

# A homogeneous model for compressible and immiscible two-phase flows: 1. Closure laws

Olivier Hurisse<sup>†</sup>

<sup>†</sup>EDF R&D MFEE, 6 quai Watier, 78400 Chatou, France.  
olivier.hurisse@edf.fr

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- 2 The thermodynamical behaviour of the mixture
  - Phasic quantites
  - The mixture entropy
  - The Gibbs relation for the mixture
  - Modeling the exchanges between the phases
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- 4 Specificity for steam/water flows
  - Specificity of the steam/water mixture
  - The heating of the phases
- 5 Some remarks
  - Other possible relaxation source terms ?
  - Energy fraction or entropy fraction ?

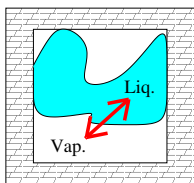
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## Outline of this part:

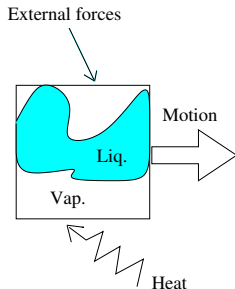
- We first focus on the thermodynamical behaviour of a small amount of a  $n$ -phase mixture ( $n \geq 1$ ).
- Then the dynamical behaviour of this mixture volume is described (always for  $n \geq 1$  phases).
- At last, the specificity of two-phase steam-liquid mixture is introduced ( $n = 2$ ).

### First step



Isolated system

### Second step



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For each phase  $k$  we have the following extensive quantities [Callen,85]:

- a volume  $\mathcal{V}_k$  (in  $m^3$ );
- a mass  $\mathcal{M}_k$  (in  $kg$ );
- a energy  $\mathcal{E}_k$  (in  $J$ ).

Then for the mixture we have:

- the mixture volume  $\mathcal{V} = \sum_k \mathcal{V}_k$  (since the phases are **immiscible** !);
- the mixture mass  $\mathcal{M} = \sum_k \mathcal{M}_k$ ;
- and the mixture internal energy  $\mathcal{E} = \sum_k \mathcal{E}_k$ .

*Remark: The surface tension and the topological arrangement of the phases are not taken into account.*

Within each phase we assume that an extensive entropy  $\eta_k$  is given (an EOS) on  $(\mathbb{R}^+)^3$ :

$$W_k \mapsto \eta_k(W_k) \quad (\text{in } J/K), \quad \text{where } W_k = (\mathcal{V}_k, \mathcal{M}_k, \mathcal{E}_k).$$

We assume that the entropy  $\eta_k$  is such that :

- $W_k \mapsto \eta_k(W_k)$  is  $C^2$ ;
- $W_k \mapsto \eta_k(W_k)$  is concave;
- $\forall a \in \mathbb{R}^+, \forall W_k \in (\mathbb{R}^+)^3, \eta_k(aW_k) = a\eta_k(W_k)$ ;
- $\forall W_k, \frac{\partial \eta_k}{\partial \mathcal{E}_k} |_{\mathcal{V}_k, \mathcal{M}_k} > 0$ .

If we assume that the “Classical Irreversible Thermodynamic” (CIT) holds, the following Gibbs relation is fulfilled for each phase:

$$T_k d(\eta_k) = d(\mathcal{E}_k) + P_k d(\mathcal{V}_k) - \mu_k d(\mathcal{M}_k),$$

where we have:

- $T_k$  is the temperature within phase  $k$ , with  $\frac{1}{T_k} = \frac{\partial \eta_k}{\partial \mathcal{E}_k} |_{\mathcal{V}_k, \mathcal{M}_k}$ ;
- $P_k$  is the pressure of phase  $k$ , with  $\frac{P_k}{T_k} = \frac{\partial \eta_k}{\partial \mathcal{V}_k} |_{\mathcal{M}_k, \mathcal{E}_k}$ ;
- and  $\mu_k$  is the Gibbs enthalpy of phase  $k$ , with  $\mathcal{M}_k \mu_k = \mathcal{E}_k + P_k \mathcal{V}_k - T_k \eta_k$ .

*Remark: Since we have assumed that  $\frac{\partial \eta_k}{\partial \mathcal{E}_k} |_{\mathcal{V}_k, \mathcal{M}_k} > 0$ , we get that  $T_k > 0$ .*

The thermodynamical behaviour of each phase is now defined.

Let's turn to the thermodynamical behaviour of the mixture.



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We assume that the extensive mixture-entropy  $\eta$ , is the sum of the extensive phasic-entropies (surface tension is neglected):

$$\eta(W) = \sum_k \eta_k(W_k), \quad \text{where } W = (W_1, W_2, \dots).$$

Thanks to the properties of the phasic entropies  $\eta_k$ , one can prove that

- $W \mapsto \eta(W)$  is  $C^2$ ;
- $W \mapsto \eta(W)$  is concave on  $(\mathbb{R}^+)^{3n}$ ;
- $\forall a \in \mathbb{R}^+, \forall W \in (\mathbb{R}^+)^{3n}, \eta(aW) = a\eta(W)$ .

Moreover, the restriction  $\tilde{\eta}$  of  $\eta$  on  $\mathcal{H}(\mathcal{M}) \subset (\mathbb{R}^+)^{3n}$  is strictly concave:

$$\mathcal{H}(\mathcal{M}) = \left\{ W \in (\mathbb{R}^+)^{3n}; \sum_k \mathcal{M}_k = \mathcal{M} \right\}.$$

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The operator  $d$ . of the previous slides can be seen as a derivative along the streamlines of the flow:

$$d\phi_k = \left( \frac{\partial \phi_k}{\partial t} + u_k \frac{\partial \phi_k}{\partial x} \right) dt,$$

where  $u_k$  is the velocity of the phase  $k$ .

**Since we have assumed that  $u_k = U$  for all  $k$ , the operator  $d$ . does not depend on  $k$ .**

We can thus write:

$$d\eta = \sum_k d\eta_k,$$

and we can then exhibit a Gibbs relation for this mixture entropy using the phasic Gibbs relations.

We then have:

$$d\eta = \sum_k d\eta_k \Leftrightarrow d\eta = \sum_k \left( \frac{1}{T_k} d\mathcal{E}_k + \frac{P_k}{T_k} d\mathcal{V}_k - \frac{\mu_k}{T_k} d\mathcal{M}_k \right),$$

which by using the chain-rule  $d\phi_k = \phi d(\phi_k/\phi) + \phi_k/\phi d\phi$  yields:

$$d\eta = \sum_k \left( \frac{\mathcal{E}_k}{\mathcal{E}} \frac{1}{T_k} \right) d\mathcal{E} + \sum_k \left( \frac{\mathcal{V}_k}{\mathcal{V}} \frac{P_k}{T_k} \right) d\mathcal{V} - \sum_k \left( \frac{\mathcal{M}_k}{\mathcal{M}} \frac{\mu_k}{T_k} \right) d\mathcal{M} \\ + \sum_k \left( \mathcal{E} \frac{1}{T_k} d \left( \frac{\mathcal{E}_k}{\mathcal{E}} \right) + \mathcal{V} \frac{P_k}{T_k} d \left( \frac{\mathcal{V}_k}{\mathcal{V}} \right) - \mathcal{M} \frac{\mu_k}{T_k} d \left( \frac{\mathcal{M}_k}{\mathcal{M}} \right) \right).$$

We can then identify:

- the mixture temperature  $T$  as  $\frac{1}{T} = \sum_k \left( \frac{\mathcal{E}_k}{\mathcal{E}} \frac{1}{T_k} \right)$ ;
- the mixture pressure  $P$  such that  $\frac{P}{T} = \sum_k \left( \frac{\mathcal{V}_k}{\mathcal{V}} \frac{P_k}{T_k} \right)$ ;
- and the mixture Gibbs enthalpy  $\mu$  such that  $\frac{\mu}{T} = \sum_k \left( \frac{\mathcal{M}_k}{\mathcal{M}} \frac{\mu_k}{T_k} \right)$ .

The Gibbs relation for the mixture is finally:

$$Td\eta - \underbrace{(d\mathcal{E} + Pd\mathcal{V} - \mu d\mathcal{M})}_{\text{"external exchange"}} = T \underbrace{\sum_k \left( \frac{\mathcal{E}}{T_k} d\left(\frac{\mathcal{E}_k}{\mathcal{E}}\right) + \frac{\mathcal{V}P_k}{T_k} d\left(\frac{\mathcal{V}_k}{\mathcal{V}}\right) - \frac{\mathcal{M}\mu_k}{T_k} d\left(\frac{\mathcal{M}_k}{\mathcal{M}}\right) \right)}_{\text{exchange between the phases}}.$$

In order to write a model, we need to define the following derivatives:

$$d\mathcal{E}, \quad d\mathcal{V}, \quad d\mathcal{M}, \quad d\left(\frac{\mathcal{E}_k}{\mathcal{E}}\right), \quad d\left(\frac{\mathcal{V}_k}{\mathcal{V}}\right), \quad d\left(\frac{\mathcal{M}_k}{\mathcal{M}}\right).$$

Let's start by the terms for the exchange between the phases, which represent the thermodynamical disequilibrium effects

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We assume in this subsection that the mixture is a closed system, that is :

$$d\mathcal{E} = d\mathcal{V} = d\mathcal{M} = 0.$$

We then define  $\mathcal{D}(\mathcal{V}, \mathcal{M}, \mathcal{E}) \subset \mathcal{H}(\mathcal{M})$  as:

$$\mathcal{D}(\mathcal{V}, \mathcal{M}, \mathcal{E}) = \left\{ W; W \in \mathcal{H}(\mathcal{M}), \sum_k \mathcal{V}_k = \mathcal{V}, \sum_k \mathcal{E}_k = \mathcal{E} \right\}.$$

We can thus consider the entropy  $\tilde{\eta}$  which is strictly concave on the closed bounded set  $\mathcal{D}(\mathcal{V}, \mathcal{M}, \mathcal{E})$ .

Hence, we get the two following properties.

- (i) There exist a unique point  $\overline{W} = (\overline{\mathcal{V}}_k, \overline{\mathcal{M}}_k, \overline{\mathcal{E}}_k)_k$  for which  $\tilde{\eta}$  is maximum on  $\mathcal{D}(\mathcal{V}, \mathcal{M}, \mathcal{E})$ .
- (ii) At any point  $W$  in  $\mathcal{D}(\mathcal{V}, \mathcal{M}, \mathcal{E})$ , the tangent plane to  $\tilde{\eta}$  at  $W$  is above  $\tilde{\eta}$ .

So that we have the inequality:

$$\tilde{\eta}(\overline{W}) \leq \tilde{\eta}(W) + \nabla_W(\tilde{\eta})(\overline{W} - W).$$



If we assume the following models for the exchange term [Barberon-Helluy, CAF, 2005]:

$$\begin{cases} d\left(\frac{\mathcal{V}_k}{\mathcal{V}}\right) = \frac{\overline{\mathcal{V}}_k - \mathcal{V}_k}{\lambda \mathcal{V}} dt; \\ d\left(\frac{\mathcal{M}_k}{\mathcal{M}}\right) = \frac{\overline{\mathcal{M}}_k - \mathcal{M}_k}{\lambda \mathcal{M}} dt; \\ d\left(\frac{\mathcal{E}_k}{\mathcal{E}}\right) = \frac{\overline{\mathcal{E}}_k - \mathcal{E}_k}{\lambda \mathcal{E}} dt; \end{cases}$$

where  $\lambda > 0$  is a time scale, we have the Gibbs relation on  $\mathcal{D}(\mathcal{V}, \mathcal{M}, \mathcal{E})$ :

$$d\tilde{\eta} = (\nabla_W(\eta) dW) = \nabla_W(\eta) \left( \frac{\overline{W} - W}{\lambda} \right) dt.$$

Due to the concavity of  $\tilde{\eta}$  this yields:

$$d\tilde{\eta} = \nabla_W(\eta) \left( \frac{\overline{W} - W}{\lambda} \right) dt \geq \frac{1}{\lambda} (\tilde{\eta}(\overline{W}) - \tilde{\eta}(W)) dt,$$

and since  $\overline{W}$  corresponds to the maximum of the entropy on  $\mathcal{D}(\mathcal{V}, \mathcal{M}, \mathcal{E})$ :

$$d\tilde{\eta} \geq \frac{1}{\lambda} (\tilde{\eta}(\overline{W}) - \tilde{\eta}(W)) dt \geq 0,$$

As a consequence, the models:

$$\left\{ \begin{array}{l} d\left(\frac{\mathcal{V}_k}{\mathcal{V}}\right) = \frac{\bar{\mathcal{V}}_k - \mathcal{V}_k}{\lambda \mathcal{V}} dt; \\ d\left(\frac{\mathcal{M}_k}{\mathcal{M}}\right) = \frac{\bar{\mathcal{M}}_k - \mathcal{M}_k}{\lambda \mathcal{M}} dt; \\ d\left(\frac{\mathcal{E}_k}{\mathcal{E}}\right) = \frac{\bar{\mathcal{E}}_k - \mathcal{E}_k}{\lambda \mathcal{E}} dt; \end{array} \right.$$

ensure that the entropy of the mixture  $\tilde{\eta}$  increases in time when the mixture is a closed system (i.e.  $d\mathcal{E} = d\mathcal{V} = d\mathcal{M} = 0$ ).

**They thus fulfill the second law of thermodynamics.**

*Remark: These models represent one choice among others. See the last section for a discussion on that point.*

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From the previous section, it remains to define  $d\mathcal{E}$ ,  $d\mathcal{V}$ , and  $d\mathcal{M}$ .

This is done in a classical manner with the following assumptions:

- the mass is conserved along the streamlines (so that we are in  $\mathcal{H}(\mathcal{M})$ ):

$$d\mathcal{M} = 0;$$

- the variation of volume  $\mathcal{V}$  is due to the divergence of the velocity field  $U$ :

$$d\mathcal{V} = \mathcal{V} \nabla_x \cdot (U) dt;$$

- the variation of the velocity  $U$  follows the Newton's law (we only consider the force due to the mixture pressure here):

$$d(\mathcal{M} U) = -\mathcal{V} \nabla_x (P) dt;$$

- the first law of thermodynamics applies to the energy  $\mathcal{E}$ :

$$d\mathcal{E} = -P d\mathcal{V} + Q dt.$$

The term  $Q$  will be discussed in an other section, and it is set to zero until that section.

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We first introduce a notation to deal with the dimension of the variables: for instance for a mass  $M$  which is in  $kg$ , we set  $M = M' \mathbb{I}_{kg}$ , where  $M'$  has no dimension and  $\mathbb{I}_{kg}$  is equal to  $1 \text{ kg}$ .

We then apply this to the phasic entropy  $\eta_k$  (in  $J/K$ ) and we use the property:

$$\forall a \in \mathbb{R}^+, \eta_k(a\mathcal{V}_k, a\mathcal{M}_k, a\mathcal{E}_k) = a\eta_k(\mathcal{V}_k, \mathcal{M}_k, \mathcal{E}_k).$$

We have:

$$\frac{1}{\mathcal{M}_k} \eta_k(\mathcal{V}_k, \mathcal{M}_k, \mathcal{E}_k) = \frac{1}{\mathbb{I}_{kg}} \eta_k \left( \frac{\mathcal{V}_k}{\mathcal{M}'_k}, \frac{\mathcal{M}_k}{\mathcal{M}'_k}, \frac{\mathcal{E}_k}{\mathcal{M}'_k} \right) = \frac{1}{\mathbb{I}_{kg}} \eta_k \left( \frac{\mathcal{V}_k}{\mathcal{M}_k} \mathbb{I}_{kg}, \mathbb{I}_{kg}, \frac{\mathcal{E}_k}{\mathcal{M}_k} \mathbb{I}_{kg} \right)$$

We can thus define a specific entropy  $s_k$  (in  $J/K/kg$ ), a specific volume  $\tau_k$  (in  $m^3/kg$ ) and a specific internal energy  $e_k$  (in  $J/kg$ ) as:

$$s_k(\tau_k, e_k) = \frac{1}{\mathbb{I}_{kg}} \eta_k(\tau_k \mathbb{I}_{kg}, \mathbb{I}_{kg}, e_k \mathbb{I}_{kg}); \quad \tau_k = \frac{\mathcal{V}_k}{\mathcal{M}_k}; \quad e_k = \frac{\mathcal{E}_k}{\mathcal{M}_k}.$$

This specific entropy  $s_k$  corresponds to the entropy for one unit of mass, so that  $s_k$  is strictly concave with respect to  $(\tau_k, e_k)$ .

Moreover, we have for the temperature:

$$\frac{1}{T_k} = \frac{\partial \eta_k}{\partial \mathcal{E}_k |_{\mathcal{V}_k, \mathcal{M}_k}} = \frac{\partial (\eta_k / \mathcal{M}_k)}{\partial (\mathcal{E}_k / \mathcal{M}_k) |_{\mathcal{V}_k, \mathcal{M}_k}} = \frac{\partial s_k}{\partial e_k |_{\tau_k}},$$

and for the pressure:

$$\frac{P_k}{T_k} = \frac{\partial s_k}{\partial \tau_k |_{e_k}}.$$

By dividing  $\eta$  by  $\mathcal{M}$ , we can also define a specific mixture entropy  $s$  as:

$$s\left(\frac{\mathcal{M}_1}{\mathcal{M}}, \tau_1, e_1, \frac{\mathcal{M}_2}{\mathcal{M}}, \tau_2, e_2, \dots\right) = \sum_k \frac{\mathcal{M}_k}{\mathcal{M}} s_k(\tau_k, e_k).$$



We define the volume fractions  $\alpha_k$ , the mass fractions  $y_k$  and the energy fractions  $z_k$  as:

$$\alpha_k = \frac{\mathcal{V}_k}{\mathcal{V}}, \quad y_k = \frac{\mathcal{M}_k}{\mathcal{M}}, \quad z_k = \frac{\mathcal{E}_k}{\mathcal{E}}.$$

We obviously have  $\sum_k \alpha_k = \sum_k y_k = \sum_k z_k = 1$ .

*Remark:  $\sum_k \alpha_k = 1$  because of the phases are immiscible !*

We define the equilibrium fractions associated with the equilibrium state  $\overline{W}$ :

$$\overline{\alpha}_k = \frac{\overline{\mathcal{V}}_k}{\overline{\mathcal{V}}}, \quad \overline{y}_k = \frac{\overline{\mathcal{M}}_k}{\overline{\mathcal{M}}}, \quad \overline{z}_k = \frac{\overline{\mathcal{E}}_k}{\overline{\mathcal{E}}}.$$

The specific volume, mixture density and specific internal energy are:

$$\tau = \frac{\mathcal{V}}{\mathcal{M}} = \sum_k y_k \tau_k, \quad \rho = \frac{1}{\tau} = \sum_k \alpha_k \rho_k, \quad e = \frac{\mathcal{E}}{\mathcal{M}} = \sum_k y_k e_k.$$

Then after some calculations ...

$d\mathcal{M} = 0;$	$\longleftrightarrow$	none
$d\left(\frac{\mathcal{V}_k}{\mathcal{V}}\right) = \frac{\bar{\mathcal{V}}_k - \mathcal{V}_k}{\lambda \mathcal{V}} dt;$	$\longleftrightarrow$	$\frac{\partial}{\partial t}(\rho \alpha_k) + \nabla_x \cdot (\rho U \alpha_k) = \rho \frac{\bar{\alpha}_k - \alpha}{\lambda};$
$d\left(\frac{\mathcal{M}_k}{\mathcal{M}}\right) = \frac{\bar{\mathcal{M}}_k - \mathcal{M}_k}{\lambda \mathcal{M}} dt;$	$\longleftrightarrow$	$\frac{\partial}{\partial t}(\rho y_k) + \nabla_x \cdot (\rho U y_k) = \rho \frac{\bar{y}_k - y}{\lambda};$
$d\left(\frac{\mathcal{E}_k}{\mathcal{E}}\right) = \frac{\bar{\mathcal{E}}_k - \mathcal{E}_k}{\lambda \mathcal{E}} dt;$	$\longleftrightarrow$	$\frac{\partial}{\partial t}(\rho z_k) + \nabla_x \cdot (\rho U z_k) = \rho \frac{\bar{z}_k - z}{\lambda};$
$d\mathcal{V} = \mathcal{V} \nabla_x \cdot (U) dt;$	$\longleftrightarrow$	$\frac{\partial}{\partial t}(\rho) + \nabla_x \cdot (\rho U) = 0;$
$d(\mathcal{M} U) = -\mathcal{V} \nabla_x (P) dt;$	$\longleftrightarrow$	$\frac{\partial}{\partial t}(\rho U) + \nabla_x \cdot (\rho U \otimes U + P I_3) = 0;$
$d\mathcal{E} = -P d\mathcal{V};$	$\longleftrightarrow$	$\frac{\partial}{\partial t}(\rho E) + \nabla_x \cdot (U(\rho E + P)) = 0,$

with the total energy  $E = e + U^2/2$ .

We get a multiphase flow model in conservative form, that allows to deal with immiscible components and accounts for the thermodynamical disequilibrium between the phases.

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In the following, we set:

- phase 1 for the steam
- phase 2 for the liquid water

Since we still have:

$$\begin{aligned}\mathcal{V} &= \mathcal{V}_1 + \mathcal{V}_2 \Rightarrow 0 = d\left(\frac{\mathcal{V}_1}{\mathcal{V}}\right) + d\left(\frac{\mathcal{V}_2}{\mathcal{V}}\right), \\ \mathcal{M} &= \mathcal{M}_1 + \mathcal{M}_2 \Rightarrow 0 = d\left(\frac{\mathcal{M}_1}{\mathcal{M}}\right) + d\left(\frac{\mathcal{M}_2}{\mathcal{M}}\right), \\ \mathcal{E} &= \mathcal{E}_1 + \mathcal{E}_2 \Rightarrow 0 = d\left(\frac{\mathcal{E}_1}{\mathcal{E}}\right) + d\left(\frac{\mathcal{E}_2}{\mathcal{E}}\right),\end{aligned}$$

and thanks to the closure laws for  $d\mathcal{V}$ ,  $d\mathcal{M}$  and  $d\mathcal{E}$ , the Gibbs relation for the mixture:

$$Td\tilde{\eta} - \underbrace{(d\mathcal{E} + Pd\mathcal{V} - \mu d\mathcal{M})}_{\text{"external exchange"}=0!} = T \underbrace{\sum_k \left( \frac{\mathcal{E}}{T_k} d\left(\frac{\mathcal{E}_k}{\mathcal{E}}\right) + \frac{\mathcal{V}P_k}{T_k} d\left(\frac{\mathcal{V}_k}{\mathcal{V}}\right) - \frac{\mathcal{M}\mu_k}{T_k} d\left(\frac{\mathcal{M}_k}{\mathcal{M}}\right) \right)}_{\text{exchange between the phases}}.$$

becomes:

$$d\tilde{\eta} = \mathcal{V} \left( \frac{P_1}{T_1} - \frac{P_2}{T_2} \right) d\left(\frac{\mathcal{V}_1}{\mathcal{V}}\right) + \mathcal{M} \left( \frac{\mu_2}{T_2} - \frac{\mu_1}{T_1} \right) d\left(\frac{\mathcal{M}_1}{\mathcal{M}}\right) + \mathcal{E} \left( \frac{1}{T_1} - \frac{1}{T_2} \right) d\left(\frac{\mathcal{E}_1}{\mathcal{E}}\right).$$

Hence, when the equilibrium between the three phases is reached, i.e. when  $d\tilde{\eta} = 0$ , i.e. when  $W = \overline{W}$ , we have:

$$\begin{aligned} P_1(\overline{\mathcal{V}}_1, \overline{\mathcal{M}}_1, \overline{\mathcal{E}}_1) &= P_2(\overline{\mathcal{V}}_2, \overline{\mathcal{M}}_2, \overline{\mathcal{E}}_2), \\ T_1(\overline{\mathcal{V}}_1, \overline{\mathcal{M}}_1, \overline{\mathcal{E}}_1) &= T_2(\overline{\mathcal{V}}_2, \overline{\mathcal{M}}_2, \overline{\mathcal{E}}_2), \\ \mu_1(\overline{\mathcal{V}}_1, \overline{\mathcal{M}}_1, \overline{\mathcal{E}}_1) &= \mu_2(\overline{\mathcal{V}}_2, \overline{\mathcal{M}}_2, \overline{\mathcal{E}}_2), \end{aligned}$$

with the constraints that

$$\begin{aligned} \overline{\mathcal{V}}_1 + \overline{\mathcal{V}}_2 &= \mathcal{V}, \\ \overline{\mathcal{M}}_1 + \overline{\mathcal{M}}_2 &= \mathcal{M}, \\ \overline{\mathcal{E}}_1 + \overline{\mathcal{E}}_2 &= \mathcal{E}, \end{aligned}$$

where  $\mathcal{V}$ ,  $\mathcal{M}$  and  $\mathcal{E}$  are fixed and known because we are in  $\mathcal{D}(\mathcal{V}, \mathcal{M}, \mathcal{E})$ .

If there is no solution for this system of equations, it means that the equilibrium state for  $(\mathcal{V}, \mathcal{M}, \mathcal{E})$  corresponds to a single phase state:

- pure liquid if  $\eta_2(\mathcal{V}, \mathcal{M}, \mathcal{E}) > \eta_1(\mathcal{V}, \mathcal{M}, \mathcal{E})$
- pure vapor if  $\eta_1(\mathcal{V}, \mathcal{M}, \mathcal{E}) > \eta_2(\mathcal{V}, \mathcal{M}, \mathcal{E})$

This pressure/temperature/Gibbs enthalpy equality defines the saturation curve. Indeed, by assuming a change of variable for the Gibbs enthalpy, we get at equilibrium:

$$\begin{aligned}P_1 &= P_2, \\T_1 &= T_2, \\ \mu_1(P_1, T_1) &= \mu_2(P_2, T_2).\end{aligned}$$

The saturation curve is then defined by the relation

$$\mu_1(P, T) = \mu_2(P, T),$$

which implicitly defines  $P_{sat}(T)$  and  $T_{sat}(P)$  as:

$$\begin{aligned}T &\mapsto P_{sat}(T), & \text{such that } \mu_1(P_{sat}(T), T) &= \mu_2(P_{sat}(T), T); \\ P &\mapsto T_{sat}(P), & \text{such that } \mu_1(P, T_{sat}(P)) &= \mu_2(P, T_{sat}(P)).\end{aligned}$$

On this saturation curve, the two phases co-exist.

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We may have to account for some external heating of the phases ( $Q$  was set to zero previously).

We assume that for each phase  $k$ :

- (i) the specific volume of each phase is constant,  $d(\tau_k) = 0$ ;
- (ii) the partial mass of each phase is constant,  $d(\alpha_k \rho_k) = 0$ ;
- (iii) the internal energy of each phase is such that,  $d(\alpha_k \rho_k e_k) = \alpha_k \rho_k q_k dt$ ;

where  $q_k$  is the specific power (in  $J/kg/s$ ) received by phase  $k$ .

Then we get that the mixture receives the heat  $\tilde{Q}$ :

$$d(\rho e) = \sum_k \alpha_k \rho_k q_k dt = \rho \tilde{Q} dt, \text{ and } \tilde{Q} = \sum_k y_k q_k,$$

and that the energy fraction of phase  $k$ ,  $z_k = (\alpha_k \rho_k e_k) / (\rho e)$ , is:

$$\rho e d(z_k) = \alpha_k \rho_k q_k dt - z_k \rho \tilde{Q} dt = \rho (y_k q_k - z_k \tilde{Q}) dt.$$

Hence, when the phases are heated by an external source  $q_k$ , system of equations becomes:

$$\left\{ \begin{array}{l} \frac{\partial}{\partial t} (\rho \alpha_k) + \nabla_x \cdot (\rho U \alpha_k) = \rho \frac{\bar{\alpha}_k - \alpha}{\lambda}, \quad k = 1..3, \\ \frac{\partial}{\partial t} (\rho y_k) + \nabla_x \cdot (\rho U y_k) = \rho \frac{\bar{y}_k - y}{\lambda}, \quad k = 1..3, \\ \frac{\partial}{\partial t} (\rho z_k) + \nabla_x \cdot (\rho U z_k) = \rho \frac{\bar{z}_k - z}{\lambda} + \rho \frac{y_k q_k - z_k \tilde{Q}}{e}, \quad k = 1..3, \\ \frac{\partial}{\partial t} (\rho) + \nabla_x \cdot (\rho U) = 0, \\ \frac{\partial}{\partial t} (\rho U) + \nabla_x \cdot (\rho U^2 + P l_3) = 0, \\ \frac{\partial}{\partial t} (\rho E) + \nabla_x \cdot (U(\rho E + P)) = \rho \tilde{Q}, \end{array} \right. \quad (1)$$

*Remark: If we omit the additionnal source term on  $z_k$ , we have:*

$$q_k = \frac{z_k}{y_k} \tilde{Q} \implies d(\alpha_k \rho_k e_k) = \alpha_k \rho_k q_k dt = \rho z_k \tilde{Q} dt,$$

*which means that the heat is dispatched between the phases with respect to the energy fractions !*

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At fixed  $\tau$  and  $e$ , they must increase the specific mixture-entropy  $s$ :

$$ds = \tau \left( \frac{P_1}{T_1} - \frac{P_2}{T_2} \right) d\alpha + \left( \frac{\mu_2}{T_2} - \frac{\mu_1}{T_1} \right) dy + e \left( \frac{1}{T_1} - \frac{1}{T_2} \right) dz.$$

It can be shown that  $(\alpha, y, z) \mapsto s(\alpha, y, z, \tau, e)$  is strictly concave. Hence starting from a point  $(\alpha_0, y_0, z_0)$ , the set

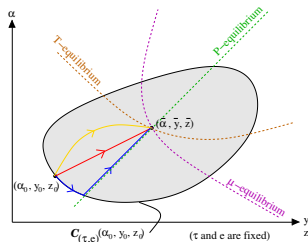
$$\mathcal{C}_{(\tau, e)}(\alpha_0, y_0, z_0) = \left\{ (\alpha, y, z) \in [0, 1]^3; s(\alpha, y, z, \tau, e) \geq s(\alpha_0, y_0, z_0, \tau, e) \right\}$$

is convex.

Moreover,  $(\bar{\alpha}, \bar{y}, \bar{z})$  only depends on  $(\tau, e)$  and  $(\bar{\alpha}, \bar{y}, \bar{z}) \in \mathcal{C}_{(\tau, e)}(\alpha_0, y_0, z_0)$ .

The model for the source terms, i.e. for  $d\alpha$ ,  $dy$ ,  $dz$  must be such that the path followed by  $(\alpha, y, z)$ :

- begins at  $(\alpha_0, y_0, z_0)$  at  $t = 0$ ;
- ends at  $(\bar{\alpha}, \bar{y}, \bar{z})$  when  $t \rightarrow \infty$ ;
- lies in  $\mathcal{C}_{(\tau, e)}(\alpha_0, y_0, z_0)$ ;
- and is such that  $ds \geq 0$  along the path.

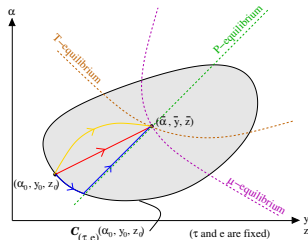


### Model chosen here:

Since the equilibrium state does only depend on  $\tau$  and  $e$ :

$$d\alpha = \frac{\bar{\alpha} - \alpha}{\lambda} dt \quad \longleftrightarrow \quad \alpha(t) = \beta \alpha_0 + (1 - \beta) \bar{\alpha}, \quad \text{with } \beta = e^{-\int_0^t 1/\lambda ds}.$$

This solution is very simple **BUT** there is only one parameter for the return to equilibrium.



## "Two-fluid" model:

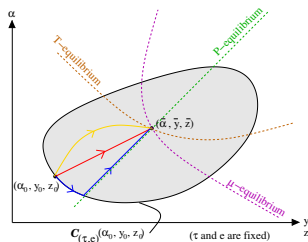
$$d\alpha = K_\alpha \left( \frac{P_1}{T_1} - \frac{P_2}{T_2} \right) dt, \quad K_\alpha > 0;$$

$$dy = K_y \left( \frac{\mu_2}{T_2} - \frac{\mu_1}{T_1} \right) dt, \quad K_y > 0;$$

$$dz = K_z \left( \frac{1}{T_1} - \frac{1}{T_2} \right) dt, \quad K_z > 0.$$

It is then possible to specify different time-scales for the pressure equilibrium, temperature equilibrium and Gibbs potential equilibrium.

**BUT**, in practice, numerical difficulties may arise and in particular vanishing-phase cases are difficult to handle.



### Instantaneous pressure-equilibrium (incomplete proposal):

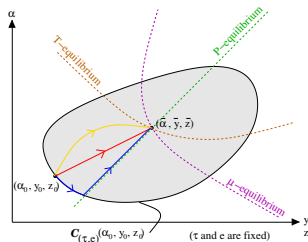
We first go from  $(\alpha_0, y_0, z_0)$  to a point  $(\alpha'_0, y'_0, z'_0)$  such that:

$$\begin{cases} s(\alpha'_0, y'_0, z'_0, \tau, e) = s(\alpha_0, y_0, z_0, \tau, e), \\ P_1(\alpha'_0, y'_0, z'_0, \tau, e) = P_2(\alpha'_0, y'_0, z'_0, \tau, e), \\ y'_0 = y_0. \end{cases}$$

Then, go from  $(\alpha'_0, y'_0, z'_0)$  to  $(\bar{\alpha}, \bar{y}, \bar{z})$  while keeping the  $P$ -equilibrium.  
Similar procedures could be proposed for  $T$ ,  $\mu$  or for  $P/T$ ,  $T/\mu$ , ...

**BUT**, does this proposal fulfil the criterion  $ds > 0$  ? does  $(\alpha'_0, y'_0, z'_0)$  exist ? Is it unique ?





### Just for fun, a stochastic procedure:

- initialization :  $(\alpha', y', z') := (\alpha_0, y_0, z_0)$  and  $C := \mathcal{C}_{(\tau,e)}(\alpha_0, y_0, z_0)$ ;
- then for  $t \rightarrow t + \delta t$  : choose randomly a point  $(\alpha', y', z')$  in the interior of  $C$ , and compute  $C := \mathcal{C}_{(\tau,e)}(\alpha', y', z')$
- continue until  $vol(C) > 0$ .

Convergence towards  $(\bar{\alpha}, \bar{y}, \bar{z})$  is ensured by the strict concavity of  $s$  and the choice of the new points inside  $C$  (no need to compute  $(\bar{\alpha}, \bar{y}, \bar{z})$  !).

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energy fraction	entropy fraction
$(\tau_k, e_k) \mapsto s_k(\tau_k, e_k)$	$(\tau_k, s_k) \mapsto e_k(\tau_k, s_k)$
$\alpha_k, y_k, z_k = y_k e_k / e$	$\alpha_k, y_k, \beta_k = y_k s_k / s$
$ds_k = de_k / T_k + P_k / T_k d\tau_k$	$de_k = T_k ds_k - P_k d\tau_k$
$P / T = \sum \alpha_k P_k / T_k$	$P = \sum \alpha_k P_k$
$1 / T = \sum z_k / T_k$	$T = \sum \beta_k T_k$
$c^2 = \text{"complex formula"}$	$c^2 = \sum y_k c_k^2$