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Citation: Phys. Fluids 25, 036101 (2013); doi: 10.1063/1.4792708
View online: http://dx.doi.org/10.1063/1.4792708
View Table of Contents: http://pof.aip.org/resource/1/PHFLE6/v25/i3
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Computational study of detonation wave propagation in narrow channels

Ashwin Chinnayya, Abdellah Hadjadj, and Davy Ngomo

CORIA, CNRS UMR 6614, INSA and University of Rouen, 76801 Saint Etienne du Rouvray, France

(Received 3 July 2012; accepted 18 December 2012; published online 7 March 2013)

A numerical study of the propagation of regular detonation waves is conducted in the context of narrow channels undergoing strong wall confinement. To deal with shock waves, chemical reactions, heat and viscous stresses, a high-order Navier-Stokes solver based on Weighted Essentially Non-Oscillatory (WENO) scheme, coupled with the Strang splitting method, is used in the framework of multi-species reacting mixtures. Results show that the wall dissipative effects decrease the speed of the detonation wave compared to the Chapman-Jouguet (CJ) detonation velocity. In addition, the multidimensional results reveal that the development of the thermo-diffusive boundary layers behind the leading shock wave induces an expansion flow, which then determines the contour of the sonic envelope. From the Master Equation and the generalized CJ condition, which are derived and compared to the results of the current simulations, the main energy withdrawals are found to be related to the streamline divergence as well as to the growth of the boundary layer. Moreover, a fraction of the released energy is trapped in the vicinity of the wall and does not contribute to drive the shock front. The influence of the channel height is also investigated. It was found that the transverse instabilities are damped when the channel is scaled down, which results in an increase of the dissipative effects. Finally, the validity of the Fay model is discussed with regard to the channel height and the curvature of the detonation front.

I. INTRODUCTION

Progress toward the miniaturization of increasingly advanced micro- and nano-electromechanical systems has highlighted the need for a better knowledge of the design of such devices. Understanding micro- and nano-pipe flows is still mandatory. In the field of energy and power, as the systems are scaled down, the thermal efficiency of conventional propellant devices is seriously reduced due to significant heat losses which can cause the combustion extinction. A promising technique for sustaining the combustion is to use shock or detonation waves in gaseous media to enhance the chemical reaction rates. Therefore in addition to the classical safety issues, possible applications of micro-detonations refer to energy production, propulsion, or actuation, for instance the predetonator of a pulsed detonation engine. With regards to energetic materials, micro-scale applications may also include detonation interaction with micro-structure.

From a theoretical viewpoint and following the classical Zel’dovich, von Neumann, Döring (ZND) model, a detonation is a self-sustaining process of a rapid burning rate, where strong shock waves raise abruptly the thermodynamic state, so that the chemical decomposition eventually turns the gaseous reactants into products. This process leads to an equilibrium state downstream of the shock, while the released energy and the induced pressure drop sustain the leading shock front.
From an experimental viewpoint, it has been shown that the viscous effects may strongly affect the propagation of the detonation wave when the length scale of the chamber is reduced. The finite thickness of the reaction zone renders the latter sensitive to the dissipative nature of the boundary layer, meaning that the diffusive transport phenomena cannot be neglected any more. This yields a decrease of the detonation velocity compared to the one inferred from the Chapman-Jouguet (CJ) theory.8

In terms of instabilities, it is well known that most explosive mixtures are unstable. These instabilities are multidimensional, exhibiting a complex shock structures, with transverse waves and Mach stems. They provide a key mechanism for the self-propagation of detonation. As a consequence, the leading shock is subjected to violent accelerations. This flow regime is particularly active when the temperature dependence of the chemical reaction rate is high. In this case, quenching behind the incident shock can occur. However, the multiple shock interactions provide hot spots, which are starting points of possible local re-ignitions and micro-explosions.9 Moreover, as a consequence of vorticity-generating mechanisms, the turbulence can enhance the mixing in the reaction zone and speed up the global chemical decomposition rate.8 Therefore, the mechanism of propagation of these unstable detonations cannot be explained solely by only the ZND theory,10 as opposed to regular detonation. In addition, the shock front appears highly wrinkled and the cellular detonation pattern shows a wide spectrum of length scales.9, 11

In the case of regular detonations, as the activation energy is lowered, the cellular pattern pertains if the heat reaction is high enough.7, 12 It becomes more regular with weaker transverse waves and exhibits a fish-like structure. Even in the absence of thermal sensitivity to chemical-kinetics,13 Clavin in his review paper14 has shown theoretically that an initial one-dimensional front is unstable with regards to multidimensional disturbances. Indeed, the deflection of the streamlines across the wrinkled shock perturbs the heat-release rate distribution and longitudinal waves are generated, which in a feedback loop, support the leading shock instabilities. This pure “hydrodynamic instability” is enhanced by the heat release and the sensitivity of the chemical rate with the temperature.

With regards to the detonation velocity, several mechanisms proposed by different authors are reviewed in Lee8 and Camargo et al.10 They are briefly recalled here. Zel’dovich15 was most probably the first to point out that heat and friction losses become more significant when the length scales are reduced. As a consequence, a one-dimensional formalism was derived by the author in which drag forces and heat losses are included. Based on this formalism, Zhang and Lee16 concluded that the energy dissipation was the main cause of detonation velocity deficit. Manson and Guénoche, and Murray17, 18 have proposed another phenomenological mechanism to account for the velocity deficit. They assumed that the chemical reactions are inhibited or significantly modified in the viscous sublayer. Two distinguished zones in the flow could then be identified: the boundary layer and the potential core flow, where the released energy sustains the detonation front. In their model, the authors considered separately the heat release in the boundary layer and in the flow core. This means that the heat release was modified in the Hugoniot equation by a fraction proportional to the section of the potential flow. Also, they noted that the sonic surface could not be strictly planar, especially in the near-wall region. Consequently, their modified conservation laws had to be considered in an average sense, the averaging process being made in the cross-section.

Both studies lead to the fact that the velocity deficit depends linearly on the inverse of the tube diameter. An improved model was proposed by Fay,19 where the two-dimensional boundary layer effects were accounted for the propagation of the detonation wave. The velocity deficit is explained by the development of the boundary layer downstream of the leading shock. After the shock passage, the fluid particles are accelerated and a boundary layer starts to develop downstream of the shock. In this model, in the coordinate system related to the shock front, the wall moves at the same velocity as the upstream flow. Due to the boundary layer growth, momentum diffusion takes place in the subsonic zone of the potential core flow. This induces a boundary layer negative displacement, which in turn causes flow divergence. The flow can then be modeled by a one-dimensional approach in a slowly diverging channel of which variation of the cross-sectional area can be determined from the integral length scale. The schematic illustration of the flow divergence is shown in Fig. 1.

In comparing the results of the Fay’s model with the experimental data, Camargo et al.10 have shown that within the uncertainty of chemical kinetics, the best agreement was obtained for stable
detonations, i.e., for gas mixtures following the ZND mechanism. In the one-dimensional modeling
of the influence of boundary layer growth on detonation wave, the net negative displacement is
modeled by a mass sink. Camargo et al.\textsuperscript{10} and Lee\textsuperscript{8} argue that in the case of stable detonations,
the velocity deficit due to boundary layer is thus identical to that of a curved detonation front, of
which theory was developed by Wood and Kirkwood\textsuperscript{20} and later by Bdzil\textsuperscript{21} for its multidimensional
description.

The present work deals with the study of stable detonation, in the case of absence of thermal
sensitivity of chemical kinetics. The aim of this paper is to shed more light on the multidimensional
structure of the viscous detonation propagating into narrow channels. The current investigation
will determine the structure of the subsonic reaction zone, the sonic envelope, the adjoining flow,
and its interaction with the boundary layer. It is then shown that the structure of the downstream
subsonic pocket is correlated to the early development of the boundary layer. The differences with
the phenomenological mechanisms proposed in the literature are highlighted. Insofar as non-ideal
detonation is concerned, the Master Equation is derived from the Navier-Stokes reactive model,
the generalized Chapman-Jouguet condition is presented and compared to the current simulations.
The different dissipative effects are then compared to each other in order to determine their relative
importance in the location of the sonic locus. Finally, a study of the influence of the channel-height
reduction on the structure of the detonation wave is presented. The velocity deficit, due to the scale
reduction, is accompanied by the damping of the hydrodynamic instabilities, which are probably the
most simple multidimensional unstable mode. The transverse waves get weakened and this leads to
the disappearance of the detonation cellular pattern.

The paper is organized as follows. In Sec. II, the mathematical model is recalled, while in
Sec. III, the main results are presented and discussed, leading to the conclusion given in Sec. IV.

\section*{II. MATHEMATICAL AND NUMERICAL MODELING}

In this study, the two-dimensional compressible Navier-Stokes equations with reactive multi-
species transport equations are used. The system of equations can be written in the conservation
form

\begin{equation}
\frac{\partial U}{\partial t} + \frac{\partial}{\partial x} [F(U) - F_e(U)] + \frac{\partial}{\partial y} [G(U) - G_e(U)] = S(U),
\end{equation}

where $U$ is the vector of conservatives variables, and $F(U)$ and $G(U)$ are the convective fluxes in $x$
and $y$ directions, respectively. $S(U)$ is the vector of chemical source terms

\begin{equation*}
U = \begin{bmatrix}
\rho \\
\rho u \\
\rho v \\
\rho E \\
\rho_1 \\
\vdots \\
\rho_{N_{sp}}
\end{bmatrix}, \quad F(U) = \begin{bmatrix}
\rho u \\
\rho u^2 + P \\
\rho uv \\
(\rho E + P)u \\
\rho_1 u \\
\vdots \\
\rho_{N_{sp}} u
\end{bmatrix}, \quad G(U) = \begin{bmatrix}
\rho v \\
\rho uv \\
\rho v^2 + P \\
(\rho E + P)v \\
\rho_1 v \\
\vdots \\
\rho_{N_{sp}} v
\end{bmatrix}, \quad S(U) = \begin{bmatrix}
0 \\
0 \\
0 \\
0 \\
\mathcal{W}_1 \dot{\omega}_1 \\
\vdots \\
\mathcal{W}_{N_{sp}} \dot{\omega}_{N_{sp}}
\end{bmatrix}.
\end{equation*}

$\rho$, $\rho_k$, $P$, $e$, $E = e + (u^2 + v^2)/2$, $\mathcal{W}_k$, and $\dot{\omega}_k$ are the density, the $k$th species-density, the pressure,
the internal and the total energy, the molar mass, and the chemical source term of the $k$th species,
respectively. $N_{sp}$ is the total number of species.
The diffusive fluxes $F_v(U)$ and $G_v(U)$ are
\[
F_v(U) = \begin{bmatrix}
0 \\
\tau_{xx} \\
\tau_{xy} \\
q_x \\
J_{x,1} \\
\vdots \\
J_{x,N_{sp}}
\end{bmatrix}, \quad G_v(U) = \begin{bmatrix}
0 \\
0 \\
\tau_{yy} \\
q_y \\
J_{y,1} \\
\vdots \\
J_{y,N_{sp}}
\end{bmatrix}.
\]

The different components of the viscous stress tensor are given by the following expressions:
\[
\tau_{xx} = 2\mu \frac{\partial u}{\partial x} - \frac{2}{3} \mu \left( \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \right), \quad \tau_{yy} = 2\mu \frac{\partial v}{\partial y} - \frac{2}{3} \mu \left( \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \right),
\]
where $\mu$ is the mixture dynamic viscosity. The diffusive flux in the species conservation law $J_{x,k}$ and $J_{y,k}$ are given by the Fick law. $Y_k = \rho_k/\rho$ is the mass fraction of the $k$th species. $D_{k,m}$ is the diffusion coefficient of the $k$th species into the mixture.
\[
J_{x,k} = \rho D_{k,m} \frac{\partial Y_k}{\partial x}, \quad J_{y,k} = \rho D_{k,m} \frac{\partial Y_k}{\partial y}.
\]

The dissipative fluxes in the total energy equation then read
\[
q_x = u\tau_{xx} + v\tau_{xy} + \lambda \frac{\partial T}{\partial x} + \rho \sum_{k=1}^{N_{sp}} h_k D_{k,m} \frac{\partial Y_k}{\partial x},
\]
\[
q_y = u\tau_{yx} + v\tau_{yy} + \lambda \frac{\partial T}{\partial y} + \rho \sum_{k=1}^{N_{sp}} h_k D_{k,m} \frac{\partial Y_k}{\partial y},
\]
where $\lambda$ is the mixture thermal conductivity. The terms $\lambda \frac{\partial T}{\partial x}$ and $\lambda \frac{\partial T}{\partial y}$ account for the Fourier conductive thermal flux. $h_k$ is the enthalpy of the $k$th species.

The system of Eq. (1) is solved using a fifth-order shock-capturing scheme, based on a Mapped-Weighted Essentially Non-Oscillatory (WENO5) method for the convective fluxes and a fourth-order compact scheme for the discretization of the diffusive fluxes. The details of the numerical method, the thermodynamics (perfect gas law and JANAF), as well as the mixture transport properties can be found in Ref. 23. A uniform Cartesian mesh is used.

## III. RESULTS AND DISCUSSION

The propagation of detonation waves in two-dimensional narrow channels is investigated. The initial pressure and temperature are $P_0 = 3$ kPa and $T_0 = 300$ K, respectively. The thermodynamic and transport properties of the working fluid have been chosen to be that of a stoichiometric propane/oxygen mixture. A single step has been used for the chemical mechanism: $F + O \rightarrow P$. A total of 9 chemical species is involved. The fuel and oxidant are, respectively, $F \equiv C_3H_6$ and $O \equiv 5O_2$. The detonation products consist of a mixture of gaseous components $P \equiv 1.047$ CO$_2 + 1.953$ CO + 2.63 H$_2$O + 1.12 OH + 0.587 H$_2$ + 0.86 O$_2$ + 0.4478 H + 0.487 O. The chemical composition is taken similar to the one given by the Chapman-Jouguet equilibrium state using the software GASEQ or as in Ref. 24 at initial conditions of 1 bar and 300 K. In this case, the reduced chemical energy $Q_r/R_0 T_0$ is equal to 78.5. The chemical time scale is $\tau_F = 15 \times 10^{-8}/[O_2]$ and the reactivity of the mixture depends linearly on the pressure. The chemical source term for $F$ is $\dot{\omega}_f = -[F]/\tau_F$. In what follows, we denote $\Delta$ as the distance from the shock within the ZND reaction zone, where the fuel mass fraction reaches 1% of its initial value. The coefficient of the chemical time scale decomposition has been calibrated such...
that $\Delta$ depends linearly on the inverse of the pressure and that $\Delta$ is equal to the results of Schultz and Shepherd.\textsuperscript{25} The hydrodynamic structure of propane-oxygen detonation exhibit very high turbulent features, which is due to its complex reaction zone.\textsuperscript{26} However, as the chemistry has been simplified, the modes of longitudinal instabilities cannot be present. $H$ is the height of the channel. Initially, left and right flow conditions are imposed. In the left part, a one-dimensional ZND solution is imposed, while a uniform state of a gas mixture at rest in initial conditions $P_0$ and $T_0$ is assumed. With regards to boundary conditions, a no-slip adiabatic conditions are imposed on solid walls, and a symmetric conditions are set on the symmetry axis of the domain. Open-boundary conditions are fixed at the left and right boundaries. Owing to the symmetry of the flow, only half of the channel is computed.

In the streamwise $x$ direction, the numerical resolution is such that there is 128 points per $\Delta$, which is equal to 1.068 mm. In the cross-streamwise $y$ direction, $N_y = 40$ has proven to be sufficient to ensure numerical convergence. The length of the computational domain is $74 \Delta$. It is assumed that no reaction takes place upstream of the shock, i.e., the chemical source is activated only for fluid particles that have passed through the shock.\textsuperscript{22, 27} The height is $H = \Delta/8 = H_{ref}$. The CJ velocity is $2.2$ km/s. During the transient phase, the detonation velocity $\sigma$ decreases and stabilizes to a constant value (see Fig. 2 (left)). The constant detonation velocity is $1.75$ km/s, i.e., a velocity deficit of about 26%. Moreover, as the detonation velocity has become constant, a subsonic region is found to be coupled to the detonation front. Its form and dimensions are also found to be self-similar. Indeed, the ordinate $y/(0.5H)$ for which the relative Mach number is equal to one, is drawn in Fig. 2 (right) at different times, after the shock detonation velocity has stabilized. The geometry and the dimensions of the contour of the sonic envelope do not vary. This feature along with the constant detonation velocity enables us to verify that a self-similar state is reached. The structure of the detonation front is then analyzed from the numerical results. The paper dwells mainly on the description of this subsonic reaction zone and associated flow.

A. Structure of the flow-field

The longitudinal flow velocity in a fixed-shock coordinate system is depicted in Fig. 3. The shock travels at $\sigma \bar{x}$. The change of coordinates from the laboratory system to the attached shock system results in $t' = t, \bar{x}' = \sigma t - x, \bar{y}' = -y$, and velocities $u' = \sigma - u, v' = -v$. In the following, for the sake of clarity, the prime will be omitted. The distance from the leading shock is scaled by $\Delta$. The velocity vectors are plotted at different sections of the channel. They are mainly parallel to the walls. This means that most of the flow is one-dimensional. On the one hand, the gas is decelerated through the passage of the leading shock and the flow becomes subsonic. So in the main core of the flow, the continuous heat release causes gas expansion and flow acceleration. On the other hand, in this coordinate system, the no-slip boundary implies that the velocity at the solid wall is equal to the shock velocity, which is much higher than the post-shock gas velocity. This means that overall, the flow is accelerated not only by the energy release but also by the momentum diffusion, due to
higher flow velocity near walls. The numerical results exhibit similar behavior as the scheme of Fay velocity deficit (see Fig. 1). However, the sonic surface, represented by the white line in Fig. 3, is not just a flat surface that is located at some distance from the leading shock.

Indeed, another implication of the no-slip boundary is that the flow is necessarily supersonic near the walls, whereas it remains subsonic in the core of the flow immediately downstream of the shock. The transition between these two flow regimes is then done through the sonic line shown in Fig. 3. Therefore, the subsonic zone leans against the detonation front, which is almost planar. A slight deviation of the velocity vector can still be observed through the shock passage. The upper edge of the sonic envelope is located at the intersection of the base of the shock with the beginning of the boundary layer. The sonic locus then meets the centerline of the channel at approximately $0.5\Delta$.

We can see that the topology of this sonic envelope looks like the one formed by the lateral expansion of detonation products in a weakly confined explosive charge. Moreover, a slight curvature of the leading shock can be inferred from the small deviation of the velocity vector, immediately downstream of the shock.

For that reason, as the flow near the wall is supersonic, the characteristic fields can be studied, following Gamezo and Oran approach. The Mach angle $\alpha_M$ between a streamline and a characteristic line can be determined from the local Mach number $M = \|u\|/c$:

$$\alpha_M = \pm \arcsin(1/M). \tag{2}$$

Through each point pass two characteristics $C^+$ and $C^-$, which correspond to $\alpha_M > 0$ and $\alpha_M < 0$, respectively. This will give the direction of pressure wave propagation. The characteristic lines are drawn based on the velocity vectors that are rotated by $\pm\alpha_M$ (see Fig. 4). The iso-Mach lines are shown in white.

We can see that there is a fan of Mach lines which emerges from the singular point where the foot of the shock meets the incipient boundary layer. This can be considered to be representative of a Prandtl-Meyer flow, even though the flow is subjected to heat release and dissipative effects. This expansion allows the flow to accelerate from the sonic locus to the high wall velocity.

In Fig. 4, we can also see that the pressure waves emanate from the walls and propagate along the characteristic lines toward the sonic locus. They clearly influence the sonic locus shape. Gradually as one moves away from the location of this singularity, the subsonic zone is less influenced by the walls. This explains the inflection point that can be observed on the structure of the subsonic pocket (see Fig. 5). Moreover, the characteristic lines are tangent to the subsonic zone. Thus the pressure waves cannot go through this sonic barrier. This means that the sonic locus limits the part of the reaction zone which influences and sustains the detonation front. Heat release also takes place in the supersonic region near wall boundaries, which implies that less energy is available to support the detonation front, as Manson and Guénoc'h have already suggested from different physical arguments.
Furthermore, as the sonic surface is approached, the angle between the characteristic lines and the streamlines, mainly horizontal should approach $\pm \pi/2$. This is clearly not the case, which means that the characteristics have singularities in the vicinity of the sonic surface. This will be examined when the Master Equation will be derived in the Subsection III C.

In the one-dimensional description, the boundary layers influence directly the subsonic core flow that goes from the shock front to the CJ generalized plane, through pressure and rarefaction waves that thereby reduce the detonation velocity. In the multidimensional description, information from the walls and the boundary layers travel along the pressure waves through the characteristics. Therefore, we can see in Fig. 4 how they are deposited on the sonic locus and influence the subsonic reactive region. These pressure waves are representative of a Prandtl-Meyer like flow. This expansion flow does not come from the lateral expansion of detonation products like in cartridge detonation process but from the beginning of the viscous boundary layer growth. The latter should induce a net negative boundary layer displacement and thereby the divergence of the flow. Section III B will then compare the evolution of the sonic locus in relation to the growth of the viscous boundary layer.

B. Boundary-layer growth

In this subsection, the development of the boundary layer is analyzed in relation to the evolution of the sonic locus. Figure 5 represents the position of the subsonic boundary, the viscous boundary...
layer thickness $\delta$, the displacement thickness $\delta^*$, and the momentum thickness $\theta$ as a function of the normalized distance from the shock $x/\Delta$. For each abscissa, $\delta(x)$ is the ordinate for which $u(x, \delta) = 0.99 u(x, H/2) = 0.99 u_\infty$. The underscript $\infty$ refers to the state at the axis of the channel, which varies with the distance from the shock. In the Fig. 5, the ordinate has been normalized by the height of the channel. $\delta$, $\delta^*$, and $\theta$ read

$$u(x, \delta) = 0.99 u(x, H/2) = 0.99 u_\infty,$$  \hfill (3)

$$\delta^* = \int_0^H \left( 1 - \frac{\rho u}{\rho_\infty u_\infty} \right) dy,$$  \hfill (4)

$$\theta = \int_0^H \frac{\rho u}{\rho_\infty u_\infty} \left( 1 - \frac{\rho u}{\rho_\infty u_\infty} \right) dy.$$  \hfill (5)

The flow can be divided into three parts. There is a first zone A in which the boundary layer is developing rapidly. Then, there is a second zone B where the boundary layer evolves slowly and which is located within the subsonic zone. Finally, there is a zone C where the flow is supersonic everywhere. This is in accordance with the results of Section III A.

Globally, the relative evolution of the different thicknesses and the sonic locus leads us to say that the development of the displacement thickness seems to coincide with the development of the sonic location. This agreement is particularly good at the beginning of zone A, where they are tangent with each other. On the other hand, in Subsection III A, the limiting characteristic of the expansion flow has been shown to determine the contour of the sonic envelope. As a consequence, this means (and confirms) that immediately downstream of the shock, the momentum diffusion from the walls, i.e., the growth of the boundary layer induces a net boundary layer displacement and a flow divergence, resulting in an expansion flow of Prandtl-Meyer type, which in turn determines the contour of the sonic envelope.

In the cases which we investigated, the Reynolds numbers $Re_x = (\rho u/\mu)_\text{axis} x$, $x$ distance from the shock and $u$ velocity relative to the shock, and $Re_H = (\rho u/\mu)_\text{axis} H$ are, respectively, below $3.5 \times 10^5$ and 2500. Thus the flow can be considered to be laminar. The skin coefficient $C_{fx} = 2 \tau_{\text{wall}}/(\rho u^2)_\text{axis}$ is shown in Fig. 6. In Fig. 7 is depicted the ratio of the boundary layer thickness over the distance from the shock as a function of the Reynolds number $Re_x$. When the numerical results are compared to classical relations, the order of magnitude is reproduced but the comparison is not as good as expected. The reasons for these discrepancies lie probably in the reactivity of the flow and in the presence of a very high pressure gradient (not shown here) in the reaction zone. The presence of a negative pressure gradient and the flow acceleration contribute to thin the boundary layer (see Fig. 7). Thus wall stress becomes more important in this case (see Fig. 6). This can be the reasons

![Image](image_url)
why Kitano et al.\textsuperscript{29} and Ishii et al.\textsuperscript{30,31} increase the friction coefficient in the Zel’ dovich model in order that their numerical results match their experimental results.

C. Master Equation

As far as we deal with non-ideal detonations, the sonicity condition is associated to the generalized CJ condition. As the detonation front is constant, the flow can be considered to be stationary in the reference coordinate system related to the shock. From the Navier-Stokes reactive model, the densities and pressure divergence can be substituted from the mass and impulse equations into the total energy equation. Therefore, we get the Master Equation

\[ \mathcal{H} + P_{\text{visq}} = (\gamma - 1) \left( -\dot{q} + \Phi + \dot{q}_{th} + \dot{q}_{\text{diff}} \right). \]  

(6)

In the local coordinate system of Frenet \((\vec{l}, \vec{n})\), the hydrodynamic contribution \(\mathcal{H}\) reads

\[ \mathcal{H} = \rho (c^2 - \|\vec{u}\|^2) \frac{\partial \|\vec{u}\|}{\partial l} + \rho c^2 \|\vec{u}\| \frac{\partial \theta}{\partial n}. \]  

(7)

The different terms of this energetic balance are listed below.

- \(\theta = (\vec{x}, \vec{l})\) is the deviation angle of the streamlines.
- \(\frac{\partial \theta}{\partial \vec{n}}\) represents the local divergence of the streamlines.
- \(P_{\text{visq}} = \vec{u} \cdot \vec{\tau}\) is the power related to the viscous stress.
- \(\Phi = \text{div}(\vec{\tau} \vec{u}) - \vec{u} \cdot \text{div}(\vec{\tau})\) is the viscous dissipation rate.
- \(\dot{q}_{th} = \text{div}(\lambda \text{grad}(T))\) is the thermal flux.
- \(\dot{q}_{\text{diff}}\) is related to the diffusive enthalpy species flux

\[ \dot{q}_{\text{diff}} = \sum_{k=1,N_{sp}} \text{div}(\rho D_{k,m} h_k \text{grad} (Y_k)) - \left( \frac{\partial e}{\partial Y_k} \right)_{\rho, P} \cdot \text{div}(\rho D_{k,m} \text{grad} (Y_k)). \]

- \(\dot{q}\) is related to the released energy or thermicity

\[ \dot{q} = \sum_{k=1,N_{sp}} \left( \frac{\partial e}{\partial Y_k} \right)_{\rho, P} \mathcal{W}_k \omega_k. \]

The derivative of the internal energy with respect to the mass fraction reads

\[ \left( \frac{\partial e}{\partial Y_k} \right)_{\rho, P} = h_k - c_{p,m} T \frac{\mathcal{W}}{\mathcal{W}_k}, \]

\[ c_{p,m} = \sum_k Y_k c_{p,k} \] is the mixture heat capacity. \(\mathcal{W} = (\sum_k Y_k/\mathcal{W}_k)^{-1}\) is the mixture molar mass.
This Eq. (6) becomes singular when the relative Mach number is one, i.e., the sonicity condition is $\| \vec{u} \| = c$. The generalized CJ condition then easily follows. Thus, at the critical location where the transition from subsonic to supersonic flow occurs, the rate of energy production coming from chemical decomposition must be balanced by the rate of energy withdrawal related to the streamline divergence and by the rate of the different dissipative energy sinks, which come from the growth of the boundary layers. The first energy loss is classical since Wood and Kirkwood,\textsuperscript{20} as the streamline divergence is somehow connected to the shock curvature, whereas the second energy loss is more specific to gaseous detonation propagation in narrow channels.

Equation (6) can be normalized as follows:

$$H' + P'_{visq} = 1,$$

such as $H' = \frac{H}{(\gamma - 1) (-\dot{q} + \Phi + \dot{q}_{th} + \dot{q}_{diff})}$ and $P'_{visq} = \frac{P_{visq}}{(\gamma - 1) (-\dot{q} + \Phi + \dot{q}_{th} + \dot{q}_{diff})}$.

The previous expression has been estimated from the numerical results when the relative Mach number is one. In Fig. 8, the subsonic zone is shown in blue and the supersonic zone in red. In this figure, the isoline in black refers to the value of the left-hand side of Eq. (8). One can see that there is a very good agreement between the sonic locus and the location where the generalized CJ condition holds.

In order to allow us to identify the predominant terms among the different energy losses, the values taken from the different terms of the energy balance of Eq. (6) are plotted in Fig. 9 as a function of the distance from the shock. They are normalized by the maximal value taken by $P_{visq}$. When one moves away from the shock, all the contributions of the Master Equation decrease. The contribution of the diffusive enthalpy species flux is always negligible.

Near the leading shock and Prandtl-Meyer flow, the contribution of the thermal flux is also negligible. The leading terms are relative to the exothermicity $\dot{q}$, the local divergence of the streamlines $H$, the power of the viscous stress $P_{visq}$, and the viscous dissipation rate $\Phi$. Thus, the growth of the viscous boundary layer and the local streamline divergence are clearly responsible for the location of the sonic line at the beginning of zone A, immediately downstream the shock.
As one moves away from the shock toward the end of the subsonic zone at the end of zone B, when the sonic line becomes close to the symmetry axis, the viscous dissipation rate gets negligible. The thermal flux cannot be neglected anymore as its contribution is of the same order of magnitude that $H'$. Therefore, the three energy sinks that come from the thermal conduction, the viscous stresses as well as the local streamline divergence are responsible for the location of the sonic line at the end of zone B.

In order to quantify its relative importance compared to the viscous contribution, the thermal contribution to the energetic balance $H'$ and $P'_{visq}$ has been taken out. The contribution from the species enthalpy diffusion is negligible. The following quantities are defined:

$$H'' = H \frac{(-\dot{q} + \Phi)}{(\gamma - 1)(\gamma - 1)}$$

$$P''_{visq} = P_{visq} \frac{(-\dot{q} + \Phi)}{(\gamma - 1)(\gamma - 1)}.$$  \hfill (9)

In Fig. 10, the isolines for which the quantity $H'' + P''_{visq}$ equals 1., 1.1, 1.2, 1.3, and 1.4, have been drawn. The subsonic zone is in black and the supersonic zone is in white. The isoline 1. lies within the subsonic zone. In zone A, the difference between the sonic line and the isoline 1. is weak. This means that the viscous dynamic effects prevail. However, as one goes away from the shock, the difference between the isoline 1. and the sonic line increases, especially toward the end of the zone B. Therefore, it seems that thermal conduction cannot be anymore completely neglected.

Indeed, in the absence of thermal conduction, the sonic envelope should \textit{a priori} be located at the vicinity of the isoline 1. However, the temperature is globally higher in the supersonic zone, as the residence time of the fuel is greater. Then the thermal conduction increases the temperature of the gas in the subsonic zone. The local sound speed increases, thereby decreasing the Mach number. Thus the sonic location is delayed downstream.

From the evaluation of the different terms of the energetic balance along the sonic locus, the main contributions come from the chemical energy production and the energy losses which are the streamline divergence and viscous as well as thermal dissipative effects. As expected, the boundary layer growth coming from viscous stress is mainly responsible for the early and subsequent development of the sonic contour. However, the thermal conduction cannot be anymore completely neglected when the sonic envelope meets the symmetry axis.

D. Streamline curvature

In the one-dimensional modeling of the influence of boundary layer growth on detonation wave, the net negative displacement is modeled by a mass sink. Then Camargo \textit{et al.}\textsuperscript{10} and Lee\textsuperscript{8} argue that in the case of stable detonations, the velocity deficit due to boundary layer is thus identical to that of a curved detonation front. Indeed, based on the computational results of Subsection III A, a slight deviation of the velocity vector is seen after the shock passage, which indicates the presence of a slight shock curvature. This comes from the growth of the boundary layer, which gives rise to an expansion Prandtl-Meyer flow at the base of the shock.

The Wood-Kirkwood\textsuperscript{20} theory of a curved detonation wave propagation in an explosive cartridge has been generalized by Bdzil.\textsuperscript{21} The author derived an equation for the streamline angle, which enables to describe the topology of the propagation of the entropy waves in the subsonic reaction zone.\textsuperscript{28} The physical assumptions used were that the explosive size charge and the radius of curvature of the shock front were very large compared to the one-dimensional reaction length. In addition, the streamline deflection angle was assumed to be small. These lead to the vorticity being negligible.
in the main core of the flow. Indeed, the vorticity generated by a curved shock is proportional to the curvature of the shock. Moreover, the study of Bdzil showed that the vorticity production was negligible, compared to the contribution of the chemical reaction. An other implication is that in the shock-oriented curvilinear coordinates (see Fig. 11), the derivative along the tangency ($\xi$) to the shock was negligible compared to the derivative along the normal ($\eta$) direction.

The physical situation studied by the latter author is very different from ours and the mechanism responsible for the slight curvature of the shock front is not the same. However, the same formalism is used to derive the streamline deflection angle equation and to figure out how the streamlines and the entropy waves can be deviated from horizontal.

If $x_s(y)$ is the position of the detonation front and $x'_s$ its derivative in the $y$ direction, the following parameterization of shock-oriented curvilinear coordinates is used (see Fig. 11):

$$\eta = x - x_s(y)$$
$$\xi = x + \int dy\frac{x'_s}{x'_s}.$$  \hspace{1cm} (10)

Thus the following approximate relationship can be derived from the following hypothesis used by Bdzil:\textsuperscript{21} in the curvilinear coordinates shown in Fig. 11, the derivative along the $\xi$ direction is considered to be negligible compared to the $\eta$ direction, and the vorticity $\Omega_z = \frac{\partial v}{\partial x} - \frac{\partial u}{\partial y}$ is considered to be negligible.

We begin with the Master Equation Eq. (6) in Section III C, derived in Appendix, with

$$f = \frac{x'_s}{\sqrt{1 + x'_s^2}}$$
and with the following equality:

$$\frac{\partial}{\partial x} \left( \frac{u}{u} \right) \approx \frac{u}{u^2} (1 - f^2)^{1/2} \left( -\dot{q} + \Phi + \dot{q}_{th} + \dot{q}_{diff} - \mathcal{P}_{visq} \right).$$  \hspace{1cm} (11)

The two assumptions were used to simplify the hydrodynamic contribution $\mathcal{H}$ in the Master Equation and Eq. (11). Then the following approximation relation can be derived:

$$\frac{\partial}{\partial x} \left( \frac{u}{u} \right) \approx \frac{u}{u^2} (1 - f^2)^{1/2} \left( -\dot{q} + \Phi + \dot{q}_{th} + \dot{q}_{diff} - \mathcal{P}_{visq} \right).$$  \hspace{1cm} (12)

The main difference from Eq. (3.1) of Ref. \textsuperscript{21} is the presence of all the dissipative terms $\Phi, \dot{q}_{th}, \dot{q}_{diff}$, and $\mathcal{P}_{visq}$, which comes from the dissipative nature of the Navier-Stokes model. This is due to the fact that the Master Equation in our case includes all these diffusive terms. If one cancels all these dissipative terms, Eq. (3.1) in the study of Bdzil\textsuperscript{21} is retrieved.

This last equation states that in reactive flows for which the vorticity can be neglected, the streamline curvature is related to the sonic character of the flow but also to the total energy release. This total energy release takes into account not only the chemical heat release but also the endothermic terms coming from the dissipative effects.

In Subsection III A, a slight deviation of the velocity vector is seen after the shock. The curvature of the shock acts to curve the streamlines away from the axis of the channel. On the one hand, exothermicity in the subsonic reaction zone acts to curve the streamline toward the symmetry axis.\textsuperscript{21} On the other hand, the pressure is quasi-uniform in each section of the channel (see Fig. 12 (top)), except near the shock, where a maximum of pressure can be seen at the intersection of the base of the shock and the beginning of the boundary layer. It is also the place where the vorticity is maximum (see Fig. 12 (bottom)). Then, in a third step, dissipative effects tend to accelerate the
alignment of the streamlines with the symmetry axis. These different steps can be clearly seen in Fig. 13 (top), where some streamlines have been traced.

If dissipative effects were absent, streamlines curvature would exhibit a change of sign near the sonic locus as the computation of Gamezo and Oran\textsuperscript{28} have shown. Here we can see in Fig. 13 (bottom) the location where \( \frac{\partial (v/u)}{\partial x} = 0 \). The change of sign is only apparent at the beginning of the development of the sonic locus.

In Fig. 14 (top), the white line depicts the locus where \( \frac{\partial (v/u)}{\partial x} = 0 \) is zero. And in Fig. 14 (bottom), the white line depicts the locus where the right-hand side of Eq. (12) equals zero. In both figures, the subsonic region is in black, the supersonic region in white. There is a qualitative agreement between the numerical results and the approximate relation. However, the location of the isoline zero is not exactly at the same place for both figures.

Thus, from Figs. 13 and 14, it can be inferred that the vorticity production cannot be completely neglected. The vorticity, which is maximum at the beginning of the boundary layer development (see Fig. 12) diffuses well into the subsonic reaction zone, and is non-negligible as the height of the channel is comparable to the reaction zone thickness.

\subsection*{E. Influence of channel height}

The structure of the detonation front has been studied for a given height. It is then natural to study the influence of the height on the structure of the detonation wave. The height of the channel is varied and in addition to the previous case, five heights have been investigated: \( 4H_{\text{ref}}, 3H_{\text{ref}}, 2H_{\text{ref}}, H_{\text{ref}}/2, H_{\text{ref}}/4 \). The same numerical initial conditions and the same spatial resolution, as in Sec. III are used.

Figure 15 represents the normalized mean detonation velocity as a function of the inverse normalized height. The detonation velocity decreases as the height of the channel is decreased.
The behavior of the velocity deficit shows another similarity with the case of confined and curved detonation. The behavior of the detonation velocity as a function of the inverse of the height is more quadratic than linear.

Figure 16 shows the contour of the subsonic zone for different heights. One can see that the size of the subsonic region decreases when the $H$ is decreased. This is due to the increased viscous effects. The velocity deficit is thus higher.

One can also see in Fig. 16 that the sonic locus for greater heights has many inflection points. This comes from the transverse instabilities. Indeed the polytropic coefficient of the reactants as well as

![Image](image_url)
the products is $1.14 \sim 1.2$, the reduced heat is 78.5 and the activation energy is zero. Erpenbeck, and Short and Stewart have shown that for a detonation overdrive of 1., a polytropic coefficient of 1.2 and a reduced heat of 50, this type of mixture does not present longitudinal instabilities but present transverse instabilities in multidimensional configurations, even in the case of absence of thermal sensitivity of chemical-kinetics. This is also consistent with Clavin’s review, who shows that these instabilities are enhanced with heat release.

With the increase of the channel height, the wall dissipative effects diminish. And the transverse instabilities which were certainly damped with height reduction reappear as they are intrinsic to the detonation propagation. The detonation velocity is then oscillatory as can be seen in Fig. 17, which depicts the instantaneous detonation velocity on the symmetry axis as a function of time, for the height channel $4H_{cr}$. This is a characteristic of the presence of multidimensional instabilities of the detonation front. Near the walls, the detonation velocity will also be oscillatory. Thus the boundary layer will be subjected to multiple accelerations. This in turn affects the subsonic region, which sees oscillations develop on its frontier (see Fig. 18).

The transverse and incident shock waves are anchored on triple points, whose trajectories in the channel determine the cellular structure of detonation. Figure 19 depicts the triple points trajectories for the different heights investigated. As the dissipative effects increase with scale reduction, the transverse waves are more difficult to be captured as they lose their intensity, being damped by dissipative effects. The cellular structure then fades until it disappears.

An analogy can be made with the attenuation of the transverse wave structure in porous walls tubes for stable detonation propagation. Radulescu et al. link this mitigation process to the mass divergence which leads to a curved detonation front. We might assume that the same mechanism

![FIG. 15. Mean detonation velocity as a function of the inverse of the height.](image1)

![FIG. 16. Contour of the subsonic region for different channel heights.](image2)
FIG. 17. Instantaneous velocity of the detonation front on the symmetry axis, for height $4H_{ref}$. The straight dashed line represents the mean velocity.

FIG. 18. Contour of the subsonic region (black dots), boundary layer thickness (red squares), displacement thickness (green diamonds), and momentum thickness (blue stars). Channel of height $4H_{ref}$.

FIG. 19. Triple point trajectories for different channel heights. From top to bottom: $H = 4H_{ref}$, $H = 2H_{ref}$, $H = 3H_{ref}$, $H = H_{ref}$.
occurs in the case of stable detonation propagation in narrow channels, i.e., the transverse structure gets attenuated because of the boundary layers, which induce a negative displacement of the walls and consequently, a flow divergence.

No extinction of the detonation was observed in our numerical simulations. Indeed, the chemical decomposition rate for the mass fraction of $F$ depends linearly on the pressure. Even if our configuration is different, the analysis of Bdzil indicates that this linear dependence cannot lead to extinction.

IV. CONCLUSION

A computational study of detonation propagation in narrow channels has been carried out. The main finding is that the detonation velocity shows a deficit. The thermodynamic and transport properties of the working fluid have been chosen to be that of a stoichiometric propane/oxygen mixture and their products. Its reactivity has been modeled to depend linearly on pressure with an absence of thermal sensitivity. Thus, in terms of instabilities, detonation shows one multidimensional unstable mode.

The flow is accelerated after the passage of the leading flow. This leads to the growth of the boundary layer. In the coordinate system attached to the shock, a subsonic reactive region is found to be coupled to the shock and to be self-similar. The structure of the flowfield, studied in Subsection III A, is found to be very similar to that proposed by Fay to explain the velocity deficit. The difference comes from the sonic locus topology, which is found to be closer to the lateral expansion of detonation products in weakly confined charges.

Indeed, immediately downstream of the shock, the momentum diffusion from the walls, i.e., the growth of the boundary layer induces a net boundary layer displacement and a flow divergence, resulting in a Prandtl-Meyer expansion flow, which in turn determines the contour of the sonic envelope. This expansion flow originates at the intersection between the beginning of the boundary layer and the foot of the shock and enables the flow to accelerate from the sonic locus to the higher wall velocity.

The Master Equation was then derived. From the evaluation of the different terms of the energy balance along the sonic locus, the main contributions come from the chemical energy production and the energy losses which are the streamline divergence and viscous as well as thermal dissipative effects. As expected, the boundary layer growth coming from viscous stress is mainly responsible for the early and subsequent development of the sonic contour. However, the thermal conduction cannot be completely neglected when the sonic envelope interacts with the centerline of the channel.

Then, the extension of the Bdzil’s formalism to our configuration has enabled us to figure out the behavior of the entropy waves in the subsonic reaction zone. The computational results show that they were at first deflected by the shock curvature from the axis, then in a second step that the exothermicity of the flow acts to curve the streamlines toward the axis and finally, that the dissipative effects act to realign the streamlines with the wall and symmetry axis.

The streamline deflection angle equation, which was derived, assuming that the vorticity is negligible was compared to current numerical data. There was only qualitative agreement, which means that the vorticity produced at the intersection of the base of the shock and the beginning of the boundary layer, diffuses well into the subsonic reactive region. This also means that in the case of viscous detonation propagation, as the height of the channel is comparable to the reaction zone thickness, vorticity cannot be completely neglected in the subsonic reactive zone.

A further study on the influence of height reduction has also been investigated. With height increase, wall dissipative effects diminish. Transverse instabilities, intrinsic to detonation propagation reappear. The subsonic region shows an oscillatory frontier. And it has been shown that the cellular structure fades until complete disappearance as the transverse waves are probably damped with increase dissipative effects. We might expect that the increased induced flow divergence could be the mechanism of the mitigation of these multidimensional instabilities, as in Radulescu et al.

The multidimensional time-averaged structure of the subsonic reactive region and its adjoining flow of a detonable mixture with higher temperature reaction sensitivity could then be analyzed, following Radulescu et al., which would give higher physical insight about the "turbulent
structure of gaseous detonations. Indeed, the losses in channels are based on the conjunction of three factors: the boundary layer growth, the Prandtl-Meyer rarefaction fan, and the shock curvature. Thus, on an average sense, the phenomenology which is highlighted in this paper can be probably transcribed in the case of unstable detonations, where the strong interaction of transverse shocks with turbulence is moreover expected.

ACKNOWLEDGMENTS

This study is supported by the French Ministry of Research and Education. Computations are performed using HPC resources from GENCI (CCRT/CINES/IDRIS) (Grant No. 2010-0211640) and CRIHAN.

APPENDIX: DERIVATION OF THE MASTER EQUATION EQ. (6)

In the Cartesian coordinates (x, y), the Navier-Stokes equations Eq. (1) read

\[ \frac{\partial U}{\partial t} + \frac{\partial}{\partial x} [F(U) - F_v(U)] + \frac{\partial}{\partial y} [G(U) - G_v(U)] = S(U). \]  

(A1)

The expressions of the different conservative vectors and fluxes as well as the source terms can be found in Sec. II. Let us consider the following change of coordinates (see Fig. 20):

\[ t' = t, \quad x' = \sigma t - x, \quad y' = -y, \quad u' = \sigma - u \quad \text{et} \quad v' = -v, \]  

(A2)

where \( \sigma \) is the mean velocity of the detonation front. The different derivatives in the shock frame are

\[ \frac{\partial}{\partial t} = \frac{\partial}{\partial t'} + \sigma \frac{\partial}{\partial x'}, \quad \frac{\partial}{\partial x} = -\frac{\partial}{\partial x'}, \quad \frac{\partial}{\partial y} = -\frac{\partial}{\partial y'}. \]  

(A3)

For example, the viscous stress can be evaluated

\[ \tau_{xx} = \frac{2}{3} \mu \left( \frac{2}{3} \frac{\partial u}{\partial x} - \frac{\partial v}{\partial y} \right) = \frac{4}{3} \mu \left( -\frac{\partial (\sigma - u')}{\partial x'} \right) - \frac{2}{3} \mu \left( -\frac{\partial (-v')}{\partial y'} \right) \]

\[ = \tau_{x'y'}. \]

In the same way, the other viscous components read \( \tau_{xy} = \tau_{x'y'} \) and \( \tau_{yy} = \tau_{y'y'} \). The continuity, impulse and species equations remain unchanged

\[ \frac{\partial \rho}{\partial t'} + \frac{\partial \rho u'}{\partial x'} + \frac{\partial \rho v'}{\partial y'} = 0, \]  

(A4)

\[ \frac{\partial \rho u'}{\partial t'} + \frac{\partial (\rho u'^2 + P)}{\partial x'} + \frac{\partial \rho u' v'}{\partial y'} = \frac{\partial \tau_{x'x'}}{\partial x'} + \frac{\partial \tau_{x'y'}}{\partial y'}, \]  

(A5)

\[ \frac{\partial \rho v'}{\partial t'} + \frac{\partial \rho u' v'}{\partial x'} + \frac{\partial (\rho u'^2 + P)}{\partial y'} = \frac{\partial \tau_{x'y'}}{\partial x'} + \frac{\partial \tau_{y'y'}}{\partial y'}, \]  

(A6)

\[ \frac{\partial \rho Y_k}{\partial t'} + \frac{\partial (\rho u' Y_k)}{\partial x'} + \frac{\partial (\rho v' Y_k)}{\partial y'} = \gamma_k \omega_k + \frac{\partial}{\partial x'} \left( \rho D_{km} \frac{\partial Y_k}{\partial x'} \right) + \frac{\partial}{\partial y'} \left( \rho D_{km} \frac{\partial Y_k}{\partial y'} \right). \]  

(A7)

FIG. 20. System of coordinates.
The total energy equation also remains unchanged
\[
\frac{\partial \rho E'}{\partial t'} + \frac{\partial}{\partial x'}(\rho E' u' + P u') + \frac{\partial}{\partial y'}(\rho E' v' + P v') = \frac{\partial}{\partial x'}(\tau_{x'y'}) + \frac{\partial}{\partial y'}(\tau_{y'x'}) + \sum_k \frac{\partial}{\partial x'}(\rho D_{k,m} h'_k) + \sum_k \frac{\partial}{\partial y'}(\rho D_{k,m} h'_k).
\]

(A8)

Indeed, the reactive Navier-Stokes model remains unchanged under translation and rotation. The total energy, in the new frame of coordinates reads \( E' = e + (u'^2 + v'^2)/2 \).

In the following, for the sake of clarity, the superscript will be omitted.

The equation of the internal energy can thus be obtained
\[
\rho \left( \frac{\partial e}{\partial t} + u \frac{\partial e}{\partial x} + v \frac{\partial e}{\partial y} \right) + P \left( \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \right) = \Phi + \dot{q}_{th} + \dot{q}_{diff} \tag{A9} \]

with the viscous dissipation rate \( \Phi \)
\[
\Phi = \tau_{xx} \frac{\partial u}{\partial x} + \tau_{xy} \frac{\partial u}{\partial y} + \tau_{yx} \frac{\partial v}{\partial x} + \tau_{yy} \frac{\partial v}{\partial y} \tag{A10}.
\]

the thermal flux \( \dot{q}_{th} \)
\[
\dot{q}_{th} = \frac{\partial}{\partial x} \left( \lambda \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left( \lambda \frac{\partial T}{\partial y} \right) \tag{A11}.
\]

and the diffusive flux for the enthalpy species \( \dot{q}_{diff} \)
\[
\dot{q}_{diff} = \sum_k \left[ \frac{\partial}{\partial x} \left( \rho D_{k,m} h_k \frac{\partial Y_k}{\partial x} \right) + \frac{\partial}{\partial y} \left( \rho D_{k,m} h_k \frac{\partial Y_k}{\partial y} \right) \right]. \tag{A12}
\]

Differentiation of the internal energy gives
\[
de = \left( \frac{\partial e}{\partial P} \right)_{\rho,Y_k} dP + \left( \frac{\partial e}{\partial \rho} \right)_{P,Y_k} d\rho + \sum_k \left( \frac{\partial e}{\partial Y_k} \right)_{P,\rho} dY_k. \tag{A13}
\]

From the equation of state of the gaseous mixture \( e = \sum_k Y_k h_k - \frac{P}{\rho} \) and \( T = \frac{P W}{R \rho} \), we obtain
\[
e = \sum_k Y_k h_k \left( \frac{P W}{R \rho} \right) - \frac{P}{\rho}. \tag{A14}
\]

Moreover as \( h_k = h_k^0 + \int_{t_0}^{T} c_{p,k}(\tau) d\tau \), the partial derivatives of the internal energy can then be cast in the following form:
\[
\left( \frac{\partial e}{\partial P} \right)_{\rho,Y_k} = \sum_k Y_k \frac{dh_k}{dT} \frac{W}{R \rho} - \frac{1}{\rho} = \left( \sum_k Y_k c_{p,k} \right) \frac{W}{R \rho} - \frac{1}{\rho} \tag{A15}
\]
\[
= c_{p,m} \frac{W}{R \rho} - \frac{1}{\rho} = \frac{1}{(\gamma - 1) \rho}
\]

and
\[
\left( \frac{\partial e}{\partial \rho} \right)_{P,Y_k} = - \sum_k Y_k \frac{dh_k}{dT} \frac{P W}{R \rho^2} + \frac{P}{\rho^2} = \frac{P}{(\gamma - 1) \rho} \tag{A16}
\]
\[
= - \frac{P}{(\gamma - 1) \rho^2}
\]
and then
\[
\left( \frac{\partial e}{\partial Y_k} \right)_{r, P} = h_k + \sum_i Y_i c_{p_i} \frac{P}{R \rho} \frac{T^2}{W_k} = h_k - c_{p_m} T \frac{T}{W_k}. \tag{A17}
\]

From the equation of the internal energy, we get the pressure equation. Thus, the equations for the primitive variables \((u, v, P)\) with the hydrodynamic contribution are
\[
\rho \left( \frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} \right) + \frac{\partial P}{\partial x} = \frac{\partial \tau_{xx}}{\partial x} + \frac{\partial \tau_{xy}}{\partial y}, \tag{A18}
\]
\[
\rho \left( \frac{\partial v}{\partial t} + u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} \right) + \frac{\partial P}{\partial y} = \frac{\partial \tau_{yx}}{\partial x} + \frac{\partial \tau_{yy}}{\partial y}, \tag{A19}
\]
\[
\frac{\partial P}{\partial t} + u \frac{\partial P}{\partial x} + v \frac{\partial P}{\partial y} + \rho c^2 \left( \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \right) = (\gamma - 1) (-\dot{q} + \Phi + \dot{q}_{th} + \dot{q}_{diff}). \tag{A20}
\]

In stationary regime, \(\partial \dot{q}/\partial t = 0\). The pressure equation allows us to get the following energetic balance:
\[
\mathcal{H} + \mathcal{P}_{visq} = (\gamma - 1) \left( -\dot{q} + \Phi + \dot{q}_{th} + \dot{q}_{diff} \right) \tag{A21}
\]
with the hydrodynamic contribution
\[
\mathcal{H} = \rho (c^2 - u^2) \frac{\partial u}{\partial x} + \rho (c^2 - v^2) \frac{\partial v}{\partial y} - \rho uv \left( \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right). \tag{A22}
\]

\(\mathcal{P}_{visq}\) is the power related to the viscous stress
\[
\mathcal{P}_{visq} = u \left( \frac{\partial \tau_{xx}}{\partial x} + \frac{\partial \tau_{xy}}{\partial y} \right) + v \left( \frac{\partial \tau_{yx}}{\partial x} + \frac{\partial \tau_{yy}}{\partial y} \right). \tag{A23}
\]
\(\dot{q}\) is the heat release, per unit time - \(\dot{\xi}\) is the progress variable of the chemical reaction
\[
\dot{q} = \sum_k \left( \frac{\partial e}{\partial Y_k} \right)_{r, P} W_k (v''_k - v'_k) \dot{\xi}. \tag{A24}
\]

The viscous dissipation rate \(\Phi\) is
\[
\Phi = \tau_{xx} \frac{\partial u}{\partial x} + \tau_{xy} \frac{\partial u}{\partial y} + \tau_{yx} \frac{\partial v}{\partial x} + \tau_{yy} \frac{\partial v}{\partial y}. \tag{A25}
\]

The thermal flux \(\dot{q}_{th}\) is
\[
\dot{q}_{th} = \frac{\partial}{\partial x} \left( \lambda \frac{\partial T}{\partial x} + \frac{\partial}{\partial y} \left( \lambda \frac{\partial T}{\partial y} \right) \right). \tag{A26}
\]

\(\dot{q}_{diff}\) is related to the species enthalpy diffusive flux
\[
\dot{q}_{diff} = \left\{ \begin{array}{l}
\sum_k \left[ \frac{\partial}{\partial x} \left( \rho D_{k,m} \frac{Y_k}{\partial x} \right) + \frac{\partial}{\partial y} \left( \rho D_{k,m} \frac{Y_k}{\partial y} \right) \right] \\
- \sum_k \left( h_k - c_{p_m} T \frac{T}{W_k} \right) \left[ \frac{\partial}{\partial x} \left( \rho D_{k,m} \frac{Y_k}{\partial x} \right) + \frac{\partial}{\partial y} \left( \rho D_{k,m} \frac{Y_k}{\partial y} \right) \right]. \tag{A27}
\end{array} \right.
\]

In the local coordinate system of Frenet \((\vec{l}, \vec{n})\), the vector \(\vec{l} = \vec{u}/\|\vec{u}\|\) is parallel to the streamlines and \(\theta = (\vec{x}, \vec{l})\) is the deviation angle of the streamlines. \(\vec{n}\) and \(\vec{l}\) form an orthonormal basis, with
\( (\vec{l}, \vec{n}) = \pi / 2 \). The following relations hold \( \pi = \| \vec{u} \| \cos \theta, \nu = \| \vec{u} \| \sin \theta \), and

\[
\left( \begin{array}{c}
\frac{\partial}{\partial x} \\
\frac{\partial}{\partial y}
\end{array} \right) = \left( \begin{array}{cc}
\cos \theta & -\sin \theta \\
\sin \theta & \cos \theta
\end{array} \right) \left( \begin{array}{c}
\frac{\partial}{\partial \vec{l}} \\
\frac{\partial}{\partial \vec{n}}
\end{array} \right)
\]

Thus Eq. (A22) becomes

\[
\mathcal{H} = \rho(c^2 - \| \vec{u} \|) \frac{\partial \| \vec{u} \|}{\partial \vec{l}} + \rho c^2 \| \vec{u} \| \frac{\partial \theta}{\partial \vec{n}}.
\]

Note that the local divergence of the streamlines \( \partial \theta/\partial \vec{n} \) enters into the mass equation

\[
\rho \| \vec{u} \| \frac{\partial \theta}{\partial \vec{n}} = 0.
\]