# Stability of Chain Branched Detonation Waves with Slow Initiation

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## 1 Introduction

Most fuels, and in particular hydrogen, are characterized by chain-branching kinetics. Typically, initiation is rather slow compared to chain-branching. In that situation, even if the von Neumann point lies inside the chain-branching region, a thin zone of intense reaction separates long initiation and completion regions [1]. Stability will then be affected mainly by modes with a frequency that resolves the main reaction zone. The current work presents a formulation in the slow initiation limit, in the framework of the stationary solution formulated by Bédard-Tremblay et al [1].

## 2 Formulation

The problem is described by the two-dimensional, transient Euler's equations, with chemistry described by [2, 3]

$$\frac{\partial \lambda_1}{\partial t} + \mathbf{u}\cdot\nabla\lambda_1 = -r_I - r_B, \frac{\partial \lambda_2}{\partial t} + \mathbf{u}\cdot\nabla\lambda_2 = r_I + r_B - r_T \tag{1}$$

in which

$$r_I = \lambda_1 k_I \exp\frac{-E_I}{T}, \quad r_B = \rho\lambda_1\lambda_2 k_B \exp\frac{-E_B}{T},$$
$$r_T = \lambda_2 k_T \tag{2}$$

Boundary conditions include the preshock state for $x \to -\infty$, On the right, boundary conditions are non-reflective, i.e. for $x \to \infty$, the left-going Riemann invariant is zero. The problem has been made dimensionless scaling density and temperature by their preshock ($x \to -\infty$) values, velocity by the preshock speed of sound, the heat release by the preshock speed of sound squared, and finally, pressure by $\gamma$ times the preshock pressure. Time is scaled by a value $\tau$ that resolves the main chain-branching zone, and length, by the preshock speed of sound times $\tau$. Rates have been scaled by $1/\tau$. Chemistry is taken to be negligible at the conditions corresponding to the left boundary conditions.

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The steady one-dimensional reference solution is then, using the local Mach number as the independent variable [1],

$$\sqrt{T} = \frac{M(\gamma M_0^2 + 1)}{M_0(\gamma M^2 + 1)}, \quad \rho = \frac{M_0^2(\gamma M^2 + 1)}{M^2(\gamma M_0^2 + 1)}, \quad u = \frac{M^2(\gamma M_0^2 + 1)}{M_0(\gamma M^2 + 1)}, \quad p = \frac{\gamma M_0^2 + 1}{\gamma(\gamma M^2 + 1)}, \tag{3}$$

and introducing the heat release $q$,

$$\Delta = \Delta_N - \frac{q}{Q}, \quad \Delta_N = \frac{(M_0^2 - 1)^2}{2M_0^2(\gamma^2 - 1)Q}, \quad \Delta = \Delta_N - 1 + \lambda_1 + \lambda_2 \tag{4}$$

$$M^2 = \frac{\gamma M_0^2 + 1 \pm \sqrt{2M_0^2(\gamma^2 - 1)Q\Delta}}{\gamma M_0^2 + 1 \mp \gamma\sqrt{2M_0^2(\gamma^2 - 1)Q\Delta}} \tag{5}$$

in which the lower, subsonic branch describes the post-shock detonation wave structure. Index N represents the von Neumann point. Introducing

$$\kappa = \frac{(\gamma - 1)(1 - \gamma M^2)}{1 - M^2}\frac{Q}{T_N} \tag{6}$$

$T$ and $q$ are related by

$$\frac{dT}{\kappa T_N} = \frac{dq}{Q} = -d\Delta = -d(\lambda_1 + \lambda_2) \tag{7}$$

Next, writing

$$\epsilon = \frac{k_I}{k_B}\exp\frac{E_B - E_I}{T_N} \tag{8}$$

$$a = \rho_N \exp\left(\frac{E_B}{T_B} - \frac{E_B}{T_N}\right) = \rho_N k_B \exp\frac{-E_B}{T_N}, \quad \theta = \frac{E_B}{T_N}\left(1 - \frac{T_N}{T}\right) = \frac{E_B}{T_N} - \frac{E_B}{T} \tag{9}$$

and assuming $\epsilon << 1$, in the initiation zone,

$$\lambda_2 = \frac{a\epsilon}{\rho_N(a-1)}\left[\exp\frac{(a-1)x}{u_N} - 1\right] \tag{10}$$

$$\lambda_1 = 1 + \frac{\epsilon a x}{M_0(a-1)} - \frac{\epsilon a^2}{\rho_N(a-1)^2}\left[\exp\frac{(a-1)x}{u_N} - 1\right] \tag{11}$$

$$\theta = \frac{E_B}{T_N}\frac{a\epsilon\kappa_N}{\rho_N(a-1)^2}\left[\exp\frac{(a-1)x}{u_N} - 1 - \frac{(a-1)x}{u_N}\right] \tag{12}$$

In the main chain-branching zone, using

$$x = \frac{-u_N \log\epsilon}{a-1} + \xi \tag{13}$$

one finds that if within the chain-branching region, i.e. if $a > 1$,

$$\lambda_1 = \exp\int_{\Delta_N}^{\Delta}\frac{\rho}{\rho_N}\frac{a}{k_T}\exp\theta d\Delta \tag{14}$$

$$\xi = \frac{u_N}{a-1}\log\frac{\rho_N(a-1)^2(\Delta_N - \Delta)}{a} - u_N\int_{\Delta_N}^{\Delta}\left[\frac{\rho_N}{\rho}\frac{1}{k_T\lambda_2} - \frac{1}{(a-1)(\Delta_N - \Delta)}\right]d\Delta \tag{15}$$

The formulation for the main reaction zone remains valid only as long as it yields positive values for $\Delta$ and $\lambda_2$. The latter would imply an underdriven wave. If that is not the case, however, $\lambda_2$ is found to return to zero before all the fuel is consumed, for $\Delta = \Delta^{**}$. Beyond that point, there is no longer any chain branching, and $\lambda_2$ becomes of order $\epsilon$ again, with value

$$\lambda_2 = \frac{\epsilon a \lambda_1 \exp E_I\theta/E_B}{k_T\rho_N - a\rho\lambda_1 \exp\theta} \tag{16}$$

and transition occurs at $\Delta = \Delta^{**}$, determined as the solution of

$$\Delta^{**} - \Delta_N + 1 = \lambda_1^{**} = \exp \int_{\Delta_N}^{\Delta^{**}} \frac{\rho a}{\rho_N k_T} \exp\theta d\Delta \tag{17}$$

## 3 Perturbation

Introducing perturbations, denoted for instance by $u'$ for velocity and likewise for the other variables, and, taking into account that the coefficients depend upon $\xi$ but not $t$ or $y$, thus writing the solution in Fourier space in time and in $y$, the perturbation problem can be written as

$$\begin{aligned} u\frac{d\rho'}{d\xi} = &-\left(i\omega + \frac{\gamma p}{\gamma p - \rho u^2}\frac{du}{d\xi}\right)\rho' + \left(\frac{\gamma p - 3\rho u^2}{\rho u^2}\frac{du}{d\xi} - i\omega\right)\frac{\rho^2 u u'}{\gamma p - \rho u^2} \\ &+\frac{ik\rho^2 u^2}{\gamma p - \rho u^2}v' + \frac{\rho}{\gamma p - \rho u^2}\left(i\omega + \gamma\frac{du}{d\xi}\right)p' - \frac{(\gamma-1)\rho^2 Q k_T}{\gamma p - \rho u^2}\lambda_2' \end{aligned} \tag{18}$$

$$(\gamma p - \rho u^2)\frac{du'}{d\xi} = \rho' u^2\frac{du}{d\xi} + \left(i\omega + 2\frac{du}{d\xi}\right)\rho u u' - i\gamma p k v' - \left(i\omega + \gamma\frac{du}{d\xi}\right)p' + (\gamma-1)\rho Q k_T\lambda_2' \tag{19}$$

$$\rho u\frac{dv'}{d\xi} = -i\omega\rho v' - ikp' \tag{20}$$

$$(\rho u^2 - \gamma p)\frac{dp'}{d\xi} = \rho' u\gamma p\frac{du}{d\xi} + \left[i\omega\gamma p + (\rho u^2 + \gamma p)\frac{du}{d\xi}\right]\rho u' - i\gamma\rho u p k v' - \left(i\omega + \gamma\frac{du}{d\xi}\right)\rho u p' + (\gamma-1)\rho^2 u Q k_T\lambda_2' \tag{21}$$

$$u\frac{d\lambda_1'}{d\xi} = -i\omega\lambda_1' - a\frac{\rho}{\rho_N}\lambda_1\lambda_2\left(\frac{\rho'}{\rho} + \frac{\lambda_1'}{\lambda_1} + \frac{\lambda_2'}{\lambda_2} + \theta' - \frac{u'}{u}\right)\exp\theta \tag{22}$$

$$u\frac{d\lambda_2'}{d\xi} = -i\omega\lambda_2' + a\frac{\rho}{\rho_N}\lambda_1\lambda_2\left(\frac{\rho'}{\rho} + \frac{\lambda_1'}{\lambda_1} + \frac{\lambda_2'}{\lambda_2} + \theta' - \frac{u'}{u}\right)\exp\theta - \lambda_2' k_T + \frac{u'}{u}\lambda_2 k_T \tag{23}$$

in which $\omega$ is the complex frequency, and $k$ is the (real) transverse wavelength.

Boundary conditions are obtained by setting to zero the Riemann variables coming from the ends into the solution domain, on both sides. Indeed, in the limit $\epsilon \to 0$, the lengths of both the initiation and the termination zone become infinite so that waves at the higher frequencies that resolve the reaction zone will never have time to reflect and return to the reaction zone. This avoid having to deal with refelction at the shock in the presence of shock oscillations, focusing the problem to the effect of the main reaction zone.

When $\xi \to -\infty$,

$$\lambda_2' \to C\exp\frac{(a-1)\xi}{u_N}\exp\frac{-i\omega\xi}{u_N} \tag{24}$$

thus the $\lambda_2$ perturbation becomes small, while other values do not. Chemistry becomes

$$i\omega\lambda_1' + u\frac{d\lambda_1'}{d\xi} = -a\lambda_2' \tag{25}$$

$$i\omega\lambda_2' + u\frac{d\lambda_2'}{d\xi} = (a-1)\lambda_2' \tag{26}$$

This suggests that we write all variables (such as $\lambda_2'$) as

$$\lambda_2' = \Lambda_2(\xi)\exp\frac{(a-1-i\omega)\xi}{u_N} \tag{27}$$

then, using symbols $\Lambda$ for mass fraction perturbations, $R$ for the density perturbation, $U$ and $V$ for velocity perturbations, $P$ for pressure, we have that

$$\frac{dX}{d\xi} = AX \tag{28}$$

in which

$$X = \begin{vmatrix} R \\ U \\ V \\ P \\ \Lambda_1 \\ \Lambda_2 \end{vmatrix}, A = \begin{vmatrix} a_{11} & a_{12} & a_{13} & a_{14} & 0 & a_{16} \\ a_{21} & a_{22} & a_{23} & a_{24} & 0 & a_{26} \\ 0 & 0 & a_{33} & a_{34} & 0 & 0 \\ a_{41} & a_{42} & a_{43} & a_{44} & 0 & a_{46} \\ a_{51} & a_{52} & 0 & a_{54} & a_{55} & a_{56} \\ a_{61} & a_{62} & 0 & a_{64} & a_{65} & a_{66} \end{vmatrix} \tag{29}$$

in which the various coefficients $a_{ij}$ are readily found from the equations above.

Finally, given that a numerical solution will be required, the domain is expressed as a function of $\Delta$ rather than $\xi$:

$$\frac{d}{d\xi} = \frac{d}{d\Delta}\frac{d\Delta}{d\xi} \tag{30}$$

thus

$$\frac{d}{d\xi} = -\frac{k_T\rho\lambda_2}{M_0}\frac{d}{d\Delta} \tag{31}$$

The system becomes

$$\frac{dX}{d\Delta} = -\frac{M_0}{k_T\rho(\Delta - \Delta_N + 1 - \lambda_1)}AX \tag{32}$$

which, given that integration now starts at $\Delta_N$, where $\lambda_1 = 1$, does not satisfy a Lipschitz condition. However, the matrix $A$ is singular, at $\Delta_N$, leaving one degree of freedom. Thus, one can express the solution as a combination of modes coming from the right, plus a constant. Integration is pursued until $\Delta = \Delta^{**}$.

## 4 Numerical solution

The eigenvalue problem requires a numerical solution. The procedure s then similar to that used by Lee & Stewart [4]. A fourth order accurate Runge-Kutta integration solves the system above for assumed frequency and assumed values of the amplitudes for the mode coming from the right. Then a carpet search identifies rough regions where eigensolutions lie. Finally, in the neighborhood of an eigensolution, an iterative scheme of Newton-Raphson type determines the eigenvalues. A continuation method is used to explore the effect of varying global input parameters.

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### References

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