to asymptotic expansions of state variables. The length scales, x_0, y_0, and the time scale, t_0, are chosen to reflect the appropriate physics of weakly non-linear waves. We assume that $\epsilon = x_0/\left(u_a t_0\right)$ is small, which means that the spatial scale of interest in the x-direction, which is related to the size of the reaction zone, is small compared to the typical distance covered by acoustic waves in time t_0. For the transverse dimension, we assume the scaling $y_0 = x_0/\sqrt{\epsilon}$. This follows from the fact that along a weakly curved front, a distance ϵ in the normal direction corresponds to a distance $O(\sqrt{\epsilon})$ in the transverse direction.

Several dimensionless groups appear upon rescaling of the governing equations. We define the Reynolds, Prandtl, and Lewis numbers, respectively, as follows: $\mathrm{Re} = \rho_a u_a x_0/\mu, \quad \mathrm{Pr} = c_p\mu/\kappa, \quad \mathrm{Le} = \kappa/\rho_a c_p d$. Writing $\mathbf{u} = \left(U,V\right)^T$, it is convenient to introduce the differential operator $L = \partial_\tau + \frac{1}{\epsilon}(U - D_0)\partial_x + \frac{1}{\sqrt{\epsilon}}V\partial_y$. Introducing the dimensionless parameters, $Q = \tilde{Q}/RT_a, \quad E = \tilde{E}/RT_a, \quad K = t_0\tilde{k}\exp\left(-E\right)$, the non-dimensional governing equations become

$$L[\rho] + \rho\left(\frac{1}{\epsilon}U_x + \frac{1}{\sqrt{\epsilon}}V_y\right) = 0, \tag{5}$$

$$\rho L[U] + \frac{1}{\epsilon}p_x = \frac{1}{3\epsilon\mathrm{Re}}\left(U_{xx} + \sqrt{\epsilon}V_{xy}\right) + \frac{1}{\epsilon\mathrm{Re}}\left(U_{xx} + \epsilon U_{yy}\right), \tag{6}$$

$$\rho L[V] + \frac{1}{\sqrt{\epsilon}}p_y = \frac{1}{3\epsilon\mathrm{Re}}\left(\sqrt{\epsilon}U_{xy} + \epsilon V_{yy}\right) + \frac{1}{\epsilon\mathrm{Re}}\left(V_{xx} + \epsilon V_{yy}\right), \tag{7}$$

$$\begin{aligned}\rho L[T] - \frac{\gamma-1}{\gamma}L[p] = {} & \frac{\gamma-1}{\gamma}\left(Q\rho W - \frac{2}{3\epsilon\mathrm{Re}}\left(U_x + \sqrt{\epsilon}V_y\right)^2 + \frac{1}{\epsilon\mathrm{Re}}\left(U_x^2 + \epsilon U_y^2 + V_x^2 + \epsilon V_y^2\right)\right) \\ & + \frac{\gamma-1}{\gamma}\frac{1}{\epsilon\mathrm{Re}}\left(U_x^2 + \sqrt{\epsilon}U_y V_x + \sqrt{\epsilon}V_x U_y + \epsilon V_y^2\right) + \frac{1}{\epsilon\mathrm{RePr}}\left(T_{xx} + \epsilon T_{yy}\right),\end{aligned} \tag{8}$$

$$\rho L[\Lambda] = \rho W + \frac{1}{\epsilon\mathrm{RePrLe}}\left(\left(\rho\Lambda_x\right)_x + \epsilon\left(\rho\Lambda_y\right)_y\right), \tag{9}$$

where W is defined as

$$W = K(1-\Lambda)\exp\left[E\left(1-\frac{1}{T}\right)\right]. \tag{10}$$

Now we make the following assumptions regarding the size of different dimensionless terms: (a) $K = k/\epsilon$, $k = O(1)$; (b) $(\gamma-1)\,Q/\gamma = \epsilon^2 q$, $q = O\,(1)$; (c) $E = \theta/\epsilon^2$, $\theta = O\,(1)$; (d) $\gamma - 1 = \epsilon$; (e) $\mathrm{Re} = O(1/\epsilon)$; (f) $\mathrm{Pr} = O(1/\epsilon)$; (g) $\mathrm{Le} = O(1)$.

Next, we expand the dependent variables as $\rho = 1+\rho_1\epsilon+\rho_2\epsilon^{3/2}+\rho_3\epsilon^2+o(\epsilon^2)$ and similarly with other variables. Inserting the expansions in (5-8), collecting respective powers of ϵ, and applying solvability conditions at each level of the expansion, we obtain that the perturbations satisfy the following system of equations,

$$u_\tau + uu_x + v_y = \frac{-T_{3x}}{2} + \mu u_{xx}, \tag{11}$$

$$v_x = u_y, \tag{12}$$

$$\lambda_x = -k(1-\lambda)\exp(\theta T_3) - d\lambda_{xx}, \tag{13}$$

$$\kappa T_{3xx} + T_{3x} = u_x + q\lambda_x + qd\lambda_{xx}, \tag{14}$$

where

$$\mu = \frac{4}{3}\frac{1}{\epsilon\mathrm{Re}}, \quad d = \frac{1}{\epsilon^2\mathrm{RePrLe}}, \quad \kappa = \frac{1}{\epsilon^2\mathrm{RePr}}$$

represent the dissipative effects due to viscosity, species diffusion, and heat conduction, respectively. The variables u and v are corrections to the flow velocity and λ is the leading order term in the expansion of the reaction-progress variable, $\Lambda = \lambda + o\,(\epsilon)$.

Integrating equation (14) twice with respect to x, and assuming all variables and their derivatives vanish in the limit $x \to \infty$, we obtain that the temperature is given by

$$T_3 = e^{\frac{-x}{\kappa}}\int_{-\infty}^{x}\frac{1}{\kappa}e^{\frac{z}{\kappa}}\left(u + q\lambda + qd\lambda_z\right)\,dz.$$

Without any further assumptions, we arrive at the following system which describes weakly nonlinear dissipative detonations:

$$u_\tau + uu_x + v_y = \frac{-T_{3x}}{2} + \mu u_{xx}, \tag{15}$$

$$v_x = u_y, \tag{16}$$

$$\lambda_x = -k(1-\lambda)\exp(\theta T_3) - d\lambda_{xx}, \tag{17}$$

$$T_3 = e^{\frac{-x}{\kappa}}\int_{-\infty}^{x}\frac{1}{\kappa}e^{\frac{z}{\kappa}}\left(u + q\lambda + qd\lambda_x\right)\,dz. \tag{18}$$

This systems retains viscous effects, species diffusion, and heat conduction.

3 Inviscid case and small κ limit

Although much simpler than the compressible reactive Navier-Stokes equations, the asymptotic system above still poses a formidable challenge from a theoretical and numerical points of view. An obvious simplification occurs when dissipative effects are completely ignored. Then, the asymptotic equations reduce to

$$u_\tau + uu_x + v_y = \frac{-T_{3x}}{2}, \tag{19}$$

$$v_x = u_y, \tag{20}$$

$$\lambda_x = -k(1-\lambda)\exp(\theta T_3), \tag{21}$$

$$T_3 = u + q\lambda. \tag{22}$$

This system has been analyzed extensively in [3], where it is shown that (19-22), capture many features of multidimensional inviscid detonations such as a complex linear stability spectrum, cellular structures, and triple points.

Somewhat between a fully dissipative and fully non-dissipative descriptions lies the limit of small, but not negligible heat dissipation. If we assume that κ is small, then Watson's lemma can be applied to the integral expression for T_3, yielding

$$T_3 = u + q\lambda + qd\lambda_x - \kappa(u_x + q\lambda_x + qd\lambda_{xx}) + o(\kappa). \tag{23}$$

The governing equations are then given by (15-17), where T is given by equation (23).

Interestingly, the effect of dissipation on the heat distribution in the small κ limit is modeled by including spatial derivatives which modify the inviscid relation, $T_3 = u + q\lambda$. As expected, these effects would only be important in places of high gradients.

The effects of viscosity, μ, and species diffusion, d, have been studied in the past, in the context of the Majda or Rosales-Majda model ([4–6]). But since these theories lump pressure, velocity, and temperature together, heat diffusion is included in the viscous parameter, μ. The theory developed in this paper, on the other hand, allows for temperature to behave differently than other primitive variables, which is key for a correct description of reactive shocks. Because of this fact, the effect of heat dissipation is no longer lumped into μ, but has a special place in the theory.

The one-dimensional traveling wave solutions with $d = 0$ and in the limit of small κ are described by the following model,

$$u_\tau + uu_x = \frac{-T_{3x}}{2} + \mu u_{xx}, \tag{24}$$

$$\lambda_x = -k(1-\lambda)\exp(\theta T_3), \tag{25}$$

$$T_3 = u + q\lambda - \kappa(u_x + q\lambda_x). \tag{26}$$

We see that if also $\kappa = 0$, then the theory of viscous detonations developed in [3, 5, 6] applies directly. For $\kappa \neq 0$, however, understanding the nature of traveling wave solutions of (24-26) is at present a completely open question.

4 Conclusions

In this work, we propose an asymptotic model for detonations wherein dissipative effects, such viscosity, species diffusion, and heat conduction, are important. Retaining higher order derivative terms in the modeling equations (i.e. compressible reactive Navier-Stokes equations), the resulting asymptotic system is found to be quite different in its mathematical structure from that of the standard weakly nonlinear theories. Because these asymptotic equations are still too complex, a further approximation is performed in order to obtain a more tractable model. The presence of dissipation is expected to bring new and interesting effects which require further exploration. Even the theory for the traveling wave solutions of (24-26) appears to be nontrivial. Analysis of these solutions, their linear stability analysis, and numerical exploration of the reduced system is of interest and is being currently pursued.

References

[1] P. Clavin and B. Denet. Diamond patterns in the cellular front of an overdriven detonation. *Phys. Rev. Let.*, 88(4):044502, 2002.

[2] P. Clavin and F. A. Williams. Dynamics of planar gaseous detonations near Chapman-Jouguet conditions for small heat release. *Combustion Theory and Modelling*, 6(1):127–139, 2002.

[3] L. M. Faria, A. R. Kasimov, and R. R. Rosales. Theory of weakly nonlinear self-sustained detonations. *arXiv preprint arXiv:1407.8466*, 2014.

[4] J. Humpherys, G. Lyng, and K. Zumbrun. Stability of viscous detonations for Majda's model. *Physica D: Nonlinear Phenomena*, 259:63–80, 2013.

[5] A. Majda. A qualitative model for dynamic combustion. *SIAM Journal on Applied Mathematics*, 41(1):70–93, 1980.

[6] R. R. Rosales and A. J. Majda. Weakly nonlinear detonation waves. *SIAM Journal on Applied Mathematics*, 43(5):1086–1118, 1983.

[7] J. Yao and D. S. Stewart. On the dynamics of multi-dimensional detonation. *J. Fluid Mech.*, 309:225–275, 1996.