A mathematical model for three dimensional detonation as pure gas-dynamic discontinuity

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1 Introduction

During the last decades very significant advances has been achieved in the theoretical understanding of the detonation. For its significance for our investigation, we may underline the research carried out by Scott Steward and his co-workers on the insight of the intrinsic relation of the detonation shock speed and its curvature, see e.g. [1], [2]. The studies performed by these authors has crystallized in the Detonation Shock Dynamic (DSD) theory in which the conditions of the so called *sonic locus* are derived under the assumption of weak curvature but including multi-dimensionality effects.

In our analysis, while keeping in mind the ideas contained in DSD theory, we to focus on the fact that the thickness of detonations is typically small compared to the characteristic scales of the fluid flow. Some modeling studies, e.g. [3], showed that the detonation process can be successfully reproduced if the 3D structure of detonation cells is resolved and that the details of the internal structure of the shock and the chemistry can be ignored. Thus, a simplified model for detonations can be conceived considering that the fuel consumption zone shrinks to an infinitely thin surface of discontinuity separating reactants and products. For deflagrations, such models exist since the pioneering works of Darrieus and Landau who derived the jump conditions across the flame based on this assumption. More recently, Matalon and Matkowsky [4] considered arbitrary flame shapes for nearly equi-diffusional flames with thermal expansion in general flow fields. The leading terms of the jump conditions were those of the Darrieus-Landau model and perturbative corrections were obtained in the next order of approximation. Class et al. [5] simplified the derivation of Matalon and Matkowsky explicitly exploiting the distinctiveness of length scales, and re-calculated and re-interpreted the Rankine-Hugoniot jump conditions.

In the present work, the authors apply the Class et al. [5] methodology to detonation. Modified Rankine-Hugoniot jump conditions are derived, implicitly including the full effect of the chemistry. For detonation, this implies that the results of the Zeldovich-von Newmann-Döring theory can be utilized as a leading order *planar* model to close the system [6] and obtain the final modified jump conditions which include perturbative correction terms.

2 Analysis

The reactive Euler equations are considered as the basis of the analysis,

$$\partial_t\tilde{\phi} + \nabla \cdot J(\tilde{\phi}) = \tilde{Q}(\tilde{\phi}), \quad J(\tilde{\phi}) = \begin{pmatrix} \tilde{\rho}\tilde{v} \\ \tilde{\rho}\tilde{v} \otimes \tilde{v} + \tilde{p}\overline{\overline{E}} \\ \tilde{\rho}\tilde{e}\tilde{v} + \tilde{p}\overline{\overline{E}} \cdot \tilde{v} \\ \tilde{\rho}\tilde{Y}\tilde{v} \end{pmatrix}, \; Q(\tilde{\phi}) = \begin{pmatrix} 0 \\ 0 \\ 0 \\ \tilde{\rho}\tilde{W} \end{pmatrix}. \tag{1}$$

with $\tilde{\phi}^T = (\tilde{\rho}, \tilde{\rho}\tilde{v}, \tilde{\rho}\tilde{e}, \tilde{\rho}\tilde{Y})$ and $\tilde{W}$ the Arrhenius chemical consumption rate. The system is made dimensionless with the use of the reference variables $\tilde{\rho}_s$, $\tilde{c}_s$ that represents the conditions at the Von Neumann peak and $\tilde{l}_f$ which is the characteristic scale of the flow motion. We assume a large ratio Z of the hydrodynamic typical length to the half detonation thickness $Z = \tilde{l}_f/\tilde{l}_c$. A thin detonation structure corresponds to an intense source term Q which is re-scaled accordingly $Q = Z/Z \cdot Q = ZQ'$. Additionally, it is convenient to transform the equations to a moving generalized curvilinear coordinate system which was already utilized in [5]. The coordinate system is attached to the discontinuity surface with its normal direction pointing towards the products and perpendicular to the surface of the flame. Its tangential direction moves with the local tangential flow. In this system, the flame is at rest with no flow along the flame surface. In the curvilinear coordinates, the system of differential equations is

$$\partial_t\left(\sqrt{g}\phi\right) + \partial_{x^j}\left(\sqrt{g}J^j(\phi)\right) = \sqrt{g}ZQ'(\phi) \tag{2}$$

with g^{ij} the contra-variant metric tensor. The flux vectors, $J^j(\phi) = (v^j - u^j)\phi$ with u^j representing the speed of the moving coordinates relative to fixed Eulerian coordinate, become according to [5],

$$J^j \begin{pmatrix} \rho \\ \rho v^i l_i \\ \rho e \\ \rho\lambda \end{pmatrix} = \begin{pmatrix} m^j \\ \left(m^j v^i + p/\gamma \cdot g^{ij}\right) l_i \\ m^j e + p/\gamma \cdot g^{ij} \cdot m^i/\rho \\ m^j\lambda \end{pmatrix}, \tag{3}$$

with mass flux $m^j = (v^j - u^j)\rho$. Decomposing the Eq. (2) in the normal and tangential directions and introducing the stretched normal spatial variable, $X = Zx^1$, Eq. (2) yields,

$$Z^{-1}\left[\partial_t\left(\sqrt{g}\phi\right) + \partial_{x^\alpha}\left(\sqrt{g}J^\alpha(\phi)\right)\right] + \partial_X\left(\sqrt{g}J^1(\phi)\right) = \sqrt{g}Q'(\phi). \tag{4}$$

Since Z, the ratio between the length of the fluid flow and the consumption zone thickness, is assumed to be asymptotically large, the variables can be expressed in terms of an asymptotic series expansion in powers of $1/Z$, i.e. $\phi \approx \sum_{n=0} Z^{-n}\phi_{(n)} \approx \phi_{(0)} + Z^{-1}\phi_{(1)} + O(Z^{-1})$. The volume element is Taylor expanded around the discontinuity $\sqrt{g} = \sqrt{g}_{(0)} + \sqrt{g}_{(1)}Z^{-1}X + o(X^2)$. Additionally, we make use of the equalities $\sqrt{g}_{(1)} = -2H$ and $\chi = \partial_t(\sqrt{g}_{(0)})/\sqrt{g}_{(0)}$ with mean curvature H and stretch χ. Substituting in Eq. (4) and collecting coefficients of zeroth, Z^0, and first order Z^{-1} terms,

$$\partial_X\left(J^1_{(0)}(\phi)\right) = Q'_{(0)}(\phi), \tag{5}$$

$$\left(\partial_t + \chi\right)\phi_{(0)} + \left(g_{(0)}\right)^{\frac{-1}{2}}\partial_{x^\alpha}\left(\sqrt{g}_{(0)}J^\alpha_{(0)}(\phi)\right) + \partial_X\left(J^1_{(1)} - 2HXJ^1_{(0)}(\phi)\right) = Q'_{(1)}(\phi) - 2HXQ'_{(0)}(\phi). \tag{6}$$

And analogously, the normal fluxes are

$$J^1_{(0)} \begin{pmatrix} \rho \\ \rho v^i l_i \\ \rho e \\ \rho\lambda \end{pmatrix} = \begin{pmatrix} m^1_{(0)} \\ m^1_{(0)}\left(v^1_{(0)}l_{1(0)} + v^\alpha_{(0)}l_{\alpha(0)}\right) + p_{(0)}/\gamma \cdot l_{1(0)} \\ m^1_{(0)}e_{(0)} + p_{(0)}/\gamma \cdot g^{i1}_{(0)} \cdot m^i_{(0)}/\rho_{(0)} \\ m^1_{(0)}\lambda_{(0)} \end{pmatrix}. \tag{7}$$

$$J^1_{(1)}\begin{pmatrix}\rho\\ \rho v^i l_i\\ \rho e\\ \rho\lambda\end{pmatrix}=\begin{pmatrix} m^1_{(1)}\\ \left(m^1_{(0)}v^i_{(1)}+m^1_{(1)}v^i_{(0)}+p_{(1)}/\gamma\cdot g^{i1}_{(0)}\right)l_{i(0)}\\ m^1_{(1)}e_{(0)}+m^1_{(0)}e_{(1)}+p_{(1)}/\gamma\cdot\left(m^i_{(0)}/\rho_{(0)}\right)+p_{(0)}/\gamma\cdot\left(m^i/\rho\right)_{(1)}\\ m^1_{(1)}\lambda_{(0)}+m^1_{(0)}\lambda_{(1)}\end{pmatrix} \tag{8}$$

The Eq. (5) combined with (7) and $Q_{(0)}=\rho_{(0)}k(1-\lambda_{(0)})e^{\left(-\theta_a/\left(p_{(0)}\Upsilon_{(0)}\right)\right)}$ in $Q\approx Q_{(0)}+Q_{(1)}Z^{-1}$ constitute an equation system for *planar* detonations. This system is equal to the known equations utilized to derive the classical results of the ZND theory of detonation, see [7]. The ZND theory provides an analytic expression for the pressure p, velocity v and specific volume Υ profiles [7] as a function of the reaction progress variable λ,

$$p=a+(1-a)(1-b\beta\lambda)^{\frac{1}{2}},\ v=(1-p)(\gamma M_S)^{-1}+M_s,\ \Upsilon=v/M_s, \tag{9}$$

where the auxiliary variables appearing in Eq.(9) are, $D=\tilde{D}/\tilde{c}_s$, $S=2\gamma D^2-(\gamma-1)$, $M_s=((\gamma-1)D^2+2)/S$, $\beta=\tilde{Q}\gamma/\tilde{c}_s^2$, $a=(\gamma D^2+1)/S$, $b=M_s^2 2\gamma(\gamma-1)/((1-a^2)(\gamma+1))$. Significantly, the equations (9) allow expressing the half reaction zone length as, $\tilde{l_c}=\tilde{c}_s k^{-1}\int_0^{1/2}v(\lambda)(1-\lambda)^{-1}e^{\theta_a/(p(\lambda)\Upsilon(\lambda))}d\lambda$ and allow for conversion to the spatial formulation, $dx/d\lambda=v(\lambda)/W(\chi)$.

A detonation can be considered as a thin layer separating the fresh mixtures of the burned products. We propose the derivation of a three dimensional *hydrodynamic* model in which the internal structure of the detonation as well as the chemical reaction is substituted by modified jump conditions. Conceptually, this construction asymptotically extends the *simplest* planar stationary theory to three-dimensional non-stationary flow. In the derivation we consider two models for the detonation simultaneously, the *hydrodynamic* and the *reactive* model, see Figure 1. Two sets of equations are handled simultaneously. From equations (5) and (6),

$$\partial_X\left(J^1_{(0)}\begin{pmatrix}\phi\\ \Phi\end{pmatrix}\right)=\begin{pmatrix}0\\ Q'_{(0)}(\Phi)\end{pmatrix}, \tag{10}$$

$$\begin{aligned}\partial_X\left(J^1_{(1)}\begin{pmatrix}\phi\\ \Phi\end{pmatrix}\right)&=\begin{pmatrix}0\\ Q'_{(1)}(\Phi)-2HXQ'_{(0)}(\Phi)\end{pmatrix}+2HJ^1_{(0)}\begin{pmatrix}\phi\\ \Phi\end{pmatrix}-\\ &-(\partial_t+\chi)\begin{pmatrix}\phi_{(0)}\\ \Phi_{(0)}\end{pmatrix}-(g_0)^{-1/2}\,\partial_{x^\alpha}\left(\sqrt{g}_{(0)}J^\alpha_{(0)}\begin{pmatrix}\phi_{(0)}\\ \Phi_{(0)}\end{pmatrix}\right),\end{aligned} \tag{11}$$

where capital letters designate the *reactive* and lower-case the *hydrodynamic* model. Away from the consumption area, these models are identical (initial, rarefaction and final states). The models exclusively differ in a thin zone surrounding the shock, i.e. between the *hydrodynamic* discontinuity and the Chapman-Jouguet point, see detailed picture. The jump conditions of the *hydrodynamic* model, particularly the position and the amplitude of the discontinuity, are determined from the internal structure of the detonation (*reactive* model). In the area of appreciable chemical reaction the *hydrodynamic* model is an extrapolation of the rarefaction wave. For simplicity, we set the origin of coordinates in the discontinuity of the *hydrodynamic* model. We perform now several manipulations with equations (10) and (11) . We subtract (10) from (11) and the difference is piecewise integrated from $-\infty$ to ∞. This finally yield,

$$-\left[J^1_{(0)}(\Phi)\right]_{VN}+\left[J^1_{(0)}(\phi)\right]_{CJ}=\int_{-\infty}^{-\infty}Q_{(0)}(\Phi), \tag{12}$$

$$\begin{aligned}-\left[J^1_{(1)}(\Phi)\right]_{VN}+\left[J^1_{(1)}(\phi)\right]_{CJ}&=\int_{-\infty}^{-\infty}\left(Q_{(1)}(\Phi)-2HXQ_{(0)}(\Phi)\right)dX+(\partial_t+\chi)\int_{-\infty}^{-\infty}\left(\Phi_{(0)}-\phi_{(0)}\right)dX+\\ &+\partial_X\left(\int_{-\infty}^{-\infty}2HX\left(J^1_{(0)}(\Phi)-J^1_{(0)}(\phi)\right)dX\right)-\int_{-\infty}^{-\infty}(g_0)^{-1/2}\,\partial_{x^\alpha}\left(\sqrt{g}_{(0)}\left(J^\alpha_{(0)}(\Phi)-J^\alpha_{(0)}(\phi)\right)\right)dX.\end{aligned} \tag{13}$$

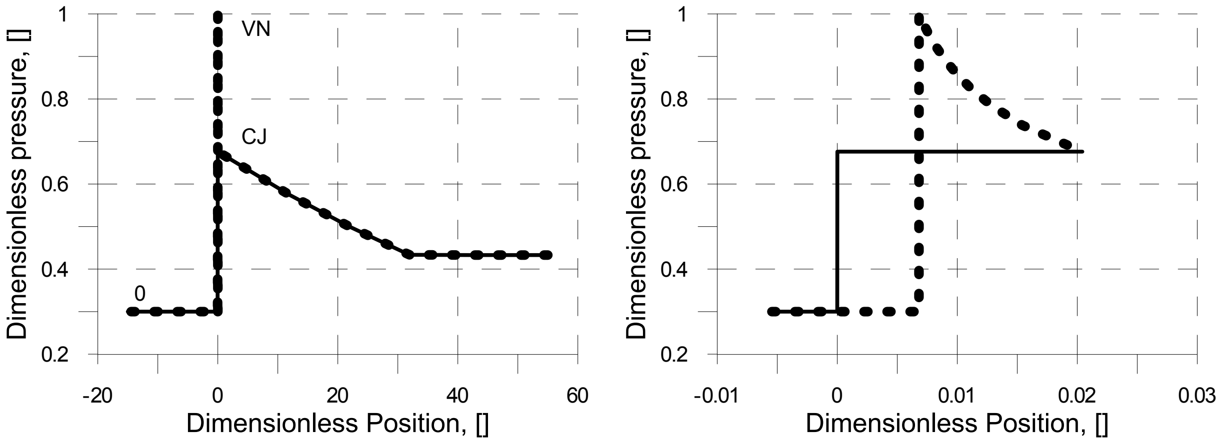

Figure 1: Profiles of *hydrodynamic* (solid) and *reactive* (dashed) detonation models. Profile obtained with ZND theory coupled with rarefaction wave, for a gas of characteristics $p_0 = 100\,kPa$, $\rho_0 = 1\,kg/m^3$, $Q = 0.1\,MJ$, $\gamma = 1.4$, $k = 1\,10^5 s^{-1}$, $E/R_g = 10000\,K$. *0* designates normal status, *VN* von Neumann peak, *CJ* Chapman-Jouget point. Left: Global view. Right: Detailed area.

We have designated with the index VN the *reactive* discontinuity and with the index CJ the *hydrodynamic*, by analogy of its conditions with the CJ point. The discontinuity in the *reactive* model is a shock, thus it is infinitely thin and the conditions governing the shock discontinuity apply, see [8]. Furthermore, the composition does not change across the discontinuity since the reaction starts at the high pressure side of the shock. This allows for strong simplification of the equations. Moreover, for the further treatment of the equations, we may define now $I_R = \int_{-\infty}^{\infty} \left(R_{(0)} - \rho_{(0)}\right) dX$, $I_\sigma = \gamma^{-1} \int_{X_{VN}}^{X_{CJ}} \left(P_{(0)} - p_{(0)}\right) dX$ and $I_\Sigma = \int_{-\infty}^{\infty} (R_{(0)} E_{(0)} - \rho_{(0)} e_{(0)}) dX$. After performing significant simplifications of Eq. (12) and (13) we combine the leading order jump conditions with the perturbative corrections and decompose the jump condition for the momentum in normal and tangential components,

$$\begin{bmatrix} m^1 \\ m^1 v^1 + p/\gamma \\ m^1 v^\beta \\ m^1 e + m^1 p/\rho\gamma \end{bmatrix}_{CJ} = -\left((\partial_t + \chi) \begin{pmatrix} I_R \\ u^1_{(0)} I_R \\ u^\beta_{(0)} I_R \\ I_\Sigma \end{pmatrix} + \begin{pmatrix} 0 \\ 2H I_\sigma \\ g^{\alpha\beta} \partial_{x^\alpha} I_\sigma \\ 0 \end{pmatrix} \right) Z^{-1} + o(Z^{-1}). \tag{14}$$

Following the methodology described in [5], we define arbitrarily the position of the artificial discontinuity in the *hydrodynamic* model requiring identical normal mass flux in the fresh and burned mixtures $\left[m^1\right]_{CJ} = 0$, which compels $I_R = 0$. The difference of slopes between rarefaction and consumption curves is asymptotically large and thus, $I_R \approx \int_{x_{VN}}^{x_{CJ}} (R_{(0)} - \rho_{CJ}) dX - (\rho_{CJ} - \rho_0) X_{VN}$. Defining $I_\rho = \int_0^1 (R^1_{(0)}(\lambda) - \rho_{CJ}) u(\lambda) \left(r(\lambda)\right)^{-1} d\lambda$, and $I_1 = Z \int_0^1 \left(P(\lambda) - p_{CJ}\right) u(\lambda) \cdot \left(r(\lambda)\right)^{-1} d\lambda = Z I_1'$, $I_\sigma = \gamma^{-1}(I_1' - (p_{CJ} - p_0)(\rho_{CJ} - \rho_0)^{-1} I_\rho) Z$, the position of the detonation shock relative to the artificial discontinuity is $x_{VN} \approx (\rho_{CJ} - \rho_0)^{-1} I_\rho$. Re-scaling $I_\Sigma = I_\Sigma' Z$, the Eq. (14) is,

$$\begin{bmatrix} m^1 \\ m^1 v^1 + p/\gamma \\ m^1 v^\beta \\ m^1 e + m^1 p/\rho\gamma \end{bmatrix}_{CJ} = -(\partial_t + \chi) \begin{pmatrix} 0 \\ 0 \\ 0 \\ I_\Sigma' \end{pmatrix} - \begin{pmatrix} 0 \\ 2H\gamma^{-1} \\ g^{\alpha\beta} \gamma^{-1} \partial_{x^\alpha} \\ 0 \end{pmatrix} \left(I_1' - \frac{p_{CJ} - p_0}{\rho_{CJ} - \rho_0} I_\rho \right) + o(Z^{-1}). \tag{15}$$

The integrals I_1 and I_ρ represent the areas contained between the detonation curve and the horizontal CJ conditions. I_1 and I_ρ depend on the chemistry model. Even numerical evaluation for complex chemistry is possible. In the present work, the explicit expressions, Eq. (9), were selected in the analysis. Finally, note that the stretch χ can be expressed as $\chi = |\nabla\rho|^{-1}\nabla\cdot\left(|\nabla\rho|\vec{u}_{(0)}\right)\big|_{X=0^+}$, see [5], and should be evaluated on the high pressure side of the *hydrodynamic* discontinuity surface (denoted by symbol $+$).

For further analysis the jump conditions (15) can be re-written in dimensional form

$$\begin{bmatrix}\tilde{m}^1\\ \tilde{m}^1\tilde{v}^1+\tilde{p}\\ \tilde{m}^1\tilde{v}^\beta\\ \tilde{m}^1\tilde{e}+\tilde{v}^1\tilde{p}\end{bmatrix}_{CJ} \approx -(\partial_{\tilde{t}}+\tilde{\chi})\begin{pmatrix}0\\0\\0\\ \tilde{I}'_\Sigma\end{pmatrix} - \begin{pmatrix}0\\ 2\tilde{H}\\ g^{\alpha\beta}\partial_{\tilde{x}^\alpha}\\ 0\end{pmatrix}\left(\tilde{I}'_1 - \frac{\tilde{p}_{CJ}-\tilde{p}_0}{\tilde{\rho}_{CJ}-\tilde{\rho}_0}\tilde{I}_\rho\right). \tag{16}$$

The system of equations corresponding to *planar* detonation (9) is a mono-parametric system dependent on D. Nevertheless, the Eq. (16) depends not only on D, but also on curvature $\tilde{H}$ and on stretch $\tilde{\chi}$. The velocity of the detonation D also suffers a change due to curvature that can be expressed through an asymptotic expansion of the form $D = D_{(0)} + D_{(1)}Z^{-1}$. The derivation of the so called *Master* equation [1], [2], a function $f(\tilde{H},\dot{\tilde{H}},\ddot{\tilde{H}},\ldots,D,\dot{D},\ddot{D},\ldots) = 0$, exceeds the scope of this paper and will be included in a forthcoming publication.

3 Virtual surface tension

The normal momentum Eq. (15) is discontinuous across the jump with linear proportionality on curvature. An analogy can be established, see [5], with an interface separating two immiscible fluids [8] in order to calculate the tension of a virtual surface representing the detonation. At the interface, $[\tilde{p}-\sigma_{nn}] = 2\tilde{H}\alpha$, where α represents the surface tension. To consider the mass transfer across the surface the formula must be modified, $\left[\tilde{m}^1\tilde{v}^1+\tilde{p}\right] = 2\tilde{H}\alpha$. We may, identify terms with eq. (16) to obtain

$$\alpha = -\left(\tilde{I}'_1 - \frac{\tilde{p}_{CJ}-\tilde{p}_0}{\tilde{\rho}_{CJ}-\tilde{\rho}_0}\tilde{I}_\rho\right) = -\tilde{l}_f\left(I'_1\frac{\rho_s c_s^2}{\gamma} - \frac{\tilde{p}_{CJ}-\tilde{p}_0}{\tilde{\rho}_{CJ}-\tilde{\rho}_0}\rho_s I_\rho\right) = \tilde{l}_f\alpha_0. \tag{17}$$

The coefficient of surface tension in an infinitely thin gas-dynamic discontinuity equivalent to a detonation is equal to the difference between the integral of the pressure between the CJ and the VN points minus the integral of the density between the same integration limits normalized by a factor. The surface tension α_0 exhibits an inverse proportionality to the initial pressure, see Figure 2. The existence of a minimum is due to the sum of the $\alpha_{01} = -I'_1\rho_s c_s^2/\gamma$ and $\alpha_{02} = (\tilde{p}_{CJ}-\tilde{p}_0)(\tilde{\rho}_{CJ}-\tilde{\rho}_0)^{-1}\rho_s I_\rho$ (dashed lines) that combined creates the final dependency. It also shows an strong direct dependence on the fuel concentration.

The existence of virtual surface tension has strong implications for the stability of the detonation. In this sense, Eq. (16) shows that the tangential momentum must not be continuous across the interface. The derivative of the surface tension (17), and the tangential derivative RHS of Eq. (16), has an analogous meaning to the Marangoni forces. From Eq. (16), the tangential derivative of the curvature can also be expressed as a function of the Marangoni forces and the derivative of the jump conditions, providing immediately the relationship between curvature of the detonation and jump conditions.

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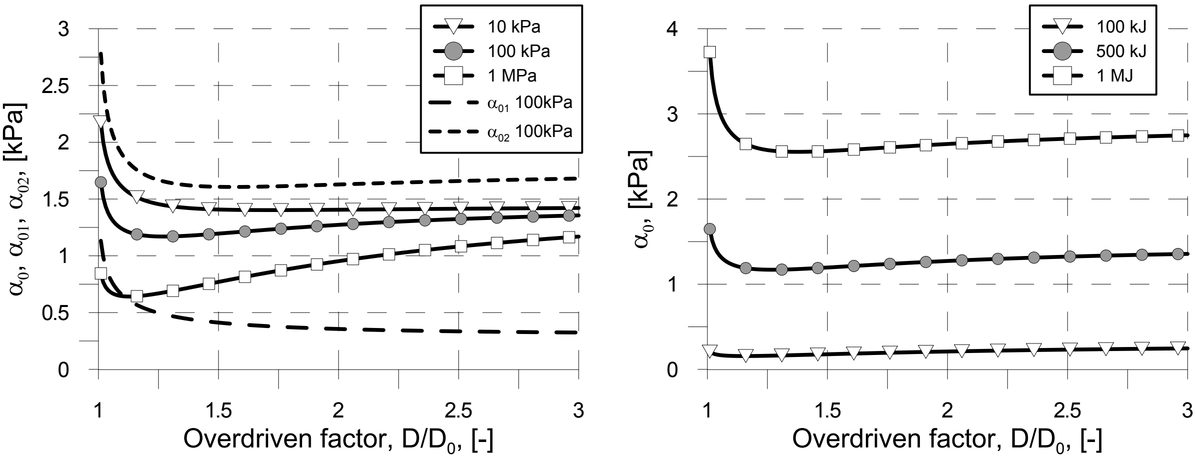

Figure 2: Left: Dependence of α_0 to the degree of over-driven detonation for a gas of characteristics $\rho_0 = 1\,kg/m^3$, $Q = 0.1\,MJ$, $\gamma = 1.4$,$k = 1\,10^5 s^{-1}$, $E/R_g = 10000\,K$ obtained for different pressures. Right: Dependence of α_0 factor to the degree of over-driven detonation for $p_0 = 100\,kPa$ obtained for different enthalpies of formation

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