An approach for building simple models for compressible turbulent flows.

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- Turbulent flows are commonly encountered in industrial applications.
- Turbulence is very important because it can strongly change the flow patterns.
- In particular, it influences mass and heat transfer in reacting flows (multiphase, combustion, ...).
- Accounting for turbulence can thus be mandatory for obtaining predictive models.
- Example for H_2 combustion[1]:
  - Laminar flame speed of H_2 in air is $\approx 1-3\ m/s$, this lead to deflagrations.
  - When the flow is turbulent near the flame front, we can get a detonation: flame speed $\approx$ speed of sound, which means $\approx 1500\ m/s$ in hot burnt gases, and $\approx 340\ m/s$ in fresh gases !

$\Longrightarrow$ **An alternative way of modeling turbulence for compressible flows** is presented in this talk with a focus on the Euler system of equations with energy (which represents the basis of a lot of the multiphase compressible models).

[1] Poster session: "A multi-component multi-temperature model for simulating laminar deflagration waves in mixtures of air and hydrogen"

Illustration of the classical RANS approach for the barotropic Euler system

$$\begin{cases} \dfrac{\partial}{\partial t}(\rho) + \dfrac{\partial}{\partial x}(\rho U) = 0, \\ \dfrac{\partial}{\partial t}(\rho U) + \dfrac{\partial}{\partial x}\left(\rho U^2 + P(\rho)\right) = 0. \end{cases} \tag{1}$$

The **statistical Reynolds average** of any quantity ϕ is denoted by $\overline{\phi}$. The **Favre "average"** reads: $\overline{\rho}\widetilde{\Psi} = \overline{\rho\Psi}$. The associated fluctuations are respectively: $\phi' = \phi - \overline{\phi}$ and $\psi^{\#} = \psi - \widetilde{\psi}$.

Applying Reynolds average to system (1) leads to (note that statistical average operators and partial derivatives commute):

$$\begin{cases} \dfrac{\partial}{\partial t}(\overline{\rho}) + \dfrac{\partial}{\partial x}\left(\overline{\rho}\ \widetilde{U}\right) = 0, \\ \dfrac{\partial}{\partial t}\left(\overline{\rho}\ \widetilde{U}\right) + \dfrac{\partial}{\partial x}\left(\overline{\rho}\ \widetilde{U}^2 + \overline{\rho}\widetilde{(U^{\#})^2} + \overline{P(\rho)}\right) = 0. \end{cases} \tag{2}$$

If we consider that $\overline{\rho}$ and $\widetilde{U}$ are the unknowns of system (2), the terms in blue should be defined with respect to these unknowns through algebraic closure laws or (more often) through additional EDP.

Remark. For a linear pressure law: $\overline{P(\rho)} = P(\overline{\rho})$, only $\widetilde{(U^{\#})^2}$ has to be closed.

Remark. The energy equation in the Euler model leads to even more additional (non-linear) terms to close.

How to model turbulence for compressible flows in industrial codes ?

- This is a complex task for incompressible flows (several decades of research and publications...), this is even more complex for compressible flows, with very few publications on rigorous derivation of models in the literature.
- Not so easy to grasp because the first theory is based on statistics ... and in common sense, turbulence often means small vortices in one particular flow !

  In a practical point of view, statistical averages used in the theory are replaced by spatial and/or time averages.

  - Ergodicity principle is used for justifying this replacement, but it could only be valid in the core of the flow (i.e. not around singularities as walls for instance) and for almost steady flows.
  - This replacement can lead to possible discrepancy between the time/space filters and time-steps/mesh-cells (in LES approach).

- A standard closure method: models for incompressible turbulence are roughly extended by considering that density varies. This is clearly not suitable for flows that endure high and rapid compression phenomena.

- One of the main challenges for modeling turbulence in compressible flows is to define shocks with a correct jump of the turbulent quantities. A conservative model is thus desirable (though not mandatory).

The classical three-scale RANS approach *versus* a "two-scale" thermodynamical approach

$$\left\{ \begin{array}{l} \dfrac{\partial}{\partial t}(\overline{\rho}) + \dfrac{\partial}{\partial x}\left(\overline{\rho}\ \widetilde{U}\right) = 0, \\ \dfrac{\partial}{\partial t}\left(\overline{\rho}\ \widetilde{U}\right) + \dfrac{\partial}{\partial x}\left(\overline{\rho}\ \widetilde{U}^2 + \overline{\rho}\widetilde{(U^{\#})^2} + \overline{P(\rho)}\right) = 0. \end{array} \right.$$

The classical RANS approach can be seen as a three-scale decomposition:

- the macro-scale represented by the velocity and the kinetic energy $\widetilde{U}^2/2$;
- the meso-scale represented by the turbulent kinetic energy $\widetilde{(U^{\#})^2}$;
- the micro-scale represented by the internal energy $e(\rho, s)$.

In the following, we propose to model both the micro-scale and meso-scale using a common thermodynamical approach.

Benefits of this point of view are associated with the mathematical properties inherited by the EDP models issued from thermodynamical-based modelling:

- hyperbolicity of the set of equations is more easy to obtain;
- conservativity is intrinsically ensured $\rightarrow$ unique shock definition;
- second law of thermodynamics.

The following models can be seen as a mixture models of two miscible phases K and L sharing the same mass.

- Let us consider a mass of fluid $\mathscr{M}$ (in kg) within a volume $\mathscr{V}$ (in m^3), with for $\phi = \{K, L\}$: $\mathscr{M}_\phi = \mathscr{M}$ and $\mathscr{V}_\phi = \mathscr{V}$.
- Thermodynamical internal energy is denoted by $\mathscr{E}_L$ (in J).
- Turbulent kinetic energy is denoted by $\mathscr{E}_K$ (in J).
- The energy is chosen as the thermodynamical potential, so that
  - EOS have to be given for $\mathscr{E}_\phi(\mathscr{M}_\phi, \mathscr{V}_\phi, \eta_\phi)$ for $\phi = \{K, L\}$,
  - where the thermodynamical entropy is denoted by η_L,
  - and the turbulent entropy by η_K (both in J/K).
- A Gibbs relation is assumed for each "phase" $\phi = \{K, L\}$:

$$d\mathscr{E}_\phi = T_\phi d\eta_\phi - P_\phi d\mathscr{V}_\phi + \mu_\phi d\mathscr{M}_\phi, \quad \text{with } \mathscr{V}_\phi = \mathscr{V} \text{ and } \mathscr{M}_\phi = \mathscr{M}.$$

- Assumption : the energy of the fluid is $\mathscr{E} = \mathscr{E}_L + \mathscr{E}_K$.
- Hence we get the Gibbs relation for the mixture:

$$d\mathscr{E} = \underbrace{T_L d\eta_L + T_K d\eta_K}_{?} - \underbrace{(P_L + P_K)}_{=P \text{ (i.e. Dalton law)}} d\mathscr{V} + \underbrace{(\mu_L + \mu_K)}_{=\mu \text{ (not used)}} d\mathscr{M}.$$

- In order to close the mixture model, we must specify how the phasic entropies η_ϕ and the mixture entropy η are linked.

Additional assumptions for the EOS

Thanks to the Gibbs relations we have:

$$P_\phi = -\frac{\partial \mathscr{E}_\phi}{\partial \mathscr{V}}_{|\mathscr{M},\eta_\phi} \quad \text{and} \quad T_\phi = \frac{\partial \mathscr{E}_\phi}{\partial \eta_\phi}_{|\mathscr{M},\mathscr{V}}.$$

Let us assume that the EOS are such that:

- $\mathscr{E}_\phi$ are convex and PH1 with respect to $(\mathscr{M}_\phi, \mathscr{V}_\phi, \eta_\phi)$,
- $\eta_L > 0$ and $\mathscr{E}_L(\mathscr{M}, \mathscr{V}, \eta_L) \geq 0$ (not always the case ! e.g. the Stiffened Gas),
- $\eta_K \geq 0$ and $\mathscr{E}_K(\mathscr{M}, \mathscr{V}, \eta_K) \geq 0$,
- $\lim_{\eta_K \to 0} (\mathscr{E}_K(\mathscr{M}, \mathscr{V}, \eta_K)) \to 0$,
- $\lim_{\eta_K \to 0} (P_K(\mathscr{M}, \mathscr{V}, \eta_K)) \to 0$,
- $\lim_{\eta_K \to 0} (T_K(\mathscr{M}, \mathscr{V}, \eta_K)) \to 0$,

The last four conditions allow to make the turbulence vanish and to retrieve the “laminar model”.

A first model issued from [2] and closely related to the one proposed in [3], though the two models make different mass assumptions for $\mathscr{M}_\phi$.

- The mixture entropy reads: $\eta = \eta_K + \eta_L$ (note that $\eta > 0$).
- We introduce a turbulent entropy fraction $\beta_K = \eta_K/\eta$ (and $\beta_L = 1 - \beta_K$).
- The mixture Gibbs relation:

$$d\mathscr{E} = \underbrace{T_L d\eta_L + T_K d\eta_K}_{?} - (P_L + P_K)d\mathscr{V} + (\mu_L + \mu_K)d\mathscr{M},$$

becomes:

$$d\mathscr{E} = \underbrace{(T_K - T_L)d\beta_K}_{\text{exchange term}} + \underbrace{(\beta_L T_L + \beta_K T_K)}_{\text{mixture temp. } T} d\eta - (P_L + P_K)d\mathscr{V} + (\mu_L + \mu_K)d\mathscr{M}.$$

- Mixture temperature T and pressure P can be identified and they read:

$$T = \beta_L T_L + \beta_K T_K \text{ and } P = P_L + P_K.$$

[2] "Modélisation de la turbulence compressible pour l'explosion", A. Toufaili, PhD Univ. Aix-Marseille, 15 march 2023, https://theses.hal.science/tel-04035905v1

[3] "Thermodynamic analysis and numerical resolution of a turbulent-fully ionized plasma flow model", R. Saurel, A. Chinnayya, F. Renaud, Shock Waves, 2003.

The volume of fluid follows a streamline defined by the velocity field U.

The variation of the volume is related to the divergence of the velocity field:

$$d\mathscr{V} = \mathscr{V}\ \nabla_x \cdot U\ dt. \tag{3}$$

We assume that the mass $\mathscr{M}$ is constant:

$$d\mathscr{M} = 0, \tag{4}$$

and that first law of thermodynamics holds for the mixture pressure forces:

$$d\mathscr{E} = -Pd\mathscr{V}. \tag{5}$$

Thanks to relations (4)-(5), the Gibbs relation:

$$d\mathscr{E} = (T_K - T_L)d\beta_K + Td\eta - Pd\mathscr{V} + (\mu_L + \mu_K)d\mathscr{M},$$

then simplifies in:

$$0 = (T_K - T_L)d\beta_K + Td\eta. \tag{6}$$

Four variables $\mathscr{V}$, $\mathscr{M}$, η and β_K (or $\mathscr{V}$, $\mathscr{M}$, η_K and η_L) BUT only three closures for their time evolution: (3), (4), (5).

→ A model has to be specified for $d\beta_K$ (or $d\eta$ thanks to (6)).

Convexity and the second law of thermodynamics

- The convexity of energies $\mathscr{E}_\phi \implies$ the convexity of the mixture energy $\mathscr{E}$.
- The convexity $\mathscr{E}$ is equivalent to the concavity of η, see [a].
- Hence the second law of thermodynamics reads here $d\eta > 0$.

[a] "Numerical approximation of hyperbolic systems of conservation laws", E. Godlewski, P.-A. Raviart, Springer, 1996.

The second law is then used for choosing admissible models for the variation of β_K.

Models for $d\beta_K$ should be such that $d\eta > 0$, which thanks to the simplified Gibbs relation, $0 = (T_K - T_L)d\beta_K + Td\eta$, leads to:

$$d\eta > 0 \iff (T_K - T_L)d\beta_K < 0.$$

Several admissible models exist. Let us choose a simple one:

$$d\beta_K = -\frac{(T_K - T_L)}{\lambda}\, dt, \quad \text{with } \lambda > 0.$$

Remark. A BGK source terms has been used in [4].

[4] "Modélisation de la turbulence compressible pour l'explosion", A. Toufaili, PhD Univ. Aix-Marseille, 15 march 2023, https://theses.hal.science/tel-04035905v1

This model has been studied in details in [5]. Let us enumerate some drawbacks of this first model.

1. The mixture temperature is a weighted formula with $\beta_K \in [0,1[$:

$$T = (1-\beta_K)T_L + \beta_K T_K.$$

   - Since $\eta_L > 0$, $\beta_K < 1$. But when $\beta_K \to 1^-$, we have $T \to T_K^-$. The energy of the model is the turbulent one, no more thermodynamical energy.
   - The mixture temperature can be less than the associated thermodynamical temperature: $T < T_L$ (typically when $T_K < T_L$).

2. The equilibrium state (long time behavior for the closed system) is:

$$T_L = T_K.$$

   Which means that turbulent kinetic energy does not vanish when equilibrium state is reached.

3. Dissipation of the turbulent energy/entropy, i.e. β_K, is associated with $(T_L - T_K)d\beta_K$, which limits the possibility of dissipation models.

$\Longrightarrow$ **The behavior of this model is not completely satisfactory.**

[5] "Modélisation de la turbulence compressible pour l'explosion", A. Toufaili, PhD Univ. Aix-Marseille, 15 march 2023, https://theses.hal.science/tel-04035905v1

A second model: let us only change the closures for the entropies.

- Assumptions for the partial masses / volumes / energies are unchanged.
- The thermodynamical and turbulent entropies now reads:

$$\eta_L = \eta, \quad \eta_K = \zeta_K \eta, \quad \text{with} \quad \zeta_K \geq 0.$$

- The mixture Gibbs relation:

$$d\mathscr{E} = \underbrace{T_L d\eta_L + T_K d\eta_K}_{?} - (P_L + P_K)d\mathscr{V} + (\mu_L + \mu_K)d\mathscr{M},$$

becomes:

$$d\mathscr{E} = \underbrace{\eta T_K d\zeta_K}_{\text{exchange term}} + \underbrace{(T_L + \zeta_K T_K)}_{\text{mixture temp. } T} d\eta - (P_L + P_K)d\mathscr{V} + (\mu_L + \mu_K)d\mathscr{M}.$$

- Mixture temperature T and pressure P can be identified and they now read:

$$T = T_L + \zeta_K T_K \text{ and } P = P_L + P_K.$$

- Thanks to early assumptions, turbulence dissipation in agreement with second law are such that $d\zeta_K \leq 0$, e.g. one can choose an exponential decrease:

$$d\zeta_K = -\frac{\zeta_K}{\nu}\, dt, \quad \text{with} \quad \nu > 0.$$

Let us compare this second model to the first one.

1. The mixture temperature is not a weighted formula:

$$T = T_L + \zeta_K T_K, \quad \text{with} \quad \zeta_K \geq 0.$$

   - When $\zeta_K \to 0$, we have $T \to T_L$. The energy of the model is the thermodynamical one, there is no more turbulent energy.
   - The mixture temperature is always greater or equal to the thermodynamical temperature: $T \geq T_L$.

2. The equilibrium state (long time behavior for the closed system) is:

$$\zeta_K = 0 \Longleftrightarrow \eta_K = 0 \Longleftrightarrow \mathscr{E}_K = P_K = T_K = 0.$$

   Which means that turbulent kinetic energy has entirely vanished when equilibrium state is reached.

$\Longrightarrow$ **The behavior of this model is in better agreement with "what could be expected".**

We already introduced the closures:

$$d\mathscr{V} = \mathscr{V}\ \nabla_x \cdot U\ dt, \quad d\mathscr{M} = 0, \quad d\mathscr{E} = -P d\mathscr{V},$$

where P is the mixture pressure $P = P_K + P_L$. We add a closure for the velocity field (in agreement with the first law of thermodynamics above) and the equation for ζ_K:

$$\mathscr{M}\, d\mathscr{U} = -\mathscr{V} \nabla_x P\ dt, \quad d\zeta_K = -\frac{\zeta_K}{\nu}\ dt.$$

We now switch from this non-conservative set of equations for extensive quantities (along streamlines) to a set of EDP in conservative form for intensive quantities, we get an Euler based model:

$$\begin{cases} \frac{\partial}{\partial t}(\rho \zeta_K) + \frac{\partial}{\partial x}(\rho U \zeta_K) = \rho \zeta_K / \nu, \\ \frac{\partial}{\partial t}(\rho) + \frac{\partial}{\partial x}(\rho U) = 0, \\ \frac{\partial}{\partial t}(\rho U) + \frac{\partial}{\partial x}\left(\rho U^2 + P(\zeta_K, \rho, s)\right) = 0, \\ \frac{\partial}{\partial t}(\rho E) + \frac{\partial}{\partial x}(U(\rho E + P(\zeta_K, \rho, s))) = 0, \end{cases}$$

where $E = e_L(\rho, s) + e_K(\rho, \zeta_K s) + U^2/2$ is the specific total energy with $e_\phi = \mathscr{E}_\phi / \mathscr{M}$, and where the unknowns are: the density $\rho = \mathscr{M}/\mathscr{V}$, the specific entropy $s = \eta / \mathscr{M}$, ζ_K and U.

Conclusion and perspectives

1. For the second model, what is the physical meaning of the closures for the entropies:

$$\eta_L = \eta, \quad \eta_K = \zeta_K \eta \quad ?$$

2. We end up with an Euler-based model with a complex mixture pressure-law and an additional advected quantity ζ_K.

3. Concerning the overall approach:

   - Benefits of thermodynamical modeling: agreement with the second law, shocks are uniquely defined, good mathematical properties.
   - Limited to isotropic turbulence which is not a "physical reality", but could be helpful on some coarse industrial settings (to be tested !).
   - Possible extension to anisotropic turbulence ?