ESAIM: PROCEEDINGS AND SURVEYS, **November 2025, Vol. 78, p.37-57**
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A CLASS OF TURBULENT *K*-MODELS FOR COMPRESSIBLE FLOWS BASED ON A THERMODYNAMICAL APPROACH.

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Abstract. This work proposes a thermodynamics-based derivation of a single-equation K model for turbulence in compressible flows. Unlike classical RANS approaches, this framework ensures hyperbolicity and well-defined shocks while avoiding complex closure modeling. The model naturally incorporates turbulence effects into temperature, which is essential for reactive flows such as premixed flame propagation. A theoretical analysis of turbulent shocks is provided, and the proposed model is compared with a classical K model, showing strong similarities under specific closures.

INTRODUCTION

Industrial applications involving flows very often require turbulence to be taken into account. One of the most common strategies for modeling turbulence in industrial codes is to apply the Reynolds Averaged Navier-Stokes (RANS) approach. On the one hand, RANS models for incompressible flows have been a widely discussed topic for several decades, and a wide range of models has been proposed in the literature. On the other hand, the literature proposing RANS models for compressible flows is more scarce [1,3,21,24]. Indeed, for compressible flows, the closure of RANS models is much more complex: more equations are involved with - in general - a higher level of nonlinearity [7,25]. This clearly makes the models more complex, with more terms whose importance must be understood.

Among the models proposed in the literature, the simple K or $K-\varepsilon$ models were first proposed, followed by more sophisticated Rotta-type models [4,11]. One of the main difficulties for compressible flows is to propose sets of closures that lead to final models that are realizable, hyperbolic and whose shocks are uniquely defined. These requirements are mandatory to keep in line with physics and to provide sets of equations that can be used for numerical simulations. In this paper, we propose to derive a K model from thermodynamic considerations. Despite the simplicity of the resulting class of models, this approach is motivated by two aspects.

Firstly, as mentioned above, models with appreciable mathematical properties can contribute to the stability of numerical simulations. The thermodynamics-based modeling framework [2] is a powerful tool for building models dedicated to multi-phase multi-component reactive flows, see for example [10, 14–16, 18,

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Article published online by EDP Sciences and available at https://www.esaim-proc.org or https://doi.org/10.1051/proc/202578037

19]. Provided that the EOS (Equation Of State) of the various components are correctly chosen, the final models are naturally hyperbolic and conservative with uniquely defined shocks. Moreover, it will be seen in the paper that tedious computations can be dispensed with to build the models. These are clearly two major advantages of this thermodynamic approach over RANS approaches.

Secondly, the thermodynamic framework is worth studying as temperature is often a key parameter in modeling reactive flows. Let's briefly recall the case of premixed flames, see for example [5, 20, 27] among many others. The propagation of premixed flames in gas clouds is driven by two phenomena: the chemical reaction (combustion) whose rate of reaction is directly associated with gas temperature by an Arrhenius law (with an exponential dependence on temperature), and the heat flux at the flame front between hot/burnt gases and fresh/unburnt gases. This heat flux increases the temperature of the fresh mixture. The reaction speed increases due to the Arrhenius law and the reaction takes place, transforming the fresh gas into burnt gas. This mechanism causes the flame front to propagate from the burnt gas zone to the fresh mixture zone. Consequently, the speed of propagation of the flame front is directly linked to this heat flux. For laminar flows, the heat flux is due to thermal conduction while turbulent mixing largely predominates for turbulent flows. One idea might therefore be to modify the temperature used in the Arrhenius's law to take account of the intensity of turbulence. This would have the effect of accelerating the flame front as turbulence increases in the flow by increasing the reaction rate, while keeping the reactive source term globally unchanged.

The document is structured as follows. In section 1, the modeling approach and physical assumptions are detailed. A class of single-equation K models is proposed to account for turbulence. The latter is described using only one equation for turbulent energy. With regard to the previous comment on premixed flames, it should be noted that the temperature of this class of models incorporates a contribution due to turbulence. This class of models inherits good mathematical properties, which are briefly recalled. Among these properties, emphasis is placed in section 2 on the definition of turbulent shocks. Theoretical studies are proposed to illustrate the behavior of pressure and temperature through shocks. Finally, a comparison is proposed in section 3 with the classical K model [24] including the closure for turbulent dissipation. It is shown that, up to certain specific closures, the class of models based on the thermodynamic approach can provide a model that is very close to the RANS model introduced in [24].

1. A SIMPLE TURBULENCE MODEL BUILT USING A THERMODYNAMICAL APPROACH

1.1. **Extensive description of the model**

Let us consider a mass of fluid $\mathscr{M}$ that occupies a volume $\mathscr{V}$, and that travels with a velocity U. This velocity represents an averaged velocity of the mass of fluid $\mathscr{M}$. We also assume that this mass of fluid is associated with three energies.

- The kinetic energy $\mathscr{M}U^2/2$ of the mass of fluid, which represents a macroscopic energy scale.
- A mesoscopic energy, denoted by $\mathscr{E}_K$, which represents the kinetic energy of small-scale fluid velocity within the volume $\mathscr{V}$. This energy is the turbulent kinetic energy.
- The microscopic energy which corresponds to the the thermodynamical internal energy, and denoted by $\mathscr{E}_L$.

In the present approach, we choose to consider that the mesoscopic energy contribution can be described using a thermodynamical approach, as in [8, 12, 22, 26]. The microscopic and mesoscopic energies, $\mathscr{E}_L$ and $\mathscr{E}_K$, are then gathered to form the energy $\mathscr{E}$ of the mass of fluid:

$$\mathscr{E} = \mathscr{E}_L + \mathscr{E}_K. \tag{1}$$

The energy $\mathscr{E}$ does not account for the kinetic energy, it represents the energy of the small scales of the mass of fluid.

Still following a thermodynamical point of view, the internal energy $\mathscr{E}_L$ and the turbulent energy $\mathscr{E}_K$ are respectively associated with an thermodynamical entropy η_L and with a turbulent entropy η_K. These entropies and the energies are assumed to be positive: $\eta_L \geq 0$, $\mathscr{E}_L \geq 0$, $\eta_K \geq 0$ and $\mathscr{E}_K \geq 0$. The total entropy of the volume of fluid is denoted by η. The turbulent and thermodynamical entropies are then defined through the relations:

$$\eta_L = \eta \quad \text{and} \quad \eta_K = \zeta \eta, \tag{2}$$

where the factor ζ is positive. In the following, energies are considered as the potentials that allow to define the thermodynamical behavior and the turbulent behavior of the fluid. We thus have to choose two Equation of States (EoS):

$$(\mathscr{M}, \mathscr{V}, \eta_\phi) \mapsto \mathscr{E}_\phi(\mathscr{M}, \mathscr{V}, \eta_\phi), \quad \text{for } \phi = \{L, K\}. \tag{3}$$

For the turbulent EoS, the following additional constraint is assumed for all $\mathscr{M}$ and $\mathscr{V}$:

$$\mathscr{E}_K(\mathscr{M}, \mathscr{V}, \eta_K) \underset{\eta_K \to 0}{\longrightarrow} 0.$$

The evolution of the different quantities is supposed to be ruled by Gibbs relations, that is:

$$d\mathscr{E}_\phi = T_\phi d\eta_\phi - P_\phi d\mathscr{V} + \mu_\phi d\mathscr{M}, \quad \text{for } \phi = \{L, K\}. \tag{4}$$

The pressure P_ϕ and the temperature T_ϕ of the thermodynamical and turbulent contributions are then defined thanks to (4) and to the EoS (3). They read:

$$P_\phi(\mathscr{M}, \mathscr{V}, \eta_\phi) = -\frac{\partial \mathscr{E}_\phi}{\partial \mathscr{V}}_{|\mathscr{M}, \eta_\phi}, \quad T_\phi(\mathscr{M}, \mathscr{V}, \eta_\phi) = \frac{\partial \mathscr{E}_\phi}{\partial \eta_\phi}_{|\mathscr{M}, \mathscr{V}}, \quad \text{for } \phi = \{L, K\}. \tag{5}$$

We assume here that the EoS are chosen so that the temperatures and the pressures are positive:

$$P_L > 0, \quad P_K \geq 0, \quad T_L > 0 \quad \text{and} \quad T_K \geq 0.$$

The Gibbs potential μ_ϕ that appears in Gibbs relations (4) will not be used in the sequel.

By using closure relations (1) and (2), we easily get a Gibbs relation for the whole volume of fluid from Gibbs relations (4). It reads:

$$d\mathscr{E} = (T_L + \zeta T_K)\, d\eta - (P_L + P_K)\, d\mathscr{V} + (\mu_L + \mu_K)\, d\mathscr{M} + \eta T_K d\zeta, \tag{6}$$

and the total pressure P and the total temperature T of the fluid can then be identified from the two first terms on the right hand side:

$$T = T_L + \zeta T_K, \quad \text{and} \quad P = P_L + P_K. \tag{7}$$

The last term on the right hand side of relation (6) models the energy exchange between the thermodynamical and the turbulent contributions. It should be noted that the pressure law for P is the same than the pressure law used in [8, 12].

Remark. The description above can be seen as the mixture of two miscible phases such that $\mathscr{V}_K = \mathscr{V}_L = \mathscr{V}$, sharing the same mass $\mathscr{M}_K = \mathscr{M}_L = \mathscr{M}$, but with different energies $\mathscr{E}_K \neq \mathscr{E}_L$ (in general). Due to the miscibility assumption $\mathscr{V}_K = \mathscr{V}_L = \mathscr{V}$, a Dalton's law is recovered for the pressures: $P = P_K + P_L$ as in [6, 13, 17, 19] for instance.

We consider now the following closure for the evolution of the mass and the energy of the fluid. The mass $\mathscr{M}$ of the volume of fluid is constant:

$$d\mathscr{M} = 0. \tag{8}$$

The first law of thermodynamics applies. When only accounting for the force due to the total pressure P on the volume, the latter reads:

$$d\mathscr{E} = -P\, d\mathscr{V}. \tag{9}$$

As a consequence, relation (6) simply gives:

$$T\, d\eta = -\eta T_K\, d\zeta. \tag{10}$$

At last, the velocity field U is introduced. It corresponds to the velocity of the center of mass of the volume of fluid $\mathscr{V}$. For the sake of simplicity, we consider here one-dimensional flows. Accordingly to (9), we restrict here to the force due to the total pressure P. Therefore, the Newton's law gives that:

$$d(\mathscr{M}U) = -\mathscr{V}\partial_x(P)\, dt. \tag{11}$$

Moreover, the flow is compressible so that the volume $\mathscr{V}$ of the fluid is modified following the divergence of the velocity field:

$$d\mathscr{V} = \mathscr{V}\partial_x(U)\, dt. \tag{12}$$

At that point, five unknowns have been introduced: $\mathscr{V}$, $\mathscr{M}$, η, ζ and U; and only four closure relations for the time evolution of the unknowns have been given: (8), (9), (12) and (11). Indeed, the time evolution of ζ has not yet been defined. This will be done in the next section.

1.2. A complete set of PDE in conservative form with intensive quantities

We turn now to a more classical description of the flow through a set of Partial Differential Equations (PDE) whose unknowns are intensive quantities. We thus define the specific volume $\tau = \mathscr{V}/\mathscr{M}$ and the density $\rho = 1/\tau$, the specific energies $e = \mathscr{E}/\mathscr{M}$, $e_K = \mathscr{E}_K/\mathscr{M}$ and $e_L = \mathscr{E}_L/\mathscr{M}$, the specific entropies $s = \eta/\mathscr{M}$, $s_K = \eta_K/\mathscr{M}$ and $s_L = \eta_L/\mathscr{M}$.

The turbulent entropy parameter $\zeta = \eta_K/\eta = s_K/s$ is already an intensive quantity. We choose here the following time evolution for ζ:

$$d\zeta = \mathscr{S}_K dt,$$

where the source term $\mathscr{S}_K$ will be defined below. Considering the velocity field U, the derivative $d\psi$ of any quantity ψ corresponds in fact to the derivative along the streamline: $d\psi = (\partial_t(\psi) + U\partial_x(\psi))dt$. Hence from the closure for ζ and from (8), (9), (12) and (11) we get the following set of four equations which is written in conservative form:

$$\begin{cases} \partial_t(\rho\zeta)+\partial_x(\rho U\zeta)=\rho\mathscr{S}_K, \\ \partial_t(\rho)+\partial_x(\rho U)=0, \\ \partial_t(\rho U)+\partial_x\left(\rho U^2+P\right)=0, \\ \partial_t(\rho E)+\partial_x(U(\rho E+P))=0, \end{cases} \tag{13}$$

where $E=e+U^2/2$ is the specific total energy. The unknowns of the system are the four intensive quantities: $\tau=1/\rho$, s, ζ and U. System (13) is then closed thanks to the results of the previous sections. Indeed, we have:

$$e=e_L(\tau_L,s_L)+e_K(\tau_K,s_K), \quad P=P_L(\tau_L,s_L)+P_K(\tau_K,s_K), \quad s_K=\zeta s, \quad s_L=s, \quad \text{and} \quad \tau_L=\tau_K=\tau, \tag{14}$$

where $(\tau_\phi,s_\phi)\mapsto e_\phi(\tau_\phi,s_\phi)$ are the EoS given in intensive form, and where:

$$P_\phi=-\frac{\partial e_\phi}{\partial\tau_\phi}_{|s_\phi}, \quad T_\phi=\frac{\partial e_\phi}{\partial s_\phi}_{|\tau_\phi}, \quad \text{for } \phi=\{K,L\}. \tag{15}$$

Moreover, the total temperature reads:

$$T=T_L(\tau,s)+\zeta T_K(\tau,\zeta s),$$

and the source term $\mathscr{S}_K$ should be defined with respect to $\tau=1/\rho$, s, ζ and U.

As noted above, it still remains to model the time evolution of ζ through the source term $\mathscr{S}_K$. We then assume that the specific energies $(\tau_L,s_L)\mapsto e_L(\tau_L,s_L)$ and $(\tau_K,s_K)\mapsto e_K(\tau_K,s_K)$ are strictly convex and that the associated temperatures fulfill $T_L(\tau_L,s_L)>0$ and $T_K(\tau_K,s_K)\geq 0$, and that the associated pressures are such that $P_L(\tau_L,s_L)>0$ and $P_K(\tau_K,s_K)\geq 0$. This implies that the entropies $(\tau_L,e_L)\mapsto s_L(\tau_L,e_L)$ and $(\tau_K,e_K)\mapsto s_K(\tau_K,e_K)$ are strictly concave [9]. We also get that the energy $(\tau,s_L,s_k)\mapsto e(\tau,s_L,s_k)$ defined by (14) is strictly convex. The entropy s can be defined implicitly with respect to (ζ,τ,e) by using the closures (14). The entropy $(\zeta,\tau,e)\mapsto s(\zeta,\tau,e)$ is thus defined by:

$$e=e_L(\tau,s)+e_K(\tau,\zeta s), \tag{16}$$

or equivalently by $\mathscr{G}(\zeta,\tau,e,s)=0$ with:

$$\mathscr{G}(\zeta,\tau,e,s)=e_L(\tau,s)+e_K(\tau,\zeta s)-e.$$

Let us consider a fixed ζ. Since the energies e_L and e_K are strictly convex, we get that $(\tau,e,s)\mapsto\mathscr{G}(\zeta,\tau,e,s)$ is also strictly convex. Moreover, the temperatures and pressures have been assumed non-negative. Therefor, we have:

$$\frac{\partial\mathscr{G}}{\partial s}_{|\zeta,\tau,e}=T_L+\zeta T_K=T>0 \quad \text{and} \quad \frac{\partial\mathscr{G}}{\partial\tau}_{|\zeta,s,e}=P_L+P_K>0.$$

Finally, considering a fixed ζ, the function $(\tau,e,s)\mapsto\mathscr{G}(\zeta,\tau,e,s)$:

- is continuous,
- is strictly convex,
- its derivative with respect to τ does not vanish,
- its derivative with respect to e is positive.

Hence, the function $(\tau,e)\mapsto s(\zeta,\tau,e)$ implicitly defined by $\mathscr{G}$ trough (16) is strictly concave. When considering a fixed (τ,e), this proof can be used to prove that the function $\zeta\mapsto s(\zeta,\tau,e)$ is strictly concave.

The equation (6) reads in intensive form:

$$(\partial_t(e)+U\partial_x(e)) = P(\partial_t(\tau)+U\partial_x(\tau))+T\ (\partial_t(s)+U\partial_x(s))+sT_K\ d\zeta. \tag{17}$$

Since the entropy s is concave, the second law of thermodynamics states that s should increase along a streamline for a closed and isolated system with $\partial_t(\tau)+U\partial_x(\tau)=\partial_t(e)+U\partial_x(e)=0$:

$$T\ (\partial_t(s)+U\partial_x(s))\geq 0. \tag{18}$$

When $\partial_t(\tau)+U\partial_x(\tau)=\partial_t(e)+U\partial_x(e)=0$, equation (17) simply gives:

$$0=T\ (\partial_t(s)+U\partial_x(s))+sT_K\ \mathscr{S}_K. \tag{19}$$

As a consequence, in order to be in agreement with the second law of thermodynamics, the source term $\mathscr{S}_K$ should fulfill the relation: $sT_K\ \mathscr{S}_K\leq 0$. Owing to the assumptions made on the EoS, we have $T>0$ and $s_K\geq 0$, hence the previous constraint reduces to $\mathscr{S}_K\leq 0$. A first straightforward choice is to choose an "exponential" decrease of the turbulent entropy along a streamline:

$$\mathscr{S}_K=-\frac{\zeta}{\lambda}, \tag{20}$$

where λ is a positive time-scale to be defined. We recall that the production of turbulent entropy has not yet been introduced in the model, this will be done in section 3.

1.3. Some properties of the model

In this section, some mathematical properties of the model of section 1.2 without source term $\mathscr{S}_K=0$ are briefly reviewed. They are directly inherited from the Euler structure of the model.

Considering the variable $Y=(\zeta,U,P,s)$, the convective part of system (13) can be written:

$$\partial_t(Y)+A(Y)\partial_x(Y)=0,$$

where the Jacobian matrix $A(Y)$ is:

$$A(Y)=\begin{pmatrix} U & 0 & 0 & 0\\ 0 & U & \tau & 0\\ O & -\tau\dfrac{\partial P}{\partial\tau}_{|\zeta,s} & U & O\\ 0 & 0 & 0 & U\end{pmatrix}. \tag{21}$$

The eigenvalues of $A(Y)$ are: $\lambda_1=U-c$, $\lambda_2=\lambda_3=U$ and $\lambda_4=U+c$, with c the sound speed defined as:

$$c^2=-\tau^2\frac{\partial P}{\partial\tau}_{|\zeta,s}=-\tau^2\frac{\partial P_L}{\partial\tau}_{|s_L}-\tau^2\frac{\partial P_K}{\partial\tau}_{|s_K}=c_L^2+c_K^2.$$

Since each energy e_L and e_K is assumed strictly convex, the associated square sound speeds c_L^2 and c_K^2 are positive. Thus, c is defined in $\mathbb{R}_*^+$ and the four eigenvalues of $A(Y)$ are real. The right eigenvalues are respectively:

$$r_1 = (0,1,-c/\tau,0),\ r_2 = (1,0,0,0),\ r_3 = (0,0,0,1),\ r_4 = (0,1,c/\tau,0).$$

Provided that $c > 0$, the set of four vectors $\{r_i, i = 1..4\}$ spans $\mathbb{R}^4$. Hence, the convective part of system (13) is hyperbolic. From the definitions above of λ_i and r_i, it can be easily checked that the field associated with:

- λ_2 and λ_3 are linearly degenerate;
- λ_1 and λ_4 are genuinely non-linear.

The waves associated with λ_1 and λ_4 can thus be either rarefaction waves or shock waves. The latter are studied in details in dedicated section 2.

1.4. **Choice for the EoS of the laminar and turbulent contributions**

In the following, model (13) is studied for a specific choice of EoS. For the laminar contribution $(\tau_L, s_L) \mapsto e_L$ we use a perfect gas law: $e_L(\tau_L, s_L) = \tau_L^{(1-\gamma)} \exp(s_L/C_v)$, where $\gamma > 1$ is the polytropic exponent and $C_v > 0$ is the specific heat capacity (in $J/kg/K$). Both have to be specified by the user depending on the fluid that is modeled. Thanks to definitions (15), this leads to the classical relations:

$$e_L(\tau_L, s_L) = C_v T_L(\tau_L, s_L), \quad \text{and} \quad P_L(\tau_L, s_L) = (\gamma - 1)\tau_L^{-\gamma} \exp(s_L/C_v) = (\gamma - 1)\frac{e_L(\tau_L, s_L)}{\tau_L}.$$

The choice for the turbulent part of the model is less classical. It is based on the EOS proposed in [8,12,22] in a framework where the turbulent entropy is a constant (i.e. a fixed parameter of the EoS). We propose here a law that extends this "isentropic" EoS while keeping the same dependence to the specific volume. As a consequence, the resulting pressure laws are identical for both EoS for a given turbulent entropy, but the temperature law differs. Hence, we introduce for the turbulent EoS:

$$(\tau_K, s_K) \mapsto e_K(\tau_K, s_K) = A\frac{s_K^2}{2}\left(\frac{\tau_K}{\tau_0}\right)^{-\beta}. \tag{22}$$

In EoS (22), three parameters are used: $A > 0$, $\beta > 0$ which plays a role similar to the γ in the perfect gas EoS, and $\tau_0 > 0$ which is normalization term that could also be included in parameter A. For EoS (22), the pressure and temperature defined thanks to (15) are:

$$e_K(\tau_K, s_K) = \frac{s_K T_K(\tau_K, s_K)}{2}, \quad \text{and} \quad P_K(\tau_K, s_K) = A\beta\frac{s_K^2}{2\tau_0}\left(\frac{\tau_K}{\tau_0}\right)^{(-\beta-1)} = \beta\frac{e_K(\tau_K, s_K)}{\tau_K}.$$

The choice of the term s_K^2 in definition (22) for e_K allows to retrieve a classical dissipation behavior as proposed by [24]. More details on that point are provided in section 3.

Using closures (14) and the two EoS defined above, we can then express the EoS for the mixture as:

$$(\zeta, \tau, s) \mapsto e(\zeta, \tau, s) = e_K(\tau, \zeta s) + e_L(\tau, s), \tag{23}$$

which gives the mixture pressure and mixture temperature law:

$$P(\zeta, \tau, s) = P_K(\tau, \zeta s) + P_L(\tau, s) \quad \text{and} \quad T(\zeta, \tau, s) = \zeta T_K(\tau, \zeta s) + T_L(\tau, s).$$

2. Rankine-Hugoniot relations and turbulence in shock waves

The Rankine-Hugoniot relations for the intensive model (13) of the previous section are:

$$\left\{\begin{array}{l} -\sigma[\rho\zeta]+[\rho U\zeta]=0, \\ -\sigma[\rho]+[\rho U]=0, \\ -\sigma[\rho U]+[\rho U^2+P]=0, \\ -\sigma[\rho E]+[U(\rho E+P)]=0, \end{array}\right. \tag{24}$$

where σ stands for the speed of the shock wave, and where the notation $[\phi]$ represents the jump of the quantity ϕ between the right r and left l side of the shock: $[\phi]=\phi_r-\phi_l$. By introducing $J=\rho(U-\sigma)$, and since $J\neq 0$ with $[J]=0$ in shock waves, relations (24) can also be written in the (classical) following manner:

$$\left\{\begin{array}{l} [\zeta]=0, \\ J[\tau]=[U], \\ [U]^2=-[\tau][P], \\ [e]+\overline{P}[\tau]=0, \end{array}\right. \tag{25}$$

where it has been set: $\overline{P}=(P_l+P_r)/2$. From relations (25), two studies are now carried on in the two sections below. First, the criterion for the admissibility of shock waves on the basis of the third equation of (25) is studied; then the variation of the pressure in the shock is investigated by the mean of the Hugoniot curve (i.e. the fourth equation of (25)). These results are compared to those obtained for the laminar Euler model (i.e. $\zeta=0$ for all (t,x)).

In order to define uniquely the shocks through relations (25) (or (24)), an additional information has to be provided see [9, 23]. In the following, we choose to use a criterion based on the entropy inequality (18), and more precisely on its weak form:

$$-\sigma[\rho s]+[\rho U s]\geq 0,$$

or equivalently:

$$J[s]\geq 0. \tag{26}$$

2.1. **The Hugoniot curve and shock definition**

In this section we focus on the Hugoniot curve which corresponds to the last relation in (25). Using closures (14) and the EoS of section 1.4, the mixture energy and the mixture pressure are respectively:

$$e(\zeta,\tau,s)=(\tau_r^{\#})^{(1-\gamma)}\exp\left(s_r/C_v\right)+A\zeta_r^2\frac{s_r^2}{2}\left(\frac{\tau_r^{\#}}{\tau_0}\right)^{-\beta},$$

and

$$P(\zeta,\tau,s)=(\gamma-1)(\tau_r^{\#})^{-\gamma}\exp\left(s_r/C_v\right)+A\beta\tau_0\zeta_r^2\frac{s_r^2}{2}\left(\frac{\tau_r^{\#}}{\tau_0}\right)^{(-\beta-1)}.$$

It should be noted that first relation of (25) gives us that $\zeta_r=\zeta_l$. We now assume that the state on the left of the shock denoted by a subscript l is known and fixed. The Hugoniot curve can be written $\mathscr{H}_l(\tau_r,s_r)=0$, with:

$$\mathscr{H}_l(\tau_r,s_r)=e(\zeta_r,\tau_r,s_r)-e(\zeta_l,\tau_l,s_l)+\frac{\tau_r-\tau_l}{2}(P(\zeta_r,\tau_r,s_r)+P(\zeta_l,\tau_l,s_l).$$

For $\tau_r = \tau_l$ we have $\mathscr{H}_l(\tau_l, s_r) = e(\zeta_r, \tau_l, s_r) - e(\zeta_l, \tau_l, s_l)$. Since we have chosen the energies such that:

$$\partial_{s_L}(e_L)_{|\tau_L} > 0 \quad \text{and} \quad \partial_{s_K}(e_K)_{|\tau_K} \geq 0,$$

we also have

$$\partial_s(e)_{|\tau,\zeta} > 0.$$

Thus, e is an increasing function of s because $\zeta \geq 0$ and we then have:

$$s_r \leq s_l \Longleftrightarrow \mathscr{H}_l(\tau_l, s_r) \leq 0. \tag{27}$$

The derivative of $\mathscr{H}_l$ with respect to τ_r reads:

$$\partial_{\tau_r}(\mathscr{H}_l)_{|s_r,\zeta_r} = -\frac{1}{2}\left((P_r - P_l) - (\tau_r - \tau_l)\partial_{\tau_r}(P_r)\right).$$

Thanks to the definition of the mixture pressure law, we have:

$$\partial_\tau(P)_{|s,\zeta} < 0 \quad \text{and} \quad \partial^2_{\tau\tau}(P)_{|s,\zeta} > 0,$$

and thus the pressure is a convex decreasing function of τ. So, the following relation holds:

$$P_r \leq P_l + (\tau_r - \tau_l)\partial_\tau(P)_{|s,\zeta}(\zeta_r, \tau_r, s_r) \Longleftrightarrow \tau_l \leq \tau_r,$$

and hence:

$$\tau_l \leq \tau_r \Longleftrightarrow \partial_{\tau_r}(\mathscr{H}_l)_{|s_r,\zeta_r} \geq 0. \tag{28}$$

Let us put together the results of relations (27) and (28). If $\tau_l \leq \tau_r$, $\mathscr{H}_l$ is a increasing function of τ_r (see (28)) and it possesses a unique zero if and only if $\mathscr{H}_l(\tau_l, s_r) \leq 0$, which thanks to (27) is equivalent to $s_r \leq s_l$. Conversely, if $\tau_l \geq \tau_r$, $\mathscr{H}_l$ is a decreasing function of τ_r (see (28)) and it possesses a unique zero if and only if $\mathscr{H}_l(\tau_l, s_r) \geq 0$, which thanks to (27) is equivalent to $s_r \geq s_l$. Hence, Hugoniot curve allows to define shock in a unique manner if and only if $[\tau][s] \leq 0$.

2.2. **Criterion for determining admissible shocks**

Third jump relation of (25) allows to define correctly the velocity jump if and only if

$$[\tau][P] \leq 0. \tag{29}$$

Let us study the criterion to be fulfilled by shock waves in order to have (29). For that purpose, we assume that the state on the left of the shock is known and we write $[P] = P_r - P_l = P(\zeta_r, \tau_r, s_r) - P(\zeta_l, \tau_l, s_l)$. First of all, the first relation of (25) gives us that $\zeta_r = \zeta_l$. The derivative of $[P]$ with respect to τ_r is:

$$\partial_{\tau_r}([P])_{|s_r,\tau_l,s_l} = \partial_{\tau_r}(P_r)_{|,s_r} = -\frac{A\beta}{2}\zeta^2 s_r^2 \tau_0^2(\beta+1)\left(\frac{\tau_r}{\tau_0}\right)^{-\beta-2} - \gamma(\gamma-1)\tau_r^{-\gamma-1}\exp\left(s_r/C_v\right)$$

Then, it straightforwardly arises that

$$\partial_{\tau_r}([P])_{|s_r,\tau_l,s_l} < 0.$$

Moreover, we also straightforwardly get the two following limits:

$$\lim_{\tau_r \to 0^+} [P] = +\infty \quad \text{and} \quad \lim_{\tau_r \to +\infty} [P] = -P_l < 0.$$

Since the function $\tau_r \mapsto [P]$ is continuous for $\tau_r > 0$, we obtain from the previous remarks that there exists a unique value $\tau_r^{\#}$ such that $P(\zeta_r, \tau_r^{\#}, s_r) = P(\zeta_l, \tau_l, s_l)$, or by using the explicit formula for the mixture pressure:

$$(\gamma-1)(\tau_r^{\#})^{-\gamma} \exp(s_r/C_v) + A\beta\tau_0\zeta_r^2 \frac{s_r^2}{2}\left(\frac{\tau_r^{\#}}{\tau_0}\right)^{(-\beta-1)} = (\gamma-1)\tau_l^{-\gamma}\exp(s_l/C_v) + A\beta\zeta_l^2\tau_0\frac{s_l^2}{2}\left(\frac{\tau_l}{\tau_0}\right)^{(-\beta-1)} \tag{30}$$

Relation (30) implicitly defines $\tau_r^{\#}$ as a function of s_r and left state l. By differentiating (30) for a fixed left state, we can obtain explicitly the derivative of $(s_r) \mapsto \tau_r^{\#}(s_r)$ with respect to s_r:

$$\frac{d\tau_r^{\#}(s_r)}{ds_r} = \frac{\frac{(\gamma-1)}{C_v}(\tau_r^{\#})^{-\gamma}\exp(s_r/C_v) + A\beta\tau_0\zeta_r^2 s_r\left(\frac{\tau_r^{\#}}{\tau_0}\right)^{(-\beta-1)}}{\gamma(\gamma-1)(\tau_r^{\#})^{-\gamma-1}\exp(s_r/C_v) + A\beta(\beta+1)\tau_0^2\zeta_r\frac{s_r^2}{2}\left(\frac{\tau_r^{\#}}{\tau_0}\right)^{(-\beta-2)}},$$

which is non-negative:

$$\frac{d\tau_r^{\#}(s_r)}{ds_r} > 0.$$

Moreover, relation (30) leads to: $\tau_r^{\#}(s_l) = \tau_l$. Therefore, since $\tau_r^{\#}$ is an increasing function of s_r, we get that:

$$s_r \le s_l \Longleftrightarrow \tau_r^{\#}(s_r) \le \tau_l$$

Let us now study the case $s_r \le s_l$. For convenience, the previous results are gathered in Figure 1. The main result is that there exist two zones for admissible shocks in agreement with relation (29):

$$0 < \tau_r \le \tau_r^{\#}(s_r) \quad \text{and} \quad \tau_r \ge \tau_l.$$

Thanks to the result of the previous section, we know that for the former zone the Hugoniot curve has no solution. Sole the latter zone thus corresponds to admissible shocks in the sense of (29). Hence, for $[s] \le 0$ we obtain in admissible shocks $[\tau] \ge 0$ and $[P] \le 0$. Moreover, the entropy jump relation (26) leads to $J \le 0$, which corresponds to a 3-shock wave.

Turning to the case $s_r \ge s_l$, the same reasoning applies and the results are summarized hereafter while the details are left to the reader. For $[s] \ge 0$ we obtain in admissible shocks $[\tau] \le 0$, $[P] \ge 0$ and $J \le 0$, which corresponds to a 1-shock wave.

Finally, it should be noted that for 1-shocks and 3-shocks we have $J[\tau] \le 0$. Hence, thanks to second relation of (25) we have $[U] \le 0$ in all the shocks. As a consequence, the velocity jump defined by third relation of (25) reads:

$$[U] = -\sqrt{-[P][\tau]}.$$

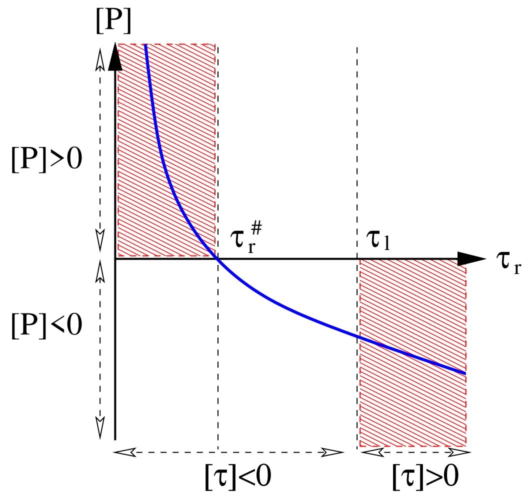

FIGURE 1. Summary of the properties of $\tau_r \mapsto [P]$ when $s_r \leq s_l$. The blue curve represents $[P]$ and the two red zones correspond to admissible shocks in the sense of relation (29).

2.3. **Pressure variation in shocks**

In this section we focus on the Hugoniot curve which corresponds to the last relation in (25). Using closures (14), it can be written by separating laminar and turbulent contributions:

$$[e]+\overline{P}[\tau] \;=\; [e_l]+\overline{P_l}[\tau] \;+\; [e_K]+\overline{P_K}[\tau] \;=\; 0. \tag{31}$$

Remark. It should be remarked that when turbulence is null on both sides of the shock, i.e. $P_K = 0 \Leftrightarrow e_K = 0$, (31) defines the classical laminar Hugoniot curve: $[e_l]+\overline{P_l}[\tau] = 0$. Hence, for purely laminar situations, laminar shocks are recovered by the model.

The specific EoS introduced in section 1.4 give the following relations between energies and pressures: $e_K\beta_K = P_K\tau$ and $e_L(\gamma-1) = P_L\tau$. Hence the Hugoniot curve (31) can be written:

$$\left[\frac{\tau P_L}{\gamma-1}\right]+\overline{P_l}[\tau] \;+\; \left[\frac{\tau P_K}{\beta_K}\right]+\overline{P_K}[\tau] \;=\; 0. \tag{32}$$

As in [23], we introduce the parameter $z = \tau_r/\tau_l$ and equation (32) is re-written in terms of z:

$$P_{K,r}\left(\frac{\beta_K+2}{\beta_K}\,z-1\right) - \,P_{K,l}\left(\frac{\beta_K+2}{\beta_K}-z\right) \;+\; P_{L,r}\left(\frac{\gamma+1}{\gamma-1}\,z-1\right) - \,P_{L,l}\left(\frac{\gamma+1}{\gamma-1}-z\right) \;=\; 0. \tag{33}$$

From relations (25) we have $[\zeta] = 0$, where thanks to the closures (14) we get $\zeta = s_K/s = s_K/s_L$. By using the EoS of section 1.4, entropies can be expressed in terms of the pressures and specific volume for both contributions:

$$s_L(\tau,P_L) = C_V \ln\left(\frac{P_L\tau^\gamma}{\gamma-1}\right) \quad \text{and} \quad s_K(\tau,P_K) = \sqrt{\frac{2\tau_0 P_K}{A\beta_K}(\tau/\tau_0)^{\beta+1}}.$$

Still using the parameter z, the jump relation $[\zeta] = 0 = [s_K/s_L]$ then gives explicitly the pressure $P_{K,r}$ as a function of z and $P_{L,r}$:

$$P_{K,r} \;=\; P_{K,l}\; z^{-\beta_K - 1} \left(\frac{\ln\left(\frac{P_{L,r} z^{\gamma} \tau_l^{\gamma}}{\gamma-1}\right)}{\ln\left(\frac{P_{L,l} \tau_l^{\gamma}}{\gamma-1}\right)} \right)^2 . \tag{34}$$

Putting relation (34) into (33) leads to an implicit definition of the pressure $P_{L,r}$ with respect to z and to the left state.

Remark. It is known from section (2.2) that a 3-shock wave is such that $[P] \leq 0 \Leftrightarrow P_{K,r} + P_{L,r} \leq P_{K,l} + P_{L,l}$. Using relation (34) one can express this inequality with respect to $P_{L,r}$, z and to the left state:

$$P_{L,r} + P_{K,l}\; z^{-\beta_K - 1} \left(\frac{\ln\left(\frac{P_{L,r} z^{\gamma} \tau_l^{\gamma}}{\gamma-1}\right)}{\ln\left(\frac{P_{L,l} \tau_l^{\gamma}}{\gamma-1}\right)} \right)^2 \leq P_{K,l} + P_{L,l}.$$

Unfortunately, this inequality defines the boundary domain of 3-shocks in an implicit manner. Obviously, the same remark holds for 1-shock wave.

2.4. **Numerical study of a family of turbulent shocks**

Shocks are thus defined by the set of non-linear equations (34)-(33), which can be reduced in a sole non-linear equation for finding $P_{L,r}$. For a given ratio z, the laminar and turbulent pressures of the left state can not be explicitly written. In the following, we focuse on 3-shocks for a given (and fixed) left state, and we propose to study the right state with respect to z in a numerical manner. System (34)-(33) is solved thanks to a bisection algorithm.

The first point is to choose EOS parameters for the laminar contribution. Two parameters have to be chosen: γ and C_v. For that purpose, a reference point with $P_{ref} = 10^5\ Pa$ and $T_{ref} = (1500 + 273)\ K$ is retained. It corresponds to a temperature that can be reached in hydrogen-air cloud deflagration. For this reference point the density is $\rho_{ref} = 0.197\ kg/m^3$ and the sound speed is $c_{ref} = 814\ m/s$. For a perfect gas EOS, we have: $\gamma = \rho_r ef * c_{ref}^2/P_{ref}$ and $C_v = P_{ref}/(\rho_{ref} T_{ref}(\gamma - 1))$, so that we can compute: $\gamma = 1.305$ and $C_v = 938.7\ J/K$. The EOS parameters for the laminar EOS are thus chosen.

Let us now define the left state of the 3-shock. It defined for a fixed total pressure $P_{K,l} + P_{L,l} = P_{ref}$ with two values of the turbulent pressure $P_{K,l} = \{0, 5000\}\ Pa$. The case $P_{K,l} = 0$ is a purely laminar case and it will be used as the reference result in the following. The left specific volume is chosen accordingly to ρ_{ref}, that is $\tau_l = 1/\rho_{ref}$. From these values of $P_{L,l}$, $P_{K,l}$ and τ_l, one can retrieve all the other quantities, and in particular the entropies: $s_{L,l} = s_L(\tau_l, P_{L,l})$ and $s_{K,l} = s_K(\tau_l, P_{K,l})$, which also give the value of $\zeta_l = s_{K,l}/s_{L,l}$.

At last, we need to define the EOS parameters for the turbulent contribution. That point is clearly more tricky. The parameter τ_0 is fixed to 1. It is indeed not very important because it could be integrated into the parameter A. Then, the shocks are computed for several values are the parameters A and β_K. The value $\beta_K = 2/3$ enables to recover the turbulent pressure law already proposed in [8, 12], which also arises in more classical compressible $K - \varepsilon$ models (see also section 3 for more details). We thus choose

$\beta_K = \{2/30, 2/3, 5/3\}$ and $A = \{0.1, 1, 10\}$ K^2kg/J.

In Figures 2-5, the right state are plotted for several couples (β_K, A) and for several values of the left pressure $P_{K,l} = 5000$ Pa. The reference situation is chosen as the laminar case $P_{K,l} = 0$, which obviously does not depend on the parameters (β_K, A). The turbulent reference parameters are here $\beta_K = 2/3$ and $A = 1$. The right states for several values of z are computed according to the results of section 2.

The results are plotted for z in $[1, z_{lim}[$, where z_{lim} is defined as the value of z for which the left pressure is equal to zero. For the laminar case, the classical definition $z_{lim} = (\gamma+1)/(\gamma-1)$ holds here. Since we have set $\gamma = 1.305$, we get $(\gamma+1)/(\gamma-1) \approx 7.557$. When turbulent pressure is not equal to zero, z_{lim} can be implicitly defined using the results of section 2.3. It should be noted that it depends on the turbulent EOS parameters which modifies the laminar limit. For the test cases considered here, the limit remains close to the laminar one. When z tends to z_{lim} in the turbulent case, the behavior becomes very stiff. In particular, the derivative of $P_{K,r}$ with respect to z tends to $-\infty$. The numerical computation of the right state is more tricky for $z \sim z_{lim}$, as shown for instance in Figure 3 for $A = 1$ and $\beta_K = 2/30$.

For all the test cases, it can be observed that accounting for the turbulence as little influence on the mean pressure. Temperatures are more sensitive to the turbulence EOS, in particular the turbulent temperature which exhibits a strong influence to the EOS parameters. The mean temperature is less influenced since the contribution of the turbulent temperature is weighted by the turbulent entropy fraction which remains small here.

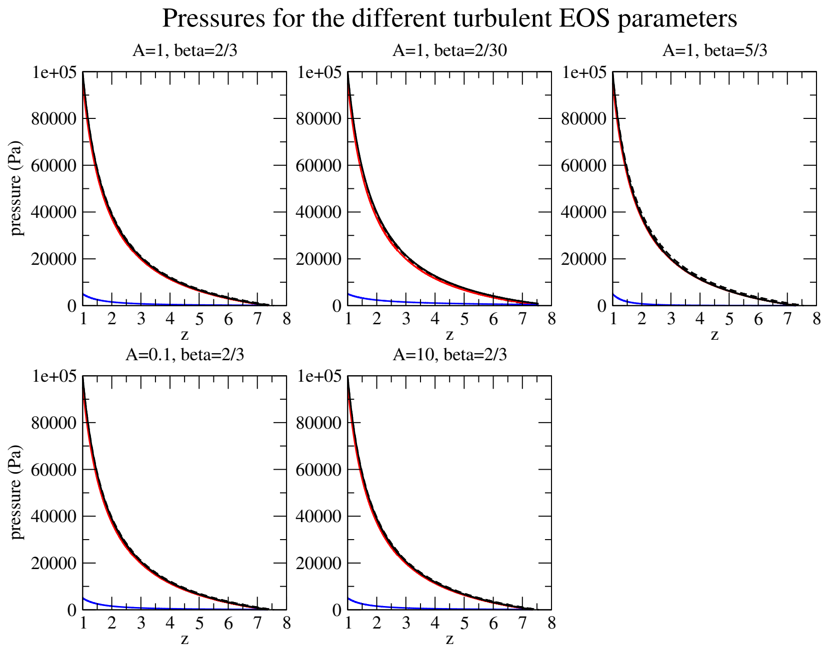

FIGURE 2. Pressure on the right of the 3-shock with respect to the ratio z for different parameters γ and A. The black dashed curve represents the pressure in the pure laminar case. The other curves are for the turbulent case: the plain black curve is the mean pressure $P_{K,r}+P_{L,r}$, the blue curve is the turbulent pressure $P_{K,r}$ and the red curve is the laminar pressure $P_{L,r}$

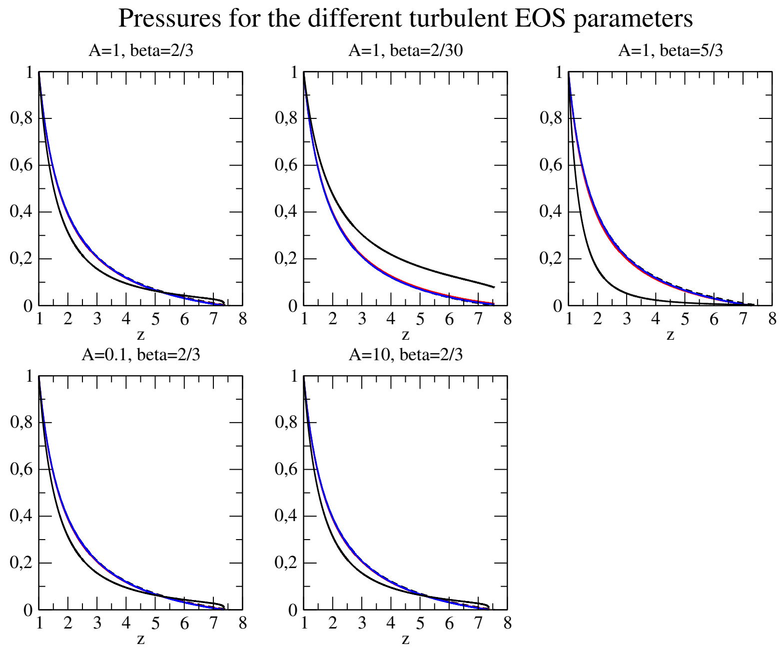

FIGURE 3. Normalized pressure on the right of the 3-shock with respect to the ratio z for different parameters γ and A. The black dashed curve represents the normalized pressure in the pure laminar case P_r/P_l. The other curves are for the turbulent case: the plain black curve is the normalized mean pressure $(P_{K,r}+P_{L,r})/P_l$, the blue curve is the normalized turbulent pressure $P_{K,r}/P_{K,l}$ and the red curve is the normalized laminar pressure $P_{L,r}/P_{L,l}$

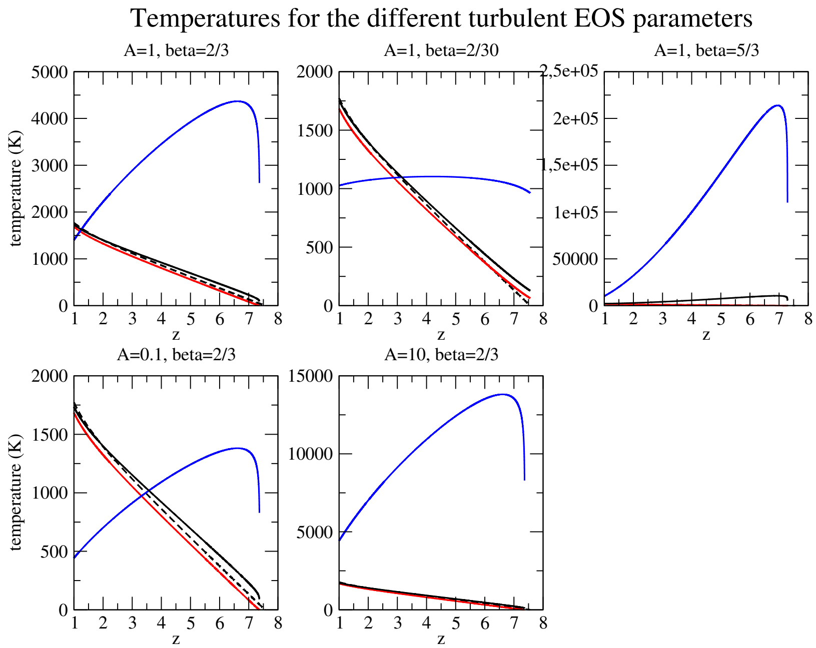

FIGURE 4. Temperature on the right of the 3-shock with respect to the ratio z for different parameters γ and A. The black dashed curve represents the temperature in the pure laminar case. The other curves are for the turbulent case: the plain black curve is the mean temperature $T_{K,r} + \zeta T_{L,r}$, the blue curve is the turbulent temperature $T_{K,r}$ and the red curve is the laminar temperature $T_{L,r}$

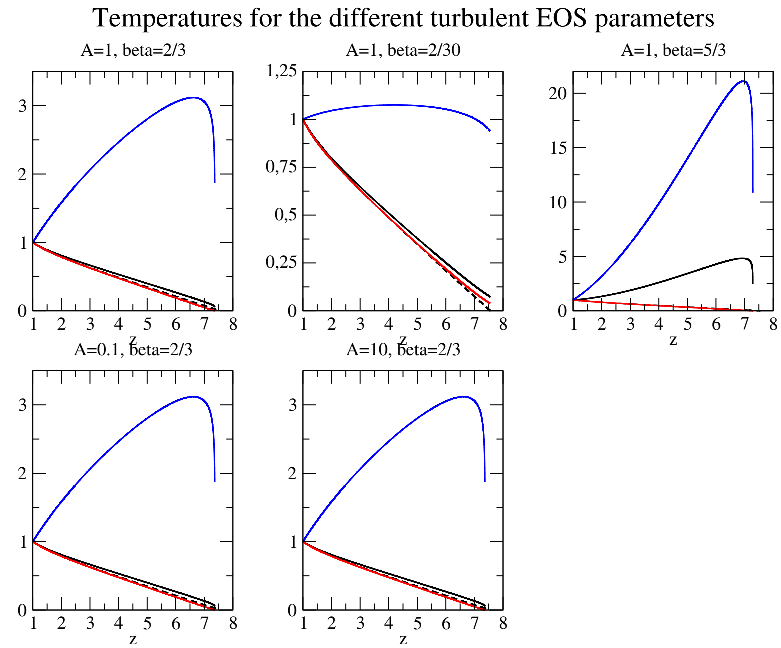

FIGURE 5. Normalized temperature on the right of the 3-shock with respect to the ratio z for different parameters γ and A. The black dashed curve represents the normalized temperature in the pure laminar case T_r/T_l. The other curves are for the turbulent case: the plain black curve is the normalized mean temperature $(T_{K,r}+\zeta T_{L,r})/T_l$, the blue curve is the normalized turbulent temperature $T_{K,r}/T_{K,l}$ and the red curve is the normalized laminar temperature $T_{L,r}/T_{L,l}$

3. Link between the thermodynamical model and a classical K-model

In order to compare the class of models proposed in the previous sections and a K-model classically derived from the RANS approach [24], a turbulent production term is first introduced in the thermodynamical-based model.

Let us now focus on the model proposed in section 1.2 and described by set of equations (13). By using the closure relations (1) and (2) and the equations of system (13), the following equations can be obtained for the turbulent energy e_K, the laminar internal energy e_L and the mean kinetic energy $e_c = U^2/2$:

$$\partial_t(\rho e_K) + \partial_x(\rho U e_K) + P_K \partial_x(U) = \rho s \frac{T_K T_L}{T} \mathscr{S}_K, \tag{35}$$

$$\partial_t(\rho e_L) + \partial_x(\rho U e_L) + P_L \partial_x(U) = -\rho s \frac{T_K T_L}{T} \mathscr{S}_K, \tag{36}$$

$$\partial_t(\rho e_c) + \partial_x(\rho U e_c) + U \partial_x(P) = 0. \tag{37}$$

Since $P = P_K + P_L$ and $E = e_K + e_L + e_c$, the total energy equation of system (13) is easily recovered by adding equations (35), (36) and (37). With these three equations, it clearly appears that in the model of section 1.2 the source term $\mathscr{S}_K = -\zeta/\lambda < 0$ leads an energy transfer from the turbulent structures to the internal energy. This corresponds to a dissipation of the turbulent energy, i.e. the meso-scale, to the internal energy, i.e. the micro-scale. The mean kinetic energy is not involved in this exchange.

We thus need to introduce here a source term that rules the exchange of energy between the mean velocity field U, i.e. the macro-scale, and the turbulent structures, i.e. the meso-scale. This source term corresponds to the so-called production term that arises in the classical models obtained through RANS approach. Equations (35) and (37) are thus modified with the production term $(\rho U \mathscr{P}_K) \geq 0$:

$$\partial_t(\rho e_K) + \partial_x(\rho U e_K) + P_K \partial_x(U) = \rho s \frac{T_K T_L}{T} \mathscr{S}_K + \rho U \mathscr{P}_K, \tag{38}$$

$$\partial_t(\rho e_L) + \partial_x(\rho U e_L) + P_L \partial_x(U) = -\rho s \frac{T_K T_L}{T} \mathscr{S}_K, \tag{39}$$

$$\partial_t(\rho e_c) + \partial_x(\rho U e_c) + U \partial_x(P) = -\rho U \mathscr{P}_K. \tag{40}$$

Obviously, the term $(\rho U \mathscr{P}_K)$ does not modify the total energy equation and the mass equation. Indeed, it represents an internal exchange within the fluid. Due to the closure laws of the model of section 1.2 for the entropies, we obtain by deriving the energies e_k and e_L:

$$T_L\ (\partial_t(s) + U \partial_x(s)) = \tau\ (\partial_t(\rho e_L) + \partial_x(\rho U e_L) + P_L \partial_x(U)),$$
$$sT_K(\partial_t(\zeta) + U \partial_x(\zeta)) + \zeta T_K\ (\partial_t(s) + U \partial_x(s)) = \tau\ (\partial_t(\rho e_K) + \partial_x(\rho U e_K) + P_K \partial_x(U)),$$

or thanks to equations (38) to (40):

$$T_L\ (\partial_t(s) + U \partial_x(s)) = -s \frac{T_K T_L}{T} \mathscr{S}_K, \tag{41}$$

$$sT_K(\partial_t(\zeta) + U \partial_x(\zeta)) + \zeta T_K\ (\partial_t(s) + U \partial_x(s)) = s \frac{T_K T_L}{T} \mathscr{S}_K + U \mathscr{P}_K. \tag{42}$$

We finally get that the entropy s does not depend on $(\rho U \mathscr{P}_K)$, which can be expected since s only depend on e_L and τ which are not influenced by $(\rho U \mathscr{P}_K)$. Equation (19) is thus recovered. On the contrary, equation

(42) for ζ becomes:

$$\partial_t(\zeta) + U\partial_x(\zeta) = \mathscr{S}_K + \frac{U}{s}\mathscr{P}_K. \tag{43}$$

Since $(\rho U \mathscr{P}_K) \geq 0$, the exchange of energy from mean kinetic energy to turbulent energy leads to an increase of the entropy fraction ζ. At last, from equation (40) one can obtain the corresponding momentum equation which includes $\mathscr{P}_K$. It can be interpreted as a volumetric force. The system accounting for the production term is now:

$$\begin{cases} \partial_t(\rho\zeta) + \partial_x(\rho U\zeta) = \rho\mathscr{S}_K + \frac{U}{s}\mathscr{P}_K, \\ \partial_t(\rho) + \partial_x(\rho U) = 0, \\ \partial_t(\rho U) + \partial_x\left(\rho U^2 + P\right) = -\rho\mathscr{P}_K, \\ \partial_t(\rho E) + \partial_x(U(\rho E + P)) = 0, \end{cases} \tag{44}$$

where all the closure laws of section 1.2 still hold:

$$E = e_K(\tau,\zeta s) + e_L(\tau,s) + U^2/2, \quad T = \zeta T_K(\tau,\zeta s) + T_L(\tau,s) \quad \text{and} \quad P = P_K(\tau,\zeta s) + P_L(\tau,s).$$

Model (44) is a three-scale model. It contains:

- a micro-scale energy represented by the thermodynamical internal (laminar) energy e_L, which corresponds to the smallest scale of the flow,
- a meso-scale (intermediate) energy e_K which gathered the energy of turbulent ”small-scale” dynamical structures,
- a macro-scale energy e_c which corresponds to the energy of the large dynamical structures.

The exchange between this levels of energy are ruled by two terms. The source term $\mathscr{S}_K$ is a dissipation term for the turbulent energy in the sense that it leads to a decrease of the turbulent energy. The amount of energy lost by the turbulent structures is transferred to the internal energy, which represents the energy contained at the thermodynamical scale. The volumetric force $\mathscr{P}_K$ gathers the effects that generate turbulent energy from the macro-scale velocity field U. Since $U\mathscr{P}_K \geq 0$, this force implies a transfer of energy from the large dynamical scales to the small dynamical scale (i.e. turbulence).

Thanks to our choice for the turbulent EOS, see section 1.4, and to the choice for $\mathscr{S}_K$, see equation (20), we have:

$$\rho s \frac{T_K T_L}{T}\mathscr{S}_K = -\rho e_K \frac{2T_L}{T}\frac{1}{\lambda},$$

and $P_K = \beta\rho e_K$. Hence equation (38) can be written:

$$\partial_t(\mathscr{E}_K) + \partial_x(\mathscr{E}_K U) + \beta\mathscr{E}_K\partial_x(U) = -\mathscr{E}_K/\lambda' + \rho U\mathscr{P}_K, \tag{45}$$

where we have set $\mathscr{E}_K = \rho e_K$ and $\lambda' = \lambda T/(2T_L)$. The equation for the turbulent energy of the model of section 1.2 written in the form (45) with the particular choice $\beta = 2/3$ is clearly very close to equation for the turbulent kinetic energy arising in the classical K-model [24]. This is at least straightforward for the convection terms. The main difference arises in the production terms. In the classical K-model it is of the form $\mu_t(\partial_x(U))^2$ whereas it reads $\rho U\mathscr{P}_K$ in (45), where $\mathscr{P}_K$ should be specified.

4. Conclusion

In this work we proposed to model turbulence using a thermodynamic point of view. The main advantage of this approach is it simplicity with regards to the process of construction of the classical turbulent models using RANS or LES approaches. The final class of models (with respect to the different possible choices for $\mathscr{S}_K$, $\mathscr{P}_K$, and for the turbulent EOS) leads to simpler models than those obtained using the classical approaches. Nevertheless, it has been shown that, up to specific closures/parameters for the turbulent EOS, a model very close to the classical K-model proposed by [24] can be written. This comparison allows to partially justify the choice of the turbulent EOS in section 1.4, but it still remains to determine some of the associated parameters which can have a great importance on the results (at least in shocks).

Moreover, the mathematical properties of the final class of models are directly inherited from the thermodynamical modeling process (hyperbolicity and realizability are ensured). At last, it should be noted that the building of the thermodynamical turbulent model has been done in 1D throughout this work, but written the 3D counterpart is straightforward. One important result of section 2.4 is that the choice of the turbulent EOS parameters has a great influence on the temperature. Hence it could be worth to extend this approach to reactive flows where reactions are driven by the temperature and enhanced by the turbulence diffusion.

Acknowledgement. The authors would like to thank Jean-Marc Hérard for fruitfull discussions on compressible turbulence models.

REFERENCES

[1] B. Audebert. *Contribution à l'analyse des modèles aux tensions de Reynolds pour l'interaction choc turbulence*. Phd thesis, Université Pierre et Marie Curie - Paris VI, Dec. 2006. https://theses.hal.science/tel-00850928/.

[2] T. Barberon and P. Helluy. Finite volume simulation of cavitating flows. *Computers and Fluids*, 34(7):832–858, 2005. https://hal.archives-ouvertes.fr/hal-00139597.

[3] C. Berthon. *Contribution a l'analyse numerique des equations de navier-stokes compressibles a deux entropies specifiques. Applications a la turbulence compressible*. PhD thesis, Paris 6, 1999.

[4] P. Chassaing and J. Herard. Second order modelling of variable density turbulent mixing. In *6th Symposium on Turbulent Shear Flows*, pages 17_8_1–17_8_6, 1987.

[5] P. Clavin. Dynamic behavior of premixed flame fronts in laminar and turbulent flows. *Progress in energy and combustion science*, 11(1):1–59, 1985.

[6] G. Faccanoni and H. Mathis. Admissible Equations of State for Immiscible and Miscible Mixtures. *ESAIM: Proceedings and Surveys*, 66:1–21, 2019. https://hal.archives-ouvertes.fr/tel-00363460.

[7] A. Favre. The equations of compressible turbulent gases. *Annual Summary Report AD0622097*, 1965.

[8] S. Gavrilyuk, J.-M. Hérard, O. Hurisse, and A. Toufaili. Theoretical and numerical analysis of a simple model derived from compressible turbulence. *Journal of Mathematical Fluid Mechanics*, 24, 2022.

[9] E. Godlewski and P.-A. Raviart. *Numerical approximation of hyperbolic systems of conservation laws*, volume 118. Springer, 1996.

[10] P. Helluy, O. Hurisse, and L. Quibel. Assessment of numerical schemes for complex two-phase flows with real equations of state. *Computers & Fluids*, 196:104347, 2020.

[11] J.-M. Hérard. Modèles au second ordre réalisables non dégénérés pour les écoulements turbulents incompressibles. *Comptes rendus Académie des Sciences. Série IIb. Mécanique*, 322(5):371–377, 1996.

[12] J.-M. Hérard. A simple turbulent model for compressible flows, https://hal.archives-ouvertes.fr/hal-02007044. Technical report, EDF R&D, 2014.

[13] J.-M. Hérard, O. Hurisse, and L. Quibel. A four-field three-phase flow model with both miscible and immiscible components. *ESAIM: Mathematical Modelling and Numerical Analysis*, 55:251–278, 2021.

[14] O. Hurisse. Numerical simulations of steady and unsteady two-phase flows using a homogeneous model. *Computers and Fluids*, 152:88–103, July 2017. https://hal.archives-ouvertes.fr/hal-01489039.

[15] O. Hurisse. A multi-component multi-temperature model for simulating laminar deflagration waves in mixtures of air and hydrogen. *Numerical Heat Transfer, Part B: Fundamentals*, pages 1–42, 2023.

[16] O. Hurisse and L. Quibel. A homogeneous model for compressible three-phase flows involving heat and mass transfer. *ESAIM: Proceedings and Surveys*, 66:81–108, 2019. https://hal.archives-ouvertes.fr/hal-01976903/.

[17] O. Hurisse and L. Quibel. Simulations of liquid-vapor water flows with non-condensable gases on the basis of a two-fluid model. *Applied Mathematical Modelling*, 99:514–537, 2021.

[18] J. Jung. *Numerical simulations of two-fluid flow on multicores accelerator*. Phd thesis, Université de Strasbourg, Oct. 2013. https://tel.archives-ouvertes.fr/tel-00876159/.

[19] H. Mathis. A thermodynamically consistent model of a liquid-vapor fluid with a gas. *ESAIM: Mathematical Modelling and Numerical Analysis*, 53(1):63–84, 2019.

[20] E. S. Oran and J. P. Boris. Detailed modelling of combustion systems. *Progress in Energy and Combustion Science*, 7(1):1–72, 1981.

[21] J. Ristorcelli. A representation for the turbulent mass flux contribution to reynolds-stress and two-equation closures for compressible turbulence. Technical report, NASA report 191569, ICASE Report No. 93-88., 1993. https://ntrs.nasa.gov/api/citations/19940018829/downloads/19940018829.pdf.

[22] R. Saurel, A. Chinnayya, and F. Renaud. Thermodynamic analysis and numerical resolution of a turbulent-fully ionized plasma flow model. *Shock Waves*, 13(4):283–297, 2003.

[23] J. Smoller. *Shock waves and reaction—diffusion equations*, volume 258. Springer Science & Business Media, 2012.

[24] P. Spalart and S. Allmaras. A one-equation turbulence model for aerodynamic flows. *La Recherche Aérospatiale*, 1:5–21, 1992.

[25] H. Tennekes and J. L. Lumley. *A first course in turbulence*. MIT press, 1972.

[26] A. Toufaili. *Modélisation de la turbulence compressible pour l'explosion*. PhD thesis, Aix-Marseille, 2023.

[27] F. A. Williams. Combustion theory: the fundamental theory of chemically reacting flow systems. Technical report, 1985.