5 First and second laws of the thermodynamics

Local volume and time averaging is used to derive rigorous energy equations for multi-phase flows in heterogeneous porous media. The flow is conditionally divided into three velocity fields. Each of the fields consists of several chemical components. Using the conservation equations for mass and momentum and the Gibbs equation, entropy equations are rigorously derived. It is shown that the use of the specific entropy as one of the dependent variables results in the simplest method for describing and modeling such a complicated thermodynamic system. A working form of the final entropy equation is recommended for general use in multi-phase flow dynamics.

5.1 Introduction

As in Chapters 1 and 2, from the large number of formulations of the conservation equations for multi-phase flows the local volume averaging as founded by *Anderson* and *Jackson, Slattery*, and *Whitaker* was selected to derive rigorously the energy conservation equations for multi-phase flows conditionally divided into three velocity fields. The heterogeneous porous-media formulation introduced by *Gentry* et al., commented by *Hirt*, and used by *Sha, Chao* and *Soo*, is then implanted into the formalism as a geometrical skeleton.

Beyond these concepts: I introduce in each of the velocity fields several constituents; The energy equations obtained in this way are then rearranged into the entropy equation using the mass and momentum equations, thereby reflecting the second law of thermodynamics; Then I perform subsequent time averaging; All interfacial integrals are suitably transformed in order to enable practical application.

This yields working equations for each of the three velocity fields that are recommended for general use in multi-phase fluid dynamic analysis.

As far as the author is aware, it was the first time in *Kolev* (1995) that a formulation of the second law of thermodynamics has been presented for such a complicated thermodynamic system as the multi-phase flows consisting of three velocity fields in porous structure, with each of these consisting of several chemical components. The most interesting result of this work is the simplicity of the local volume and time-averaged entropy equation (5.125) finally obtained

$$\rho_l\left[\alpha_l\gamma_v\frac{\partial s_l}{\partial\tau}+\left(\alpha_l^e\mathbf{V}_l\gamma\cdot\nabla\right)s_l\right]-\frac{1}{T_l}\nabla\cdot\left(\alpha_l^e\lambda_l^*\gamma\nabla T_l\right)$$

$$-\nabla.\left\{\alpha_l^e\rho_l\gamma\left[\sum_{i=2}^{i_{\max}}\left(s_{il}-s_{1l}\right)D_{il}^*\nabla C_{il}\right]\right\}=\gamma_v\left[\frac{1}{T_l}DT_l^N+\sum_{i=1}^{i_{\max}}\mu_{il}\left(s_{il}-s_l\right)\right]\quad\text{for }\alpha_l\geq 0,$$

where

$$DT_l^N=\alpha_l\rho_l\left[\delta_l\left(P_{k,l}+\varepsilon_{\eta,l}\right)+\varepsilon_l'\right]+\dot{q}'''+\sum_{i=1}^{i_{\max}}\mu_{iwl}\left(h_{iwl}-h_{il}\right)+\sum_{\substack{m=1\\m\neq l}}^{l_{\max}}\left[\begin{array}{c}\mu_{Mml}\left(h_{Ml}^{\sigma}-h_{Ml}\right)\\ \\ +\sum\limits_{n=1}^{n_{\max}}\mu_{nml}\left(h_{nm}-h_{nl}\right)\end{array}\right]$$

$$+\frac{1}{2}\left[\begin{array}{l}\mu_{wl}\left(\mathbf{V}_{wl}-\mathbf{V}_l\right)^2-\mu_{lw}\left(\mathbf{V}_{lw}-\mathbf{V}_l\right)^2+\sum\limits_{m=1}^{3}\mu_{ml}\left(\mathbf{V}_m-\mathbf{V}_l\right)^2\\ \\ +\mu_{wl}\overline{\left(\mathbf{V}_{wl}'-\mathbf{V}_l'\right)^2}-\mu_{lw}\overline{\left(\mathbf{V}_{lw}'-\mathbf{V}_l'\right)^2}+\sum\limits_{m=1}^{3}\mu_{ml}\overline{\left(\mathbf{V}_m'-\mathbf{V}_l'\right)^2}\end{array}\right].$$

This equation is more suitable for general use than the various forms of the energy equation e.g. Eq. (5.109) written in terms of the specific internal energy,

$$\frac{\partial}{\partial\tau}\left(\alpha_l\rho_l e_l\gamma_v\right)+\nabla\cdot\left(\alpha_l^e\rho_l e_l\mathbf{V}_l\gamma\right)+p_l\left[\frac{\partial}{\partial\tau}\left(\alpha_l\gamma_v\right)+\nabla\cdot\left(\alpha_l^e\mathbf{V}_l\gamma\right)\right]$$

$$-\nabla\cdot\left(\alpha_l^e\rho_l D_l^e\gamma\cdot\nabla e_l\right)+\overline{p_l'\nabla\cdot\left(\alpha_l^e\mathbf{V}_l'\gamma\right)}=\gamma_v De_l^*,$$

where

$$De_l^*=\alpha_l\rho_l\left[\delta_l\left(P_{k,l}+\varepsilon_{\eta,l}\right)+\varepsilon_l'\right]+\dot{q}'''+\frac{1}{2}\left[\begin{array}{l}\mu_{wl}\left(\mathbf{V}_{wl}-\mathbf{V}_l\right)^2-\mu_{lw}\left(\mathbf{V}_{lw}-\mathbf{V}_l\right)^2\\ \\ +\sum\limits_{m=1}^{3}\mu_{ml}\left(\mathbf{V}_m-\mathbf{V}_l\right)^2\end{array}\right]$$

$$+\frac{1}{2}\left[\mu_{wl}\overline{\left(\mathbf{V}_{wl}'-\mathbf{V}_l'\right)^2}-\mu_{lw}\overline{\left(\mathbf{V}_{lw}'-\mathbf{V}_l'\right)^2}+\sum_{m=1}^{3}\mu_{ml}\overline{\left(\mathbf{V}_m'-\mathbf{V}_l'\right)^2}\right]$$

$$+\sum_{i=1}^{i_{\max}}\left(\mu_{iwl}h_{iwl}-\mu_{ilw}h_{il}\right)+\sum_{m=1}^{3}\left[\mu_{Mml}h_{Ml}^{\sigma}+\sum_{n=1}^{n_{\max}}\left(\mu_{nml}h_{nm}-\mu_{nlm}h_{nl}\right)\right]$$

or Eq. (5.176) written in terms of temperature

$$\rho_l c_{pl}\left[\alpha_l\gamma_v\frac{\partial T_l}{\partial\tau}+\left(\alpha_l^e\mathbf{V}_l\gamma\cdot\nabla\right)T_l\right]-\left[1-\rho_l\left(\frac{\partial h_l}{\partial p}\right)_{T_l,all\_C's}\right]\left[\alpha_l\gamma_v\frac{\partial p}{\partial\tau}+\left(\alpha_l^e\mathbf{V}_l\gamma\cdot\nabla\right)p\right]$$

$$-\nabla\cdot\left(\alpha_l^e\lambda_l^*\gamma\nabla T\right)+T_l\sum_{i=2}^{i_{\max}}\Delta s_{il}^{np}\nabla\left(\alpha_l^e\rho_l D_{il}^*\gamma\nabla C_{il}\right)=\gamma_v\left[DT_l^N-T_l\sum_{i=2}^{i_{\max}}\Delta s_{il}^{np}\left(\mu_{il}-C_{il}\mu_l\right)\right],$$

or Eq. (5.115) written in terms of specific enthalpy

$$\frac{\partial}{\partial\tau}\left(\alpha_l\rho_l h_l\gamma_v\right)+\nabla\cdot\left(\alpha_l^e\rho_l\mathbf{V}_l h_l\gamma\right)-\left(\alpha_l\gamma_v\frac{\partial p_l}{\partial\tau}+\alpha_l^e\mathbf{V}_l\gamma\cdot\nabla p_l\right)$$

$$-\nabla\cdot\left\{\alpha_l^e\left[\lambda_l^*\nabla T_l+\rho_l\sum_{i=2}^{i_{\max}}\left(h_{il}-h_{1l}\right)D_{il}^*\nabla C_{il}\right]\gamma\right\}-\alpha_l^e\overline{\mathbf{V}_l'\gamma\cdot\nabla p_l'}$$

$$+\delta_l\left(\alpha_l^e\gamma\nabla p_l\right)\cdot\sum_{i=1}^{i_{\max}}D_{il}^l\nabla\ln C_{il}=\gamma_v DT_l^N+\gamma_v\sum_{\substack{m=1\\m\neq l}}^{3,w}\sum_{i=1}^{i_{\max}}\left(\mu_{iml}-\mu_{ilm}\right)h_{il}.$$

Another important result is the so called volume conservation equation

$$\frac{\gamma_v}{\rho a^2}\frac{\partial p}{\partial\tau}+\sum_{l=1}^{l_{\max}}\frac{\alpha_l}{\rho_l a_l^2}\left(\mathbf{V}_l\gamma\cdot\nabla\right)p+\nabla\cdot\sum_{l=1}^{l_{\max}}\left(\alpha_l\mathbf{V}_l\gamma\right)=\sum_{l=1}^{l_{\max}}D\alpha_l-\frac{\partial\gamma_v}{\partial\tau},$$

where

$$D\alpha_l=\frac{1}{\rho_l}\left\{\gamma_v\mu_l-\frac{1}{\rho_l}\left[\left(\frac{\partial\rho_l}{\partial s_l}\right)_{p,all\_C_{li}'s}Ds_l^N+\sum_{i=2}^{i_{\max}}\left(\frac{\partial\rho_l}{\partial C_{li}}\right)_{p,s,all\_C_{li}'s\_except\_C_{l1}}DC_{il}^N\right]\right\}$$

$$DC_{il}^N=\nabla\left(\alpha_l\rho_l D_{il}^*\gamma\nabla C_{il}\right)+\gamma_v\left(\mu_{il}-C_{il}\mu_l\right),$$

$$Ds_l^N=\frac{1}{T_l}\nabla\cdot\left(\alpha_l^e\lambda_l^*\gamma\nabla T_l\right)+\nabla.\left\{\alpha_l^e\rho_l\gamma\left[\sum_{i=1}^{i_{\max}}s_{il}D_{il}^*\nabla C_{il}\right]\right\}$$

$$+\gamma_v\left[\frac{1}{T_l}DT_l^N+\sum_{i=1}^{i_{\max}}\mu_{il}\left(s_{il}-s_l\right)\right].$$

This equation can be used instead of the one of the field mass conservation equations.

This Chapter is an extended version of the work published in *Kolev* (1995, 1997a).

5.2 Instantaneous local volume average energy equations

The energy principle formulated for a volume occupied by the velocity field *l* only is as follows:

> The sum of the rates of energy added to the velocity field from the surroundings due to conduction and convection plus the rate of work done on the velocity field is equal to the rate of change in the energy of the velocity field as it flows through a volume occupied by this velocity field.

The instantaneous energy conservation equation written per unit field volume is thus

$$\sum_{i=1}^{i_{\max}} \left\{ \frac{\partial}{\partial \tau} \left[\rho_{il} \left(e_{il}^{\tau} + \frac{1}{2} V_{il}^{\tau 2} \right) \right] + \nabla \cdot \left[\rho_{il} \left(e_{il}^{\tau} + p_{il}^{\tau} / \rho_{il} + \frac{1}{2} V_{il}^{\tau 2} \right) \mathbf{V}_{il}^{\tau} \right] \right\}$$

$$- \nabla \cdot \left(\mathbf{T}_{\eta,l}^{\tau} \cdot \mathbf{V}_{l}^{\tau} \right) - \nabla \cdot \left(\lambda_{l}^{l} \nabla T_{l} \right) + \rho_{l} \mathbf{g} \cdot \mathbf{V}_{l}^{\tau} = 0 , \qquad (5.1)$$

where $V_{il}^{\tau 2} = \mathbf{V}_{il}^{\tau} \cdot \mathbf{V}_{il}^{\tau}$ is a scalar. The scalar λ_{l}^{l} in the *Fourier*'s law of heat conduction $\dot{q}_{l}'' = -\lambda_{l}^{l} \nabla T_{l}$ is called isotropic thermal conductivity. There is no doubt about the validity of equation (5.1) for velocities much less than the velocity of light. In contrast to the *Sha* et al. (1984) derivation, a multi-component velocity field is considered here instead of a single component. This will allow for derivation of mixture properties for the field that are strictly consistent with the first law of thermodynamics.

The *specific enthalpy* of each component

$$h_{il}^{\tau} = e_{il}^{\tau} + p_{il}^{\tau} / \rho_{il} \qquad (5.2)$$

naturally arises in the second differential term. Historically, the specific enthalpy was introduced as a very convenient variable to describe steady-state processes. We replace the specific internal energy also in the first differential term by using

$$e_{il}^{\tau} = h_{il}^{\tau} - p_{il}^{\tau} / \rho_{il} . \qquad (5.3)$$

Performing local volume averaging on Eq. (5.1) as already described in Chapter 1, one obtains

$$\sum_{i=1}^{i_{\max}} \left\{ \left\langle \frac{\partial}{\partial \tau} \left[\rho_{il} \left(h_{il}^{\tau} + \frac{1}{2} V_{il}^{\tau 2} \right) \right] \right\rangle + \left\langle \nabla \cdot \left[\rho_{il} \left(h_{il}^{\tau} + \frac{1}{2} V_{il}^{\tau 2} \right) \mathbf{V}_{il}^{\tau} \right] \right\rangle - \left\langle \frac{\partial p_{il}^{\tau}}{\partial \tau} \right\rangle \right\}$$

$$- \left\langle \nabla \cdot \left(\mathbf{T}_{\eta,l}^{\tau} \cdot \mathbf{V}_{l}^{\tau} \right) + \nabla \cdot \left(\lambda_{l}^{l} \nabla T_{l} \right) \right\rangle + \left\langle \rho_{l} \mathbf{g} \cdot \mathbf{V}_{l}^{\tau} \right\rangle = 0 . \qquad (5.4)$$

The time derivative of the pressure is averaged using Eq. (1.32) (*Leibnitz* rule) as follows:

$$-\left\langle \frac{\partial p_{il}^{\tau}}{\partial \tau} \right\rangle = -\frac{\partial}{\partial \tau}\left(\gamma_v \alpha_{il} \left\langle p_{il}^{\tau} \right\rangle^{il} \right) + \frac{1}{Vol} \int\limits_{F_{l\sigma}+F_{lw}} p_{il}^{\tau} \mathbf{V}_{il\sigma}^{\tau} \cdot \mathbf{n}_l dF . \tag{5.5}$$

As in Chapter 2, the pressure at the interface $F_{l\sigma}$ is expressed in the form of the sum of bulk averaged pressure, which is independent on the location of the interface, and of the deviation from the bulk pressure, which depends on the location of the surface:

$$p_{il}^{\tau} = \left\langle p_{il}^{\tau} \right\rangle^{il} + \Delta p_{il\sigma}^{\tau} \tag{5.6}$$

An analogous separation can be performed at the structure interface F_{lw}

$$p_{il}^{\tau} = \left\langle p_{il}^{\tau} \right\rangle^{il} + \Delta p_{ilw}^{\tau} . \tag{5.7}$$

Substituting Eqs. (5.6) and (5.7) into Eq. (5.5), and using Eq. (1.33), the following is obtained

$$\frac{1}{Vol} \int\limits_{F_{l\sigma}+F_{lw}} p_{il}^{\tau} \mathbf{V}_{il\sigma}^{\tau} \cdot \mathbf{n}_l dF$$

$$= \left\langle p_{il}^{\tau} \right\rangle^{il} \frac{1}{Vol} \int\limits_{F_{l\sigma}+F_{lw}} \mathbf{V}_{il\sigma}^{\tau} \cdot \mathbf{n}_l dF + \frac{1}{Vol} \int\limits_{F_{l\sigma}} \Delta p_{il\sigma}^{\tau} \mathbf{V}_{il\sigma}^{\tau} \cdot \mathbf{n}_l dF + \frac{1}{Vol} \int\limits_{F_{lw}} \Delta p_{ilw}^{\tau} \mathbf{V}_{ilw}^{\tau} \cdot \mathbf{n}_l dF$$

$$= \left\langle p_{il}^{\tau} \right\rangle^{il} \frac{\partial}{\partial \tau}\left(\alpha_{il} \gamma_v \right) + \frac{1}{Vol} \int\limits_{F_{l\sigma}} \Delta p_{il\sigma}^{\tau} \mathbf{V}_{il\sigma}^{\tau} \cdot \mathbf{n}_l dF + \frac{1}{Vol} \int\limits_{F_{lw}} \Delta p_{ilw}^{\tau} \mathbf{V}_{ilw}^{\tau} \cdot \mathbf{n}_l dF . \tag{5.8}$$

The first term is the power introduced into the velocity field due to a change of the field component volume per unit time and unit control volume (expansion or compression power). Thus, the final result for the averaging of the time derivative of the pressure is

$$-\left\langle \frac{\partial p_{il}^{\tau}}{\partial \tau} \right\rangle = -\frac{\partial}{\partial \tau}\left(\gamma_v \alpha_{il} \left\langle p_{il}^{\tau} \right\rangle^{il} \right) + \left\langle p_{il}^{\tau} \right\rangle^{il} \frac{\partial}{\partial \tau}\left(\alpha_{il} \gamma_v \right)$$

$$+ \frac{1}{Vol} \int\limits_{F_{l\sigma}} \Delta p_{il\sigma}^{\tau} \mathbf{V}_{il\sigma}^{\tau} \cdot \mathbf{n}_l dF + \frac{1}{Vol} \int\limits_{F_{lw}} \Delta p_{ilw}^{\tau} \mathbf{V}_{ilw}^{\tau} \cdot \mathbf{n}_l dF$$

$$= -\alpha_{il} \gamma_v \frac{\partial}{\partial \tau} \left\langle p_{il}^{\tau} \right\rangle^{il} + \frac{1}{Vol} \int\limits_{F_{l\sigma}} \Delta p_{il\sigma}^{\tau} \mathbf{V}_{il\sigma}^{\tau} \cdot \mathbf{n}_l dF + \frac{1}{Vol} \int\limits_{F_{lw}} \Delta p_{ilw}^{\tau} \mathbf{V}_{ilw}^{\tau} \cdot \mathbf{n}_l dF . \tag{5.9}$$

Applying Eqs. (1.28), (1.25) and (1.32) to the other terms of Eq. (5.4), and taking into account Eq. (5.9), one obtains

$$\sum_{i=1}^{i_{\max}} \left\{ \begin{array}{l} \dfrac{\partial}{\partial \tau}\left[\gamma_v \alpha_{il} \left\langle \rho_{il} \left(h_{il}^{\tau} + \dfrac{1}{2} V_{il}^{\tau 2} \right) \right\rangle^{il} \right] \\ +\nabla \cdot \left[\gamma \alpha_{il}^{e} \left\langle \rho_{il} \left(h_{il}^{\tau} + \dfrac{1}{2} V_{il}^{\tau 2} \right) \mathbf{V}_{il}^{\tau} \right\rangle^{ile} \right] - \gamma_v \alpha_{il} \dfrac{\partial}{\partial \tau} \left\langle p_{il}^{\tau} \right\rangle^{il} \end{array} \right\}$$

$$-\nabla \cdot \left(\alpha_l^e \gamma \left\langle \mathbf{T}_{\eta,l}^{\tau} \cdot \mathbf{V}_l^{\tau} \right\rangle^{le} \right) - \nabla \cdot \left(\alpha_l^e \gamma \left\langle \lambda_l^l \nabla T_l \right\rangle^{le} \right) + \alpha_l \gamma_v \left\langle \rho_l \left(\mathbf{g} \cdot \mathbf{V}_l^{\tau} \right) \right\rangle^{l}$$

$$+\frac{1}{Vol} \int\limits_{F_{l\sigma}+F_{lw}} \left[\sum_{i=1}^{i_{\max}} \rho_{il} \left(h_{il}^{\tau} + \frac{1}{2} V_{il}^{\tau 2} \right) \left(\mathbf{V}_{il}^{\tau} - \mathbf{V}_{il\sigma}^{\tau} \right) \cdot \mathbf{n}_l dF \right]$$

$$+\frac{1}{Vol} \int\limits_{F_{l\sigma}} \Delta p_{l\sigma}^{\tau} \mathbf{V}_{l\sigma}^{\tau} \cdot \mathbf{n}_l dF + \frac{1}{Vol} \int\limits_{F_{lw}} \Delta p_{lw}^{\tau} \mathbf{V}_{lw}^{\tau} \cdot \mathbf{n}_l dF$$

$$-\frac{1}{Vol} \int\limits_{F_{l\sigma}+F_{lw}} \mathbf{T}_{\eta,l}^{\tau} \cdot \mathbf{V}_l^{\tau} \cdot \mathbf{n}_l dF - \frac{1}{Vol} \int\limits_{F_{l\sigma}+F_{lw}} \lambda_l^l \nabla T_l \cdot \mathbf{n}_l dF = 0 . \tag{5.10}$$

The δ_l -identifier for the dispersed field is now introduced into the heat conduction term, which thus becomes

$$\nabla \cdot \left(\alpha_l^e \gamma \delta_l \left\langle \lambda_l^l \nabla T_l \right\rangle^{le} \right). \tag{5.11}$$

The above simply means that there is no heat transfer through heat conduction for dispersed field, δ_l = 0, and that heat conduction is taken into account for a continuous field, δ_l = 1.

The heat source term

$$\frac{1}{Vol} \int\limits_{F_{l\sigma}+F_{lw}} \lambda_l^l \nabla T_l \cdot \mathbf{n}_l dF = \gamma_v \left(\dot{q}_{wl}''' + \sum_{\substack{m=1 \\ m \neq l}}^{3} \dot{q}_{m\sigma l}''' \right) = \gamma_v \dot{q}_l''' \tag{5.12}$$

takes into account the sum of the heat power per unit control volume introduced into the velocity field through the interface, $\gamma_v \dot{q}_{m\sigma l}'''$, and through the wall, $\gamma_v \dot{q}_{wl}'''$.

The integral terms containing the velocity difference $\mathbf{V}_{il}^{\tau} - \mathbf{V}_{il\sigma}^{\tau}$ represent the energy transfer due to (a) evaporation, or (b) condensation, or (c) entrainment, or (d) deposition at the interface $F_{l\sigma}$, or (e) due to injection or (f) suction through the solid interface F_{lw}. It is very important to note that h_{il}^{τ} under the interface integral is taken *inside the field l* at the immediate interface neighborhood denoted with σ. The subscript *M* is introduced here to designate the non-inert component within the field. n used to designate the inert component. The total number of inert components in each field is $i_{\max} - 1$.

Consequently

$$h_{Ml}^{\tau\sigma} = h''\left(T_{12}^{\sigma}\right) \quad \text{or} \quad h_{Ml}^{\tau\sigma} = h''\left(T_{13}^{\sigma}\right) \quad \text{for } l = 1, \tag{5.13}$$

$$h_{M2}^{\tau\sigma} = h'\left(p\right) \quad \text{for } l = 2, \tag{5.14}$$

$$h_{M3}^{\tau\sigma} = h'\left(p\right) \quad \text{for } l = 3\,, C_{M3} > 0, \tag{5.15}$$

for all mass flows entering field l. Mass flows leaving field l possess the l-properties. One now assumes that $\mathbf{V}_{il}^{\tau} = \mathbf{V}_{l}^{\tau}$ at the l side of the interface, with these terms then split into non-negative components. It is necessary to distinguish between mass transfer due to change in the state of aggregate, and mass transfer such as entrainment, deposition, etc. resulting from mechanical macroscopic forces.

(a) The mass transfer term at the field-solid interface is decomposed as follows:

$$-\frac{1}{Vol}\int_{F_{lw}}\left[\sum_{i=1}^{i_{\max}}\rho_{il}\left(h_{il}^{\tau}+\frac{1}{2}V_{il}^{\tau 2}\right)\left(\mathbf{V}_{il}^{\tau}-\mathbf{V}_{il\sigma}^{\tau}\right)\cdot\mathbf{n}_{l}dF\right]$$

$$=\gamma_{v}\left\{\sum_{i=1}^{i_{\max}}\left[\left(\mu_{iwl}^{\tau}\left\langle h_{iw}^{\tau}\right\rangle^{iw}-\mu_{ilw}^{\tau}\left\langle h_{il}^{\tau}\right\rangle^{il}\right)\right]+\mu_{wl}^{\tau}\frac{1}{2}\left\langle V_{wl}^{\tau 2}\right\rangle^{we}-\mu_{lw}^{\tau}\frac{1}{2}\left\langle V_{lw}^{\tau 2}\right\rangle^{le}\right\}; \tag{5.16}$$

(b) The mass transfer term at the field interface is decomposed as follows

$$-\frac{1}{Vol}\int_{F_{l\sigma}}\left[\sum_{i=1}^{i_{\max}}\rho_{il}\left(h_{il}^{\tau}+\frac{1}{2}V_{il}^{\tau 2}\right)\left(\mathbf{V}_{il}^{\tau}-\mathbf{V}_{il\sigma}^{\tau}\right)\cdot\mathbf{n}_{l}dF\right]$$

$$=\gamma_{v}\left\{\begin{array}{l}\sum_{m=1}^{3}\left\{\left(\mu_{Mml}^{\tau}h_{Ml}^{\tau\sigma}-\mu_{Mlm}^{\tau}\left\langle h_{Ml}^{\tau}\right\rangle^{Ml}\right)+\sum_{n=1}^{n_{\max}}\left(\mu_{nml}^{\tau}\left\langle h_{nm}^{\tau}\right\rangle^{nm}-\mu_{nlm}^{\tau}\left\langle h_{nl}^{\tau}\right\rangle^{nl}\right)\right\}\\ +\mu_{ml}^{\tau}\frac{1}{2}\left\langle V_{m}^{\tau 2}\right\rangle^{me}-\mu_{lm}^{\tau}\frac{1}{2}\left\langle V_{l}^{\tau 2}\right\rangle^{le}\end{array}\right\}; \tag{5.17}$$

Attention: The interfacial mass transfer is either convective or is a change of the state of aggregate (evaporation or condensation). Eq. (5.17) is strictly valid for convective interfacial mass transfer. In case of evaporation or condensation the specific enthalpy of the leaving mass flow rate may be different than the volume averaged field enthalpy resulting in: $\sum_{m=1}^{3}\left[\left(\mu_{Mml}^{\tau}h_{Ml}^{\tau\sigma}-\mu_{Mlm}^{\tau}h_{Ml}^{\tau\sigma}\right)+...\right]...$

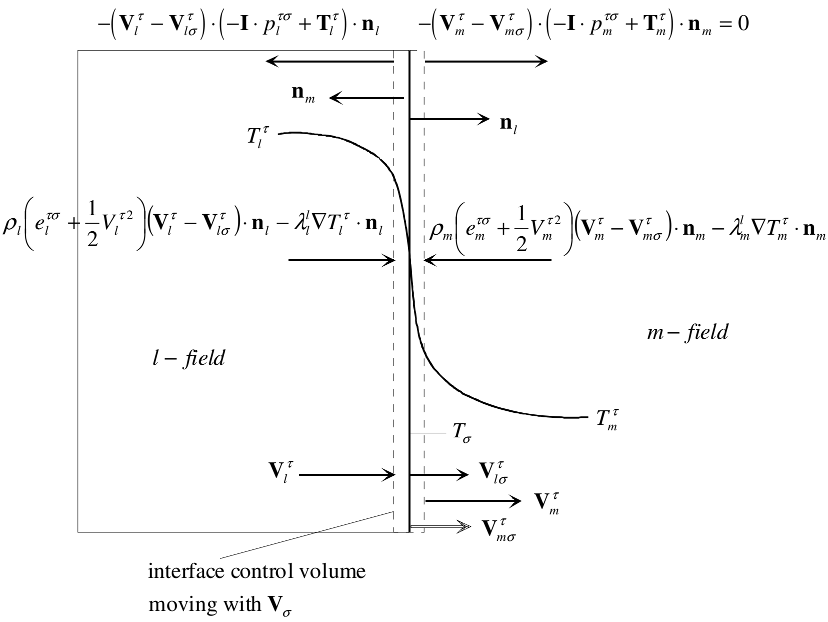

Fig. 5.1 Interfacial energy transfer

The sum of Eqs. (5.12), (5.16) and (5.17) gives

$$q_l^* = \dot{q}_l''' + \sum_{i=1}^{i_{\max}}\left[\left(\mu_{iwl}^\tau\left\langle h_{iw}^\tau\right\rangle^{iw} - \mu_{ilw}^\tau\left\langle h_{il}^\tau\right\rangle^{il}\right)\right]$$

$$+\sum_{m=1}^{3}\left\{\left(\mu_{Mml}^\tau h_{Ml}^{\tau\sigma} - \mu_{Mlm}^\tau\left\langle h_{Ml}^\tau\right\rangle^{Ml}\right) + \sum_{n=1}^{n_{\max}}\left(\mu_{nml}^\tau\left\langle h_{nm}^\tau\right\rangle^{nm} - \mu_{nlm}^\tau\left\langle h_{nl}^\tau\right\rangle^{nl}\right)\right\}$$

$$+\mu_{wl}^\tau\frac{1}{2}\left\langle V_{wl}^{\tau 2}\right\rangle^{we} - \mu_{lw}^\tau\frac{1}{2}\left\langle V_{lw}^{\tau 2}\right\rangle^{le} + \frac{1}{2}\sum_{m=1}^{3}\left(\mu_{ml}^\tau\left\langle V_m^{\tau 2}\right\rangle^{me} - \mu_{lm}^\tau\left\langle V_l^{\tau 2}\right\rangle^{le}\right). \quad (5.18)$$

The *interfacial energy jump condition* is introduced at this point, with interface *lm* considered as *non-material*, see Fig. 5.1,

$$\rho_l\left(e_l^{\tau\sigma} + \frac{1}{2}V_l^{\tau 2}\right)\left(\mathbf{V}_l^\tau - \mathbf{V}_{l\sigma}^\tau\right)\cdot\mathbf{n}_l - \lambda_l^l\nabla T_l^\tau\cdot\mathbf{n}_l$$

$$+\rho_m\left(e_m^{\tau\sigma} + \frac{1}{2}V_m^{\tau 2}\right)\left(\mathbf{V}_m^\tau - \mathbf{V}_{m\sigma}^\tau\right)\cdot\mathbf{n}_m - \lambda_m^l\nabla T_m^\tau\cdot\mathbf{n}_m$$

$$-\left(\mathbf{V}_l^\tau - \mathbf{V}_{l\sigma}^\tau\right)\cdot\left(-\mathbf{I}\cdot p_l^{\tau\sigma} + \mathbf{T}_l^\tau\right)\cdot\mathbf{n}_l - \left(\mathbf{V}_m^\tau - \mathbf{V}_{m\sigma}^\tau\right)\cdot\left(-\mathbf{I}\cdot p_m^{\tau\sigma} + \mathbf{T}_m^\tau\right)\cdot\mathbf{n}_m = 0 \quad (5.19)$$

or

$$\begin{bmatrix} \rho_l \left(h_l^{\tau\sigma} + \frac{1}{2} V_l^{\tau 2} \right) \left(\mathbf{V}_l^\tau - \mathbf{V}_{l\sigma}^\tau \right) - \rho_m \left(h_m^{\tau\sigma} + \frac{1}{2} V_m^{\tau 2} \right) \left(\mathbf{V}_m^\tau - \mathbf{V}_{m\sigma}^\tau \right) \\ \\ -\lambda_l^l \nabla T_l^\tau + \lambda_m^l \nabla T_m^\tau - \left(\mathbf{V}_l^\tau - \mathbf{V}_{l\sigma}^\tau \right) \cdot \mathbf{T}_l^\tau + \left(\mathbf{V}_m^\tau - \mathbf{V}_{m\sigma}^\tau \right) \cdot \mathbf{T}_m^\tau \end{bmatrix} \cdot \mathbf{n}_l = 0 . \quad (5.20)$$

Using Eqs. (1.42b) and (1.42c), Eq. (5.20) can be simplified as follows

$$\begin{bmatrix} \left[h_l^{\tau,m\sigma} - h_m^{\tau,l\sigma} + \frac{1}{2} \left(V_l^{\tau 2} - V_m^{\tau 2} \right) \right] \frac{\rho_m \rho_l}{\rho_l - \rho_m} \left(\mathbf{V}_m^\tau - \mathbf{V}_l^\tau \right) \\ \\ -\lambda_l^l \nabla T_l^\tau + \lambda_m^l \nabla T_m^\tau + \frac{\rho_l \rho_m}{\rho_l - \rho_m} \left(\mathbf{V}_m^\tau - \mathbf{V}_l^\tau \right) \cdot \left(\frac{\mathbf{T}_m^\tau}{\rho_m} - \frac{\mathbf{T}_l^\tau}{\rho_l} \right) \end{bmatrix} \cdot \mathbf{n}_l = 0 , \quad (5.21)$$

or

$$\left[h_l^{\tau,m\sigma} - h_m^{\tau,l\sigma} + \frac{1}{2} \left(V_l^{\tau 2} - V_m^{\tau 2} \right) + \frac{\mathbf{T}_m^\tau}{\rho_m} - \frac{\mathbf{T}_l^\tau}{\rho_l} \right] \left(\rho w \right)_{lm}^\tau + \left(\lambda_m^l \nabla T_m^\tau - \lambda_l^l \nabla T_l^\tau \right) \cdot \mathbf{n}_l = 0 .$$

or

$$\left(\rho w \right)_{lm}^\tau = - \frac{\left(\lambda_m^l \nabla T_m^\tau - \lambda_l^l \nabla T_l^\tau \right) \cdot \mathbf{n}_l}{h_l^{\tau,m\sigma} - h_m^{\tau,l\sigma} + \frac{1}{2} \left(V_l^{\tau 2} - V_m^{\tau 2} \right) + \frac{\mathbf{T}_m^\tau}{\rho_m} - \frac{\mathbf{T}_l^\tau}{\rho_l}} .$$

We realize that if there is no mass transfer across the interfacial contact discontinuity heat conduction is the only mechanism transferring energy across. In the simple case of no heat conduction at both sides of the interface and zero stress tensors the energy jump condition simplifies to

$$h_l^{\tau\sigma} - h_m^{\tau\sigma} + \frac{1}{2} \left(V_l^{\tau 2} - V_m^{\tau 2} \right) = 0 . \quad (5.22)$$

Integrating Eq. (5.20) over the interface inside the control volume and dividing by the control volume we obtain

$$\frac{1}{Vol} \int\limits_{F_{l\sigma}+F_{lw}} \begin{bmatrix} \rho_l \left(h_l^{\tau\sigma} + \frac{1}{2} V_l^{\tau 2} \right) \left(\mathbf{V}_l^\tau - \mathbf{V}_{l\sigma}^\tau \right) - \rho_m \left(h_m^{\tau\sigma} + \frac{1}{2} V_m^{\tau 2} \right) \left(\mathbf{V}_m^\tau - \mathbf{V}_{m\sigma}^\tau \right) \\ \\ -\lambda_l^l \nabla T_l^\tau + \lambda_m^l \nabla T_m^\tau - \left(\mathbf{V}_l^\tau - \mathbf{V}_{l\sigma}^\tau \right) \cdot \mathbf{T}_l^\tau + \left(\mathbf{V}_m^\tau - \mathbf{V}_{m\sigma}^\tau \right) \cdot \mathbf{T}_m^\tau \end{bmatrix} \cdot \mathbf{n}_l dF = 0 .$$

$$(5.23)$$

In the event of evaporation or condensation this yields

$$\mu_{Ml}^{\tau}\left(h_{Ml}^{\tau\sigma}+\frac{1}{2}V_{l}^{\tau 2}\right)-\dot{q}_{m\sigma l}^{\prime\prime\prime}-\mu_{Mm}^{\tau}\left(h_{Mm}^{\tau\sigma}+\frac{1}{2}V_{m}^{\tau 2}\right)-\dot{q}_{l\sigma m}^{\prime\prime\prime}$$

$$+\frac{1}{Vol}\int\limits_{F_{l\sigma}+F_{lw}}\left[-\left(\mathbf{V}_{l}^{\tau}-\mathbf{V}_{l\sigma}^{\tau}\right)\cdot\mathbf{T}_{l}^{\tau}+\left(\mathbf{V}_{m}^{\tau}-\mathbf{V}_{m\sigma}^{\tau}\right)\cdot\mathbf{T}_{m}^{\tau}\right]\cdot\mathbf{n}_{l}dF=0. \tag{5.24}$$

Postulating the weighted average

$$\left\langle\rho_{il}h_{il}^{\tau}\right\rangle^{il}/\left\langle\rho_{il}\right\rangle^{il}=\left\langle h_{il}^{\tau}\right\rangle^{il}, \tag{5.25}$$

$$\left\langle\rho_{il}V_{il}^{\tau 2}\right\rangle^{ile}/\left\langle\rho_{il}\right\rangle^{ile}=\left\langle V_{il}^{\tau 2}\right\rangle^{ile}, \tag{5.26}$$

$$\left\langle\rho_{il}V_{il}^{\tau 2}\mathbf{V}_{il}^{\tau}\right\rangle^{ile}/\left\langle\rho_{il}\right\rangle^{ile}=\left\langle V_{il}^{\tau 2}\right\rangle^{ile}\left\langle\mathbf{V}_{il}^{\tau}\right\rangle^{ile}, \tag{5.27}$$

one can then write the *conservative form* of the energy conservation equation in the following form

$$\sum_{i=1}^{i_{\max}}\left\{\begin{array}{l}\dfrac{\partial}{\partial\tau}\left[\gamma_{v}\alpha_{il}\left\langle\rho_{il}\right\rangle^{il}\left(\left\langle h_{il}^{\tau}\right\rangle^{il}+\dfrac{1}{2}\left\langle V_{il}^{\tau 2}\right\rangle^{ile}\right)\right]\\ \\ +\nabla\cdot\left[\gamma\alpha_{il}^{e}\left\langle\rho_{il}\right\rangle^{il}\left\langle\mathbf{V}_{il}^{\tau}\right\rangle^{ile}\left(\left\langle h_{il}^{\tau}\right\rangle^{il}+\dfrac{1}{2}\left\langle V_{il}^{\tau 2}\right\rangle^{ile}\right)\right]-\gamma_{v}\alpha_{il}\dfrac{\partial}{\partial\tau}\left\langle p_{il}^{\tau}\right\rangle^{il}\end{array}\right\}$$

$$-\nabla\cdot\left(\alpha_{l}^{e}\gamma\left\langle\mathbf{T}_{\eta,l}^{\tau}\cdot\mathbf{V}_{l}^{\tau}\right\rangle^{le}\right)-\nabla\cdot\left(\alpha_{l}^{e}\gamma\delta_{l}\left\langle\lambda_{l}^{l}\nabla T_{l}\right\rangle^{le}\right)+\alpha_{l}\gamma_{v}\left\langle\rho_{l}\left(\mathbf{g}\cdot\mathbf{V}_{l}^{\tau}\right)\right\rangle^{l}$$

$$+\frac{1}{Vol}\int\limits_{F_{l\sigma}}\Delta p_{l\sigma}^{\tau}\mathbf{V}_{l\sigma}^{\tau}\cdot\mathbf{n}_{l}dF+\frac{1}{Vol}\int\limits_{F_{lw}}\Delta p_{lw}^{\tau}\mathbf{V}_{lw}^{\tau}\cdot\mathbf{n}_{l}dF-\frac{1}{Vol}\int\limits_{F_{l\sigma}+F_{lw}}\mathbf{T}_{l}^{\tau}\cdot\mathbf{V}_{l}^{\tau}\cdot\mathbf{n}_{l}dF=\gamma_{v}q_{l}^{*}. \tag{5.28}$$

Using the chain rule, differentiation can now be performed on the first two terms. Comparing them with the mass conservation equations (1.38) one then obtains the *non-conservative form* of the energy equation:

$$\sum_{i=1}^{i_{\max}}\left\{\left\langle\rho_{il}\right\rangle^{il}\left[\begin{array}{l}\alpha_{il}\gamma_{v}\dfrac{\partial}{\partial\tau}\left(\left\langle h_{il}^{\tau}\right\rangle^{il}+\dfrac{1}{2}\left\langle V_{il}^{\tau 2}\right\rangle^{ile}\right)\\ \\ +\alpha_{il}^{e}\left\langle\mathbf{V}_{il}^{\tau}\right\rangle^{ile}\gamma\cdot\nabla\left(\left\langle h_{il}^{\tau}\right\rangle^{il}+\dfrac{1}{2}\left\langle V_{il}^{\tau 2}\right\rangle^{ile}\right)\end{array}\right]-\gamma_{v}\alpha_{il}\frac{\partial}{\partial\tau}\left\langle p_{il}^{\tau}\right\rangle^{il}\right\}$$

$$-\nabla\cdot\left(\alpha_{l}^{e}\gamma\left\langle\mathbf{T}_{\eta,l}^{\tau}\cdot\mathbf{V}_{l}^{\tau}\right\rangle^{le}\right)-\nabla\cdot\left(\alpha_{l}^{e}\gamma\delta_{l}\left\langle\lambda_{l}^{l}\nabla T_{l}\right\rangle^{le}\right)+\alpha_{l}\gamma_{v}\left\langle\rho_{l}\left(\mathbf{g}\cdot\mathbf{V}_{l}^{\tau}\right)\right\rangle^{l}$$

$$+\frac{1}{Vol}\int\limits_{F_{l\sigma}} \Delta p_{l\sigma}^{\tau}\mathbf{V}_{l\sigma}^{\tau}\cdot\mathbf{n}_l dF+\frac{1}{Vol}\int\limits_{F_{lw}} \Delta p_{lw}^{\tau}\mathbf{V}_{lw}^{\tau}\cdot\mathbf{n}_l dF-\frac{1}{Vol}\int\limits_{F_{l\sigma}+F_{lw}} \mathbf{T}_l^{\tau}\cdot\mathbf{V}_l^{\tau}\cdot\mathbf{n}_l dF=\gamma_v q_l^{*N} \tag{5.29}$$

where

$$q_l^{*N}=\dot{q}_l'''+\sum_{i=1}^{i_{\max}}\mu_{iwl}^{\tau}\left(\left\langle h_{iw}^{\tau}\right\rangle^{iw}-\left\langle h_{il}^{\tau}\right\rangle^{il}\right)$$

$$+\sum_{m=1}^{3}\left[\mu_{Mml}^{\tau}\left(h_{Ml}^{\tau\sigma}-\left\langle h_{Ml}^{\tau}\right\rangle^{Ml}\right)+\sum_{n=1}^{n_{\max}}\mu_{nml}^{\tau}\left(\left\langle h_{nm}\right\rangle^{nm}-\left\langle h_{nl}^{\tau}\right\rangle^{nl}\right)\right]$$

$$+\mu_{wl}^{\tau}\frac{1}{2}\left(\left\langle V_{wl}^{\tau 2}\right\rangle^{we}-\left\langle V_l^{\tau 2}\right\rangle^{le}\right)-\mu_{lw}^{\tau}\frac{1}{2}\left(\left\langle V_{lw}^{\tau 2}\right\rangle^{le}-\left\langle V_l^{\tau 2}\right\rangle^{le}\right)$$

$$+\frac{1}{2}\sum_{m=1}^{3}\mu_{ml}^{\tau}\left(\left\langle V_m^{\tau 2}\right\rangle^{me}-\left\langle V_l^{\tau 2}\right\rangle^{le}\right). \tag{5.30}$$

The superscript *N* stands here to remember that this RHS belongs to the non-conservative notation of the energy conservation equation.

5.3 *Dalton* and *Fick*'s laws, center of mass mixture velocity, caloric mixture properties

As mentioned in Chapter 1, for a gas mixture it follows from the *Dalton*'s law that $\alpha_{il}=\alpha_l$, whereas for mixtures consisting of liquid and macroscopic solid particles $\alpha_{il}\neq\alpha_l$. The instantaneous mass concentration of the component *i* in *l* is defined by Eq. (1.49) ,

$$C_{il}^{\tau}=\alpha_{il}\left\langle\rho_{il}\right\rangle^{l}/\left(\alpha_l\left\langle\rho_l\right\rangle^{l}\right). \tag{5.31}$$

The center of mass (c. m.) velocity is given by intrinsic surface-averaged field velocity $\left\langle\mathbf{V}_l^{\tau}\right\rangle^{le}$. Equation (1.50) can be rewritten as

$$\alpha_l\left\langle\rho_l\right\rangle^{l}\left\langle\mathbf{V}_l^{\tau}\right\rangle^{le}=\sum_{i=1}^{i_{\max}}\alpha_{il}\left\langle\rho_{il}\right\rangle^{l}\left\langle\mathbf{V}_{il}^{\tau}\right\rangle^{le}=\alpha_l\left\langle\rho_l\right\rangle^{l}\sum_{i=1}^{i_{\max}}C_{il}^{\tau}\left\langle\mathbf{V}_{il}^{\tau}\right\rangle^{le}. \tag{5.32}$$

Consequently

$$\left\langle\mathbf{V}_l^{\tau}\right\rangle^{le}=\sum_{i=1}^{i_{\max}}C_{il}^{\tau}\left\langle\mathbf{V}_{il}^{\tau}\right\rangle^{le}. \tag{5.33}$$

As for the derivation of the mass conservation equation, it is convenient for description of transport of the microscopic component *il* in the velocity field *l* to replace the velocity component $\left\langle \mathbf{V}_{il}^{\tau} \right\rangle^{le}$ by the sum of the center of mass velocity for the particular field $\left\langle \mathbf{V}_{l}^{\tau} \right\rangle^{le}$ and the deviation from the c. m. velocity or the so called *diffusion velocity* of the inert component $\delta_i \left\langle \mathbf{V}_{l}^{\tau} \right\rangle^{le}$, this yielding the following

$$\left\langle \mathbf{V}_{il}^{\tau} \right\rangle^{le} = \left\langle \mathbf{V}_{l}^{\tau} \right\rangle^{le} + \left(\delta \left\langle \mathbf{V}_{l}^{\tau} \right\rangle^{le} \right)_i . \tag{5.34}$$

Fick (1855) noticed that the mass flow rate of the inert component with respect to the total mass flow rate of the continuous mixture including the inert component is proportional to the gradient of the concentration of this inert component

$$\alpha_{il} \left\langle \rho_{il} \right\rangle^{l} \left(\delta \left\langle \mathbf{V}_{l}^{\tau} \right\rangle^{le} \right)_i = -\alpha_l^e \delta_l D_{il}^l \nabla \left\langle \rho_{il} \right\rangle^{il} = -\alpha_l \left\langle \rho_l \right\rangle^{l} \delta_l D_{il}^l \nabla \left\langle C_{il}^{\tau} \right\rangle^{il} , \tag{5.35}$$

or divided by the component density

$$\alpha_{il}^e \delta \mathbf{V}_{il}^{\tau} = -\alpha_l^e \delta_l D_{il}^l \frac{1}{\left\langle C_{il}^{\tau} \right\rangle^{il}} \nabla \left\langle C_{il}^{\tau} \right\rangle^{il} = -\alpha_l^e \delta_l D_{il}^l \nabla \ln \left\langle C_{il}^{\tau} \right\rangle^{il} . \tag{5.36}$$

The coefficient of proportionality, D_{il}^l, is known as the *isotropic coefficient of molecular diffusion*. The diffusion mass flow rate is directed from regions with higher concentration to regions with lower concentration, with this reflected by the minus sign in the assumption made by *Fick* (which has subsequently come to be known as *Fick*'s law), because many processes in nature and industrial equipment are successfully described mathematically by the above approach – so called diffusion processes. Here $\delta_l = 1$ for a continuous field and $\delta_l = 0$ for a disperse field. Molecular diffusion has microscopic character, as it is caused by molecular interactions. The special theoretical treatment and the experimental experience of how to determine the molecular diffusion constant in multi-component mixtures, is a science in its own right. This topic is beyond the scope of this chapter. In this context, it should merely be only noted that in line with the thermodynamics of irreversible processes, the thermal diffusivity and the diffusion coefficients influence each other. The interested reader can find useful information in *Reid* et al. (1982).

One should keep in mind that there is no molecular net mass diffusively transported across a cross section perpendicular to the strongest concentration gradient. This is mathematically expressed as follows

$$\sum_{i=1}^{i_{\max}} \left(D_{il}^l \nabla \left\langle C_{il}^{\tau} \right\rangle^{il} \right) = 0 , \tag{5.37}$$

or

$$D_{1l}^{l}\nabla\left\langle C_{1l}^{\tau}\right\rangle^{il}=-\sum_{i=2}^{i_{\max}}\left(D_{il}^{l}\nabla\left\langle C_{il}^{\tau}\right\rangle^{il}\right). \tag{5.38}$$

Therefore, the diffusion can be considered as volumetric replacement of groups of molecules of one specie with group of molecules of other specie. The compensating volumetric flow is called sometimes *Stefan*'s flow, *Stefan* (1874).

The caloric mixture properties naturally arise after summing all the energy conservation equations in conservative form. These are defined as follows

$$\left\langle\varphi_{l}^{\tau}\right\rangle^{l}=\frac{\sum\limits_{i=1}^{i_{\max}}\alpha_{il}\left\langle\rho_{il}\right\rangle^{il}\left\langle\varphi_{il}^{\tau}\right\rangle^{il}}{\alpha_{l}\left\langle\rho_{l}\right\rangle^{l}}=\sum_{i=1}^{i_{\max}}\left(\left\langle C_{il}\right\rangle^{il}\left\langle\varphi_{il}^{\tau}\right\rangle^{il}\right), \tag{5.39}$$

where

$$\varphi=h,e,s\,. \tag{5.40}$$

5.4 Enthalpy equation

For practical applications it is extremely convenient to simplify the energy equation in a way that the mechanical energy terms disappear. The resulting equation is called the *enthalpy equation*. The enthalpy equation will now be derived.

The non-conservative form of the momentum equation (2.31) using Eq. (1.38) is

$$\begin{aligned}&\left\langle\rho_{l}\right\rangle^{l}\left[\alpha_{l}\gamma_{v}\frac{\partial}{\partial\tau}\left\langle\mathbf{V}_{l}^{\tau}\right\rangle^{le}+\alpha_{l}^{e}\left\langle\mathbf{V}_{l}^{\tau}\right\rangle^{le}\gamma\nabla\cdot\left\langle\mathbf{V}_{l}^{\tau}\right\rangle^{le}\right]-\nabla\cdot\left(\alpha_{l}^{e}\gamma\left\langle\mathbf{T}_{\eta,l}^{\tau}\right\rangle^{le}\right)+\alpha_{l}^{e}\gamma\nabla\cdot\left\langle p_{l}^{\tau}\right\rangle^{le}\\&+\frac{1}{Vol}\int\limits_{F_{l\sigma}}\Delta p_{l\sigma}^{\tau}\cdot\mathbf{n}_{l\sigma}dF+\alpha_{l}\gamma_{v}\left\langle\rho_{l}\right\rangle^{l}\mathbf{g}+\frac{1}{Vol}\int\limits_{F_{lw}}\Delta p_{lw}^{\tau}\cdot\mathbf{n}_{l\sigma}dF-\frac{1}{Vol}\int\limits_{F_{l\sigma}+F_{lw}}\mathbf{T}_{l}^{\tau}\cdot\mathbf{n}_{l}dF\\&=\gamma_{v}\left\{\mu_{wl}^{\tau}\left(\left\langle\mathbf{V}_{wl}^{\tau}\right\rangle^{we}-\left\langle\mathbf{V}_{l}^{\tau}\right\rangle^{le}\right)-\mu_{lw}^{\tau}\left(\left\langle\mathbf{V}_{lw}^{\tau}\right\rangle^{we}-\left\langle\mathbf{V}_{l}^{\tau}\right\rangle^{le}\right)+\sum_{m=1}^{3}\mu_{ml}^{\tau}\left(\left\langle\mathbf{V}_{m}^{\tau}\right\rangle^{me}-\left\langle\mathbf{V}_{l}^{\tau}\right\rangle^{le}\right)\right\}.\end{aligned} \tag{5.41}$$

Here, Eqs. (5.6) and (5.7) are used, and the integral containing $\left\langle p_{l}^{\tau}\right\rangle^{le}$ is rearranged using Eq. (1.29). The scalar product of Eq. (5.41) is constructed with the field velocity. The result is a scalar expressing the mechanical energy balance. Subtracting this result from the energy equation and bearing in mind that

$$\frac{1}{2}\left(\left\langle V_{m}^{\tau 2}\right\rangle^{me}-\left\langle\mathbf{V}_{l}^{\tau 2}\right\rangle^{le}\right)-\left\langle\mathbf{V}_{l}^{\tau}\right\rangle^{le}\cdot\left(\left\langle V_{m}^{\tau}\right\rangle^{me}-\left\langle\mathbf{V}_{l}^{\tau}\right\rangle^{le}\right)=\frac{1}{2}\left(\left\langle V_{m}^{\tau}\right\rangle^{me}-\left\langle\mathbf{V}_{l}^{\tau}\right\rangle^{le}\right)^{2}, \tag{5.42}$$

and

$$\mu_{wl}^{\tau}\frac{1}{2}\left(\left\langle V_{wl}^{\tau 2}\right\rangle^{we}-\left\langle V_{l}^{\tau 2}\right\rangle^{le}\right)-\mu_{lw}^{\tau}\frac{1}{2}\left(\left\langle V_{lw}^{\tau 2}\right\rangle^{we}-\left\langle V_{l}^{\tau 2}\right\rangle^{le}\right)$$

$$-\left\langle \mathbf{V}_{l}^{\tau}\right\rangle^{le}\left[\mu_{wl}^{\tau}\left(\left\langle \mathbf{V}_{wl}^{\tau}\right\rangle^{we}-\left\langle \mathbf{V}_{l}^{\tau}\right\rangle^{le}\right)-\mu_{lw}^{\tau}\left(\left\langle \mathbf{V}_{lw}^{\tau}\right\rangle^{we}-\left\langle \mathbf{V}_{l}^{\tau}\right\rangle^{le}\right)\right]$$

$$=\mu_{wl}^{\tau}\frac{1}{2}\left(\left\langle \mathbf{V}_{wl}^{\tau}\right\rangle^{we}-\left\langle \mathbf{V}_{l}^{\tau}\right\rangle^{le}\right)^{2}-\mu_{lw}^{\tau}\frac{1}{2}\left(\left\langle \mathbf{V}_{lw}^{\tau}\right\rangle^{we}-\left\langle \mathbf{V}_{l}^{\tau}\right\rangle^{le}\right)^{2}, \qquad (5.43)$$

one then obtains the *non-conservative form of the enthalpy equation*:

$$\sum_{i=1}^{i_{\max}}\left\{\begin{array}{l}\left\langle \rho_{il}\right\rangle^{il}\left[\alpha_{il}\gamma_{v}\dfrac{\partial}{\partial\tau}\left\langle h_{il}^{\tau}\right\rangle^{il}+\alpha_{il}^{e}\left\langle \mathbf{V}_{il}^{\tau}\right\rangle^{ile}\gamma\cdot\nabla\left\langle h_{il}^{\tau}\right\rangle^{il}\right]\\ \\ -\left[\alpha_{il}\gamma_{v}\dfrac{\partial}{\partial\tau}\left\langle p_{il}^{\tau}\right\rangle^{il}+\alpha_{il}^{e}\left\langle \mathbf{V}_{il}^{\tau}\right\rangle^{ile}\gamma\cdot\nabla\left\langle p_{il}^{\tau}\right\rangle^{il}\right]\end{array}\right\}$$

$$-\nabla\cdot\left(\alpha_{l}^{e}\gamma\left\langle \lambda_{l}^{l}\nabla T_{l}\right\rangle^{le}\right)=\gamma_{v}\left(\alpha_{l}\rho_{l}P_{\eta,l}^{\tau}+q_{l}^{\tau N}\right)+E_{l}^{*\tau}. \qquad (5.44)$$

where

$$q_{l}^{\tau N}=\dot{q}_{l}'''+\sum_{i=1}^{i_{\max}}\mu_{iwl}^{\tau}\left(\left\langle h_{iw}^{\tau}\right\rangle^{iw}-\left\langle h_{il}^{\tau}\right\rangle^{il}\right)$$

$$+\sum_{m=1}^{3}\left[\mu_{Mml}^{\tau}\left(h_{Ml}^{\tau\sigma}-\left\langle h_{Ml}^{\tau}\right\rangle^{Ml}\right)+\sum_{n=1}^{n_{\max}}\mu_{nml}^{\tau}\left(\left\langle h_{nm}\right\rangle^{nm}-\left\langle h_{nl}^{\tau}\right\rangle^{nl}\right)\right]$$

$$-\sum_{\substack{m=1\\ m\neq l}}^{3}\left[\mu_{Mlm}^{\tau}\left(h_{Ml}^{\tau\sigma}-\left\langle h_{Ml}^{\tau}\right\rangle^{Ml}\right)+\sum_{n=1}^{n_{\max}}\mu_{nlm}^{\tau}\left(\left\langle h_{nl}\right\rangle^{nl}-\left\langle h_{nl}^{\tau}\right\rangle^{nl}\right)\right]$$

$$+\mu_{wl}^{\tau}\frac{1}{2}\left(\left\langle \mathbf{V}_{wl}^{\tau}\right\rangle^{we}-\left\langle \mathbf{V}_{l}^{\tau}\right\rangle^{le}\right)^{2}-\mu_{lw}^{\tau}\frac{1}{2}\left(\left\langle \mathbf{V}_{lw}^{\tau}\right\rangle^{le}-\left\langle \mathbf{V}_{l}^{\tau}\right\rangle^{le}\right)^{2}$$

$$+\frac{1}{2}\sum_{m=1}^{3}\mu_{ml}^{\tau}\left(\left\langle \mathbf{V}_{m}^{\tau}\right\rangle^{me}-\left\langle \mathbf{V}_{l}^{\tau}\right\rangle^{le}\right)^{2}. \qquad (5.45)$$

The corresponding conservative form is

$$\sum_{i=1}^{i_{\max}}\left\{\begin{array}{l}\dfrac{\partial}{\partial\tau}\left(\alpha_{il}\left\langle\rho_{il}\right\rangle^{il}\left\langle h_{il}^{\tau}\right\rangle^{il}\gamma_v\right)+\nabla\cdot\left(\alpha_{il}^{e}\left\langle\rho_{il}\right\rangle^{il}\left\langle\mathbf{V}_{il}^{\tau}\right\rangle^{ile}\left\langle h_{il}^{\tau}\right\rangle^{il}\gamma\right)\\ \\ -\left[\alpha_{il}\gamma_v\dfrac{\partial}{\partial\tau}\left\langle p_{il}^{\tau}\right\rangle^{il}+\alpha_{il}^{e}\left\langle\mathbf{V}_{il}^{\tau}\right\rangle^{ile}\gamma\cdot\nabla\left\langle p_{il}^{\tau}\right\rangle^{il}\right]\end{array}\right\}$$

$$-\nabla\cdot\left(\alpha_l^e\gamma\delta_l\left\langle\lambda_l^l\nabla T_l\right\rangle^{le}\right)=\gamma_v\left(\alpha_l\rho_l P_{\eta,l}^{\tau}+q_l\right)+E_l^{*\tau}, \qquad (5.46)$$

where

$$q_l=\dot{q}_l'''+\sum_{i=1}^{i_{\max}}\left(\mu_{iwl}^{\tau}\left\langle h_{iw}^{\tau}\right\rangle^{iw}-\mu_{ilw}^{\tau}\left\langle h_{il}^{\tau}\right\rangle^{il}\right)$$

$$+\sum_{m=1}^{3}\left[\left(\mu_{Mml}^{\tau}h_{Ml}^{\tau\sigma}-\mu_{Mlm}^{\tau}\left\langle h_{Ml}^{\tau}\right\rangle^{Ml}\right)+\sum_{n=1}^{n_{\max}}\left(\mu_{nml}^{\tau}\left\langle h_{nm}^{\tau}\right\rangle^{nm}-\mu_{nlm}^{\tau}\left\langle h_{nl}^{\tau}\right\rangle^{nl}\right)\right]$$

$$+\mu_{wl}^{\tau}\frac{1}{2}\left(\left\langle\mathbf{V}_{wl}^{\tau}\right\rangle^{we}-\left\langle\mathbf{V}_{l}^{\tau}\right\rangle^{le}\right)^2-\mu_{lw}^{\tau}\frac{1}{2}\left(\left\langle\mathbf{V}_{lw}^{\tau}\right\rangle^{le}-\left\langle\mathbf{V}_{l}^{\tau}\right\rangle^{le}\right)^2$$

$$+\frac{1}{2}\sum_{m=1}^{3}\mu_{ml}^{\tau}\left(\left\langle\mathbf{V}_{m}^{\tau}\right\rangle^{me}-\left\langle\mathbf{V}_{l}^{\tau}\right\rangle^{le}\right)^2\equiv q_l^{\tau N}+\sum_{i=1}^{i_{\max}}\mu_{il}^{\tau}\left\langle h_{il}\right\rangle^{il}. \qquad (5.47)$$

Here

$$\gamma_v\alpha_l\rho_l P_{\eta,l}^{\tau}=\nabla\cdot\left(\alpha_l^e\gamma\left\langle\mathbf{T}_{\eta,l}^{\tau}\cdot\mathbf{V}_l^{\tau}\right\rangle^{le}\right)-\left\langle\mathbf{V}_l^{\tau}\right\rangle^{le}\cdot\nabla\cdot\left(\alpha_l^e\gamma\left\langle\mathbf{T}_{\eta,l}^{\tau}\right\rangle^{le}\right)$$

$$=\alpha_l^e\gamma\cdot\left\langle\mathbf{T}_{\eta,l}^{\tau}:\nabla\cdot\mathbf{V}_l^{\tau}\right\rangle^{le}, \qquad (5.48)$$

is the *irreversible bulk viscous dissipation.* The term,

$$E_l^{*\tau}=\frac{1}{Vol}\int_{F_{l\sigma}}\Delta p_{l\sigma}^{\tau}\left(\left\langle\mathbf{V}_l^{\tau}\right\rangle^{le}-\mathbf{V}_{l\sigma}^{\tau}\right)\cdot\mathbf{n}_l dF+\frac{1}{Vol}\int_{F_{lw}}\Delta p_{lw}^{\tau}\left(\left\langle\mathbf{V}_l^{\tau}\right\rangle^{le}-\mathbf{V}_{lw}^{\tau}\right)\cdot\mathbf{n}_l dF$$

$$-\frac{1}{Vol}\int_{F_{l\sigma}+F_{lw}}\mathbf{T}_l^{\tau}\cdot\left(\left\langle\mathbf{V}_l^{\tau}\right\rangle^{le}-\mathbf{V}_l^{\tau}\right)\cdot\mathbf{n}_l dF=\frac{1}{Vol}\int_{F_{l\sigma}}\frac{\Delta p_{l\sigma}^{\tau}}{\rho_l}\rho_l\left(\mathbf{V}_l^{\tau}-\mathbf{V}_{l\sigma}^{\tau}\right)\cdot\mathbf{n}_l dF$$

$$+\frac{1}{Vol}\int_{F_{lw}}\frac{\Delta p_{lw}^{\tau}}{\rho_l}\rho_l\left(\mathbf{V}_l^{\tau}-\mathbf{V}_{lw}^{\tau}\right)\cdot\mathbf{n}_l dF-\frac{1}{Vol}\int_{F_{l\sigma}}\left(-\Delta p_{l\sigma}^{\tau}+\mathbf{T}_l^{\tau}\right)\cdot\left(\left\langle\mathbf{V}_l^{\tau}\right\rangle^{le}-\mathbf{V}_l^{\tau}\right)\cdot\mathbf{n}_l dF$$

$$-\frac{1}{Vol}\int_{F_{lw}}\left(-\Delta p_{lw}^{\tau}+\mathbf{T}_l^{\tau}\right)\cdot\left(\left\langle\mathbf{V}_l^{\tau}\right\rangle^{le}-\mathbf{V}_l^{\tau}\right)\cdot\mathbf{n}_l dF \qquad (5.49)$$

is the irreversible power dissipation caused by the interface mass transfer between two regions with different velocities. A good approximation of the last two terms is obtained if one assumes

$$\mathbf{V}_l^\tau \approx \left\langle \mathbf{V}_m^\tau \right\rangle^{me} \quad \text{at} \quad F_{l\sigma} \tag{5.50}$$

and

$$\mathbf{V}_l^\tau = 0 \quad \text{at} \quad F_{lw} \tag{5.51}$$

(non-slip condition), namely

$$-\frac{1}{Vol}\int\limits_{F_{l\sigma}} \left(-\Delta p_{l\sigma}^\tau + \mathbf{T}_l^\tau\right)\cdot\left(\left\langle \mathbf{V}_l^\tau \right\rangle^{le} - \mathbf{V}_l^\tau\right)\cdot \mathbf{n}_l dF$$

$$\approx -\left(\left\langle \mathbf{V}_l^\tau \right\rangle^{le} - \left\langle \mathbf{V}_m^\tau \right\rangle^{me}\right)\frac{1}{Vol}\int\limits_{F_{l\sigma}} \left(-\Delta p_{l\sigma}^\tau + \mathbf{T}_l^\tau\right)\cdot \mathbf{n}_l dF \tag{5.52}$$

and

$$-\frac{1}{Vol}\int\limits_{F_{lw}} \left(-\Delta p_{lw}^\tau + \mathbf{T}_l^\tau\right)\cdot\left(\left\langle \mathbf{V}_l^\tau \right\rangle^{le} - \mathbf{V}_l^\tau\right)\cdot \mathbf{n}_l dF \approx -\left\langle \mathbf{V}_l^\tau \right\rangle^{le}\frac{1}{Vol}\int\limits_{F_{lw}} \left(-\Delta p_{lw}^\tau + \mathbf{T}_l^\tau\right)\cdot \mathbf{n}_l dF\ . \tag{5.53}$$

The order of magnitude of the first two terms in Eq. (5.49) is

$$\frac{1}{Vol}\int\limits_{F_{l\sigma}} \Delta p_{l\sigma}^\tau \left(\left\langle \mathbf{V}_l^\tau \right\rangle^{le} - \mathbf{V}_{l\sigma}^\tau\right)\cdot \mathbf{n}_l dF + \frac{1}{Vol}\int\limits_{F_{lw}} \Delta p_{lw}^\tau \left(\left\langle \mathbf{V}_l^\tau \right\rangle^{le} - \mathbf{V}_{lw}^\tau\right)\cdot \mathbf{n}_l dF$$

$$\approx \sum_{m=1}^{3,w} \frac{\overline{\Delta p_{lm\sigma}^\tau}}{\rho_l}\left(\mu_{ml} - \mu_{lm}\right), \tag{5.54}$$

where $\Delta p_{lm\sigma}^\tau / \rho_l$ is an averaged pressure difference between the bulk pressure and the boundary layer pressure inside the velocity field *l*.

Performing the summation in Eq. (5.46), using the *Dalton*'s law, substituting the *Fick*'s laws in the thus obtained equation, and applying the definitions given in Chapter 3 yields

$$\frac{\partial}{\partial \tau}\left(\alpha_l \left\langle \rho_l \right\rangle^l \left\langle h_l^\tau \right\rangle^l \gamma_v\right) + \nabla\cdot\left(\alpha_l^e \left\langle \rho_l \right\rangle^l \left\langle \mathbf{V}_l^\tau \right\rangle^{le} \left\langle h_l^\tau \right\rangle^l \gamma\right)$$

$$-\left[\alpha_l \gamma_v \frac{\partial}{\partial \tau}\left\langle p_l^\tau \right\rangle^l + \alpha_l^e \left\langle \mathbf{V}_l^\tau \right\rangle^{le} \gamma\cdot\nabla\left\langle p_l^\tau \right\rangle^l\right]$$

$$
-\nabla \cdot \left\{ \alpha_l^e \gamma \delta_l \left[\left\langle \lambda_l^l \nabla T_l \right\rangle^{le} + \left\langle \rho_l \right\rangle^l \sum_{i=1}^{i_{\max}} \left(\left\langle h_{il}^\tau \right\rangle^{il} D_{il}^l \nabla \left\langle C_{il}^\tau \right\rangle^{il} \right) \right] \right\}
$$

$$
+ \delta_l \left(\alpha_l^e \gamma \nabla \left\langle p_l^\tau \right\rangle^l \right) \cdot \sum_{i=1}^{i_{\max}} D_{il}^l \nabla \ln \left\langle C_{il}^\tau \right\rangle^{il} = \gamma_v \left(\alpha_l \rho_l \varepsilon_{\eta,l}^\tau + q_l \right) + E_l^{*\tau} . \qquad (5.55)
$$

The non-conservative form of the equation (5.55) is readily obtained by differentiating the first two terms and comparing them with the field mass conservation equation. The result is

$$
\boxed{
\begin{aligned}
& \alpha_l \left\langle \rho_l \right\rangle^l \gamma_v \frac{\partial \left\langle h_l^\tau \right\rangle^l}{\partial \tau} + \alpha_l^e \left\langle \rho_l \right\rangle^l \left\langle \mathbf{V}_l^\tau \right\rangle^{le} \gamma \nabla \left\langle h_l^\tau \right\rangle^l \\
& - \left[\alpha_l \gamma_v \frac{\partial}{\partial \tau} \left\langle p_l^\tau \right\rangle^l + \alpha_l^e \left\langle \mathbf{V}_l^\tau \right\rangle^{le} \gamma \cdot \nabla \left\langle p_l^\tau \right\rangle^l \right] \\
& - \nabla \cdot \left\{ \alpha_l^e \gamma \delta_l \left[\left\langle \lambda_l^l \nabla T_l \right\rangle^{le} + \sum_{i=1}^{i_{\max}} \left(\left\langle \rho_{il} \right\rangle^{il} \left\langle h_{il}^\tau \right\rangle^{il} D_{il}^l \nabla \ln \left\langle C_{il}^\tau \right\rangle^{il} \right) \right] \right\} \\
& + \delta_l \left(\alpha_l^e \gamma \nabla \left\langle p_l^\tau \right\rangle^l \right) \cdot \sum_{i=1}^{i_{\max}} D_{il}^l \nabla \ln \left\langle C_{il}^\tau \right\rangle^{il} = \gamma_v \left(\alpha_l \rho_l \varepsilon_{\eta,l}^\tau + q_l - \mu_l^\tau \left\langle h_l^\tau \right\rangle^l \right) + E_l^{*\tau} . \\
& \hfill (5.56)
\end{aligned}
}
$$

Remember that the sum of all *C*’s inside the velocity field is equal to one so that one of the concentrations depends on all the others.

5.5 Internal energy equation

Engineers sometimes have in their personal library approximations for the state variables and transport properties in terms of the specific internal energy. For practical use in this case, Eq. (5.46) can be rewritten in terms of the specific internal energy:

$$
\sum_{i=1}^{i_{\max}} \left\{
\begin{array}{l}
\dfrac{\partial}{\partial \tau} \left(\alpha_{il} \left\langle \rho_{il} \right\rangle^{il} \left\langle e_{il}^\tau \right\rangle^{il} \gamma_v \right) + \nabla \cdot \left(\alpha_{il}^e \left\langle \rho_{il} \right\rangle^{il} \left\langle \mathbf{V}_{il}^\tau \right\rangle^{ile} \left\langle e_{il}^\tau \right\rangle^{il} \gamma \right) \\
\\
- \left\langle p_{il}^\tau \right\rangle^{il} \left[\dfrac{\partial}{\partial \tau} \left(\alpha_{il} \gamma_v \right) + \nabla \left(\alpha_{il}^e \left\langle \mathbf{V}_{il}^\tau \right\rangle^{ile} \gamma \right) \right]
\end{array}
\right\}
$$

$$-\nabla\cdot\left(\alpha_l^e\gamma\delta_l\left\langle\lambda_l^l\nabla T_l\right\rangle^{le}\right)=\gamma_v\left(\alpha_l\rho_l P_{\eta,l}^{\tau}+q_l\right)+E_l^{*\tau}, \tag{5.57}$$

or using the definitions introduced in Chapter 3

$$\boxed{\begin{aligned}
&\frac{\partial}{\partial\tau}\left(\alpha_l\left\langle\rho_l\right\rangle^l\left\langle e_l^{\tau}\right\rangle\gamma_v\right)+\nabla\cdot\left(\alpha_l^e\left\langle\rho_l\right\rangle^l\left\langle\mathbf{V}_l^{\tau}\right\rangle^{le}\left\langle e_l^{\tau}\right\rangle\gamma\right)\\
&-\left\langle p_l^{\tau}\right\rangle^l\left[\frac{\partial}{\partial\tau}\left(\alpha_l\gamma_v\right)+\nabla\left(\alpha_l^e\left\langle\mathbf{V}_l^{\tau}\right\rangle^{le}\gamma\right)\right]\\
&-\nabla\cdot\left\{\alpha_l^e\gamma\delta_l\left[\left\langle\lambda_l^l\nabla T_l\right\rangle^{le}+\left\langle\rho_l\right\rangle^l\sum_{i=1}^{i_{\max}}\left(\left\langle e_{il}^{\tau}\right\rangle^{il}D_{il}^l\nabla\left\langle C_{il}^{\tau}\right\rangle^{il}\right)\right]\right\}\\
&+\delta_l\sum_{i=1}^{i_{\max}}\left[\left\langle p_{il}^{\tau}\right\rangle^{il}\nabla\left(\alpha_l^e D_{il}^l\gamma\nabla\ln\left\langle C_{il}^{\tau}\right\rangle^{il}\right)\right]=\gamma_v\left(\alpha_l\rho_l\varepsilon_{\eta,l}^{\tau}+q_l\right)+E_l^{*\tau}.
\end{aligned}} \tag{5.58}$$

5.6 Entropy equation

The basic idea of the *Legendre* transformation is briefly introduced here: If f is a function of n variables, $x_1, x_2, ..., x_n$, $f = f\left(x_1, x_2, ..., x_n\right)$, and for j of them the partial derivatives $\partial f/\partial x_i$ are known, the *Legendre* transformation z is defined by

$$z = f - \sum_{i=1}^{j}\frac{\partial f}{\partial x_i}x_i = z\left(\frac{\partial f}{\partial x_1},\frac{\partial f}{\partial x_2},...,\frac{\partial f}{\partial x_j},x_{j+1},...,x_n\right),$$

for which the differential is dz is defined as follows

$$dz = \sum_{i=j+1}^{n}\frac{\partial f}{\partial x_i}dx_i - \sum_{i=1}^{j}x_i d\frac{\partial f}{\partial x_i}.$$

So if the specific volume is a function of the specific entropy and internal energy $v = e\left(s, e\right)$ the specific internal energy $e = e\left(s, v\right)$ is its *Legendre* transformation. The derivatives of e are measurable variables $\left(\partial e/\partial s\right)_v = T$ and $\left(\partial e/\partial v\right)_s = -p$. The differential de is then $de = Tds - pdv$ or

$$Tds = de + pdv. \tag{5.59}$$

This equation is called *Gibbs* equation (1878). The thermodynamic definitions of temperature T (absolute temperature - *Kelvin* 1848) and of the thermodynamic pressure p are used here. This is a differential equation of state which is extremely important in the thermodynamic theory of compressible substances. It relates the difference in entropy between any two infinitesimally separated states to the infinitesimal differences in internal energy and volume between those states. Note that the *Gibbs* equation is valid only if s is a *smooth* function of e and v, i.e. where the differentials de and dv are uniquely defined (smooth equation of state), see in *Gibbs* (1892). Using the definition of enthalpy (a mixture of thermodynamic and mechanical properties)

$$h = e + pv \tag{5.60}$$

the *Gibbs* equation can be written as

$$T\rho ds = \rho dh - dp \, . \tag{5.61}$$

After substituting for $\left\langle \rho_{il} \right\rangle^{il} d\left\langle h_{il}^{\tau} \right\rangle^{il} - d\left\langle p_{il}^{\tau} \right\rangle^{il}$ in Eq. (5.44) with the *Gibbs* definitions of the *specific entropy* of the corresponding components,

$$\left\langle \rho_{il} \right\rangle^{il} d\left\langle h_{il}^{\tau} \right\rangle^{il} - d\left\langle p_{il}^{\tau} \right\rangle^{il} = T_l \left\langle \rho_{il} \right\rangle^{il} d\left\langle s_{il}^{\tau} \right\rangle^{il} , \tag{5.61}$$

one obtains

$$T_l \sum_{i=1}^{i_{\max}} \left\{ \left\langle \rho_{il} \right\rangle^{il} \left[\alpha_{il} \gamma_v \frac{\partial}{\partial \tau} \left\langle s_{il}^{\tau} \right\rangle^{il} + \alpha_{il}^{e} \left\langle \mathbf{V}_{il}^{\tau} \right\rangle^{ile} \gamma \cdot \nabla \left\langle s_{il}^{\tau} \right\rangle^{il} \right] \right\}$$

$$-\nabla \cdot \left(\alpha_l^e \gamma \left\langle \lambda_l^l \nabla T_l \right\rangle^{le} \right) = \alpha_l^e \gamma \cdot \left\langle \mathbf{T}_{\eta,l}^{\tau} : \nabla \cdot \mathbf{V}_l^{\tau} \right\rangle^{le} + E_l^{*\tau} + \gamma_v q_l^N \, . \tag{5.62}$$

The following rearrangements are performed to give the conservative form of Eq. (5.62). Each of the mass conservation equations is multiplied by the corresponding component-specific entropy and field temperature. All the mass conservation equations are then added to Eq. (5.62). The differential terms are lumped together using the reverse chain rule of differentiation. The resulting *conservative form* is:

$$T_l \left\{ \frac{\partial}{\partial \tau} \left[\gamma_v \sum_{i=1}^{i_{\max}} \left(\alpha_{il} \left\langle \rho_{il} \right\rangle^{il} \left\langle s_{il}^{\tau} \right\rangle^{il} \right) \right] + \nabla \cdot \left[\gamma \sum_{i=1}^{i_{\max}} \left(\alpha_{il}^{e} \left\langle \rho_{il} \right\rangle^{il} \left\langle \mathbf{V}_{il}^{\tau} \right\rangle^{ile} \left\langle s_{il}^{\tau} \right\rangle^{il} \right) \right] \right\}$$

$$-\nabla \cdot \left(\alpha_l^e \gamma \delta_l \left\langle \lambda_l^l \nabla T_l \right\rangle^{le} \right) = \gamma_v \left(\alpha_l \rho_l P_{\eta,l}^{\tau} + q_l^N + T_l \sum_{\substack{m=1 \\ m \neq l}}^{3,w} \sum_{i=1}^{i_{\max}} \left(\mu_{iml}^{\tau} - \mu_{ilm}^{\tau} \right) \left\langle s_{il}^{\tau} \right\rangle^{il} \right) + E_l^{*\tau} \, . \tag{5.63}$$

After replacing the instantaneous values of the component velocities with the sums of the c. m. field velocities plus the deviations from the c. m. velocities, Eq. (5.34), and applying *Fick*'s law, Eq. (5.36) and keeping in mind that there is no molecular net mass diffusively transported across a cross section perpendicular to the strongest concentration gradient, Eqs. (5.37, 5.38), defining the *specific mixture entropy of the velocity field,* $\left\langle s_l^\tau \right\rangle^l$, by Eq. (5.39), introducing the *Prandtl* number

$$\mathrm{Pr}_l^l = \rho_l c_{pl} \nu_l^l / \lambda_l^l , \tag{5.64}$$

and dividing by T_l, the following form for the local instantaneous entropy equations is obtained:

$$\boxed{\begin{aligned}
&\frac{\partial}{\partial \tau}\left(\alpha_l \left\langle \rho_l \right\rangle^l \left\langle s_l^\tau \right\rangle^l \gamma_v \right) + \nabla \cdot \left(\alpha_l^e \left\langle \rho_l \right\rangle^l \left\langle s_l^\tau \right\rangle^l \left\langle \mathbf{V}_l^\tau \right\rangle^{le} \gamma \right) \\
&-\nabla . \left[\alpha_l^e \delta_l \left\langle \rho_l \right\rangle^l \gamma \left(\sum_{i=2}^{i_{\max}} \left(\left\langle s_{il}^\tau \right\rangle^{il} - \left\langle s_{1l}^\tau \right\rangle^{1l} \right) D_{il}^l \nabla \left\langle C_{il}^\tau \right\rangle^{il} \right) \right] \\
&- \frac{1}{T_l} \nabla \cdot \left(\alpha_l^e \gamma \delta_l \left\langle \rho_l c_{pl} \frac{\nu_l^l}{\mathrm{Pr}_l^l} \nabla T_l \right\rangle^{le} \right) \\
&= \gamma_v \left[\left(\alpha_l \rho_l \varepsilon_{\eta,l}^\tau + q_l^N \right) / T_l + \sum_{\substack{m=1 \\ m \neq l}}^{3,w} \sum_{i=1}^{i_{\max}} \left(\mu_{iml}^\tau - \mu_{ilm}^\tau \right) \left\langle s_{il}^\tau \right\rangle^{il} \right] + E_l^{*\tau} . \qquad (5.65)
\end{aligned}}$$

Observe the form of the RHS of Eq. (5.65).

$$\left(\alpha_l \rho_l \varepsilon_{\eta,l}^\tau + q_l^N \right) / T_l + \sum_{\substack{m=1 \\ m \neq l}}^{3,w} \sum_{i=1}^{i_{\max}} \left(\mu_{iml}^\tau - \mu_{ilm}^\tau \right) \left\langle s_{il}^\tau \right\rangle^{il}$$

$$= \frac{\dot{q}_l'''}{T_l} + \sum_{i=1}^{i_{\max}} \left[\mu_{iwl}^\tau \left(\frac{\left\langle h_{iw}^\tau \right\rangle^{iw} - \left\langle h_{il}^\tau \right\rangle^{il}}{T_l} + \left\langle s_{il}^\tau \right\rangle^{il} \right) + \mu_{ilw}^\tau \left(\frac{\left\langle h_{il}^\tau \right\rangle^{il} - \left\langle h_{il}^\tau \right\rangle^{il}}{T_l} + \left\langle s_{il}^\tau \right\rangle^{il} \right) \right]$$

$$+ \sum_{m=1}^{3} \left[\mu_{Mml}^\tau \left(\frac{h_{Ml}^{\tau\sigma} - \left\langle h_{Ml}^\tau \right\rangle^{Ml}}{T_l} + \left\langle s_{Ml}^\tau \right\rangle^{Ml} \right) + \sum_{n=1}^{n_{\max}} \mu_{nml}^\tau \left(\frac{\left\langle h_{nm} \right\rangle^{nm} - \left\langle h_{nl}^\tau \right\rangle^{nl}}{T_l} + \left\langle s_{nl}^\tau \right\rangle^{nl} \right) \right]$$

$$-\sum_{\substack{m=1\\m\neq l}}^{3}\left[\mu_{Mlm}^{\tau}\left(\frac{h_{Ml}^{\tau\sigma}-\left\langle h_{Ml}^{\tau}\right\rangle^{Ml}}{T_l}+\left\langle s_{Ml}^{\tau}\right\rangle^{Ml}\right)+\sum_{n=1}^{n_{\max}}\mu_{nlm}^{\tau}\left(\frac{\left\langle h_{nl}\right\rangle^{nl}-\left\langle h_{nl}^{\tau}\right\rangle^{nl}}{T_l}+\left\langle s_{nl}^{\tau}\right\rangle^{nl}\right)\right]$$

$$+\frac{1}{T_l}\left[\alpha_l\rho_l\varepsilon_{\eta,l}^{\tau}+\mu_{wl}^{\tau}\frac{1}{2}\left(\left\langle \mathbf{V}_{wl}^{\tau}\right\rangle^{we}-\left\langle \mathbf{V}_{l}^{\tau}\right\rangle^{le}\right)^2-\mu_{lw}^{\tau}\frac{1}{2}\left(\left\langle \mathbf{V}_{lw}^{\tau}\right\rangle^{le}-\left\langle \mathbf{V}_{l}^{\tau}\right\rangle^{le}\right)^2\right].$$

Obviously *if and only if* the pressure at the boundary inside the field is equal to the field averaged pressure the sources can be rewritten as follows

$$\left(\alpha_l\rho_l\varepsilon_{\eta,l}^{\tau}+q_l^{N}\right)/T_l+\sum_{\substack{m=1\\m\neq l}}^{3,w}\sum_{i=1}^{i_{\max}}\left(\mu_{iml}^{\tau}-\mu_{ilm}^{\tau}\right)\left\langle s_{il}^{\tau}\right\rangle^{il}=\frac{\dot{q}_l'''}{T_l}+\sum_{i=1}^{i_{\max}}\left[\mu_{iwl}^{\tau}\left\langle s_{iw}^{\tau}\right\rangle^{iw}-\mu_{ilw}^{\tau}\left\langle s_{il}^{\tau}\right\rangle^{il}\right]$$

$$+\sum_{\substack{m=1\\m\neq l}}^{3}\left[\mu_{Mml}^{\tau}s_{Ml}^{\tau\sigma}-\mu_{Mlm}^{\tau}s_{Ml}^{\tau\sigma}+\sum_{n=1}^{n_{\max}}\left(\mu_{nml}^{\tau}\left\langle s_{nm}\right\rangle^{nm}-\mu_{nlm}^{\tau}\left\langle s_{nl}\right\rangle^{nl}\right)\right]$$

$$+\frac{1}{T_l}\left[\alpha_l\rho_l\varepsilon_{\eta,l}^{\tau}+\mu_{wl}^{\tau}\frac{1}{2}\left(\left\langle \mathbf{V}_{wl}^{\tau}\right\rangle^{we}-\left\langle \mathbf{V}_{l}^{\tau}\right\rangle^{le}\right)^2-\mu_{lw}^{\tau}\frac{1}{2}\left(\left\langle \mathbf{V}_{lw}^{\tau}\right\rangle^{le}-\left\langle \mathbf{V}_{l}^{\tau}\right\rangle^{le}\right)^2\right].$$

Otherwise, the primary form has to be used.

We discussed in Chapter 4 a variety of notations of the energy conservation principle for single-phase flow. All of them are more complicated than the entropy notation. As for the single-phase flow comparing the multi-phase entropy equation (5.65) with the energy conservation equations in terms of specific enthalpy and specific internal energy (5.56, 5.58), it is evident that the computational effort required to approximate

1 time derivative,
1 divergence term,
2 diffusion terms, and
1 tensor product

is much less than the computational effort required to discretize

2 time derivatives,
2 divergence terms,
2 diffusion terms, and
1 tensor product.

Bearing in mind that each divergence term contains at least 3 differential terms, it is obvious that *for computational analysis the use of the entropy equation instead of energy equation in any of its variants is the most cost effective way for the numerical modeling of flows.*

CONCLUSION: The use of the specific entropies as components of the dependent variable vector, *the entropy concept, gives the simplest form for the mathematical description of the flow.* The use of any other state variables instead of the entropies makes the description more complicated.

5.7 Local volume- and time-averaged entropy equation

The procedure we use to obtain a time-averaged entropy equation will be used also for deriving the time-averaged enthalpy, or specific internal energy equations. Here we introduce the time averaging rules. The instantaneous surface-averaged velocity of the field *l*, $\left\langle \mathbf{V}_l^\tau \right\rangle^{le}$, can be expressed as the sum of the surface-averaged velocity which is subsequently time averaged,

$$V_l := \overline{\left\langle \mathbf{V}_l^\tau \right\rangle^{le}} \tag{5.66}$$

and a fluctuation component V_l',

$$\left\langle \mathbf{V}_l^\tau \right\rangle^{le} = V_l + V_l' \tag{5.67}$$

as proposed by *Reynolds*. The same is performed for the pressure

$$\left\langle p_l^\tau \right\rangle^l = p_l + p_l', \tag{5.68}$$

and for any specific property

$$\left\langle \varphi_{il}^\tau \right\rangle^l = \varphi_{il} + \varphi_{il}', \tag{5.69}$$

where $\varphi = s, h, e, T, C$. Here the fluctuations of densities, volume fractions are neglected as they are only of small magnitude relative to the velocity and entropy fluctuations.

The time averaging rules we use are:

$$\overline{\alpha_l \left\langle \rho_l \right\rangle^l \varphi_{il}} = \alpha_l \left\langle \rho_l \right\rangle^l \varphi_{il}, \tag{5.70}$$

$$\overline{\alpha_l \left\langle \rho_l \right\rangle^l \varphi_{il}'} = 0, \tag{5.71}$$

$$\overline{\alpha_l^e \left\langle \rho_l \right\rangle^l \varphi_{il} \mathbf{V}_l} = \alpha_l^e \left\langle \rho_l \right\rangle^l \varphi_{il} \mathbf{V}_l, \tag{5.72}$$

$$\overline{\alpha_l^e \left\langle \rho_l \right\rangle^l \varphi_{il} \mathbf{V}_l'} = 0, \tag{5.73}$$

$$\overline{\alpha_l^e \left\langle \rho_l \right\rangle^l \varphi_{il}' \mathbf{V}_l} = 0, \tag{5.74}$$

$$\overline{\varphi_{il}' D_{il}^l \nabla C_{il}} = 0, \tag{5.75}$$

$$\overline{\varphi_{il} D_{il}^l \nabla C_{il}'} = 0, \tag{5.76}$$

$$\overline{\varphi_{il} D_{il}^l \nabla C_{il}} = \varphi_{il} D_{il}^l \nabla C_{il}, \tag{5.77}$$

$$\overline{\left(\mu_{iml}^\tau - \mu_{ilm}^\tau\right)\left\langle \varphi_{il}^\tau \right\rangle^{il}} = \left(\mu_{iml} - \mu_{ilm}\right)\varphi_{il} \tag{5.78}$$

$$\overline{\mu_{il}^\tau} = \mu_{il}, \tag{5.79}$$

$$\overline{\mu_{ml}^\tau \left(\mathbf{V}_m' + \mathbf{V}_m' - \mathbf{V}_l - \mathbf{V}_l'\right)^2} = \mu_{ml}\overline{\left(\mathbf{V}_m - \mathbf{V}_l\right)^2} + \mu_{ml}\overline{\left(\mathbf{V}_m' - \mathbf{V}_l'\right)^2}, \tag{5.80}$$

$$\overline{\mathbf{T}_l' : \nabla \cdot \mathbf{V}_l} = \overline{\mathbf{T}_l'} : \nabla \cdot \overline{\mathbf{V}_l}, \tag{5.81}$$

$$\overline{\mathbf{T}_l : \nabla \cdot \mathbf{V}_l'} = 0, \tag{5.82}$$

$$\overline{\mathbf{T}_l : \nabla \cdot \mathbf{V}_l} = \overline{\mathbf{T}_l} : \nabla \cdot \overline{\mathbf{V}_l}, \tag{5.83}$$

$$\overline{\mu_{iwl}^\tau \left(\left\langle h_{iw}^\tau \right\rangle^{iw} - \left\langle h_{il}^\tau \right\rangle^{il}\right)} = \mu_{iwl}\left(h_{iw} - h_{il}\right) \tag{5.84}$$

$$\overline{\mu_{Mml}^\tau \left(h_{Ml}^{\tau\sigma} - \left\langle h_{Ml}^\tau \right\rangle^{Ml}\right)} = \mu_{Mml}\left(h_{Ml}^\sigma - h_{Ml}\right) \tag{5.85}$$

$$\overline{\mu_{nml}^\tau \left(\left\langle h_{nm}^\tau \right\rangle^{nm} - \left\langle h_{nl}^\tau \right\rangle^{nl}\right)} = \mu_{nml}\left(h_{nm} - h_{nl}\right) \tag{5.86}$$

$$\overline{q_l^{\tau N}} = q_l^N \tag{5.87}$$

$$\begin{aligned}
q_l^N &= \dot{q}_l''' + \sum_{i=1}^{i_{\max}} \mu_{iwl}\left(h_{iw} - h_{il}\right) + \sum_{m=1}^{3}\left[\mu_{Mml}\left(h_{Ml}^\sigma - h_{Ml}\right) + \sum_{n=1}^{n_{\max}} \mu_{nml}\left(h_{nm} - h_{nl}\right)\right] \\
&+ \frac{1}{2}\left[\mu_{wl}\left(\mathbf{V}_{wl} - \mathbf{V}_l\right)^2 - \mu_{lw}\left(\mathbf{V}_{lw} - \mathbf{V}_l\right)^2 + \sum_{m=1}^{3}\mu_{ml}\left(\mathbf{V}_m - \mathbf{V}_l\right)^2\right] \\
&+ \frac{1}{2}\left[\mu_{wl}\overline{\left(\mathbf{V}_{wl}' - \mathbf{V}_l'\right)^2} - \mu_{lw}\overline{\left(\mathbf{V}_{lw}' - \mathbf{V}_l'\right)^2} + \sum_{m=1}^{3}\mu_{ml}\overline{\left(\mathbf{V}_m' - \mathbf{V}_l'\right)^2}\right]
\end{aligned} \tag{5.88}$$

Substituting in Eq. (5.65) the above mentioned variables as consisting of mean values and fluctuations and performing time averaging following the above rules we obtain

$$\frac{\partial}{\partial \tau}\left(\alpha_l \rho_l s_l \gamma_v\right) + \nabla \cdot \left(\alpha_l^e \rho_l s_l \mathbf{V}_l \gamma\right)$$

$$-\frac{1}{T_l}\nabla\cdot\left(\alpha_l^e\gamma\delta_l\rho_l c_{pl}\frac{\nu_l^l}{\mathrm{Pr}_l^l}\nabla T_l\right)-\nabla.\left[\alpha_l^e\delta_l\rho_l\gamma\left(\sum_{i=1}^{i_{\max}}s_{il}D_{il}^l\nabla C_{il}\right)\right]$$

$$+\nabla\cdot\left[\alpha_l^e\rho_l\left(\overline{s_l'\mathbf{V}'}_l-\sum_{i=1}^{i_{\max}}\overline{s_{il}'\,D_{il}^l\nabla C_{il}'}\right)\gamma\right]=\gamma_v\frac{1}{T_l}DT_l^N+\gamma_v\sum_{\substack{m=1\\m\neq l}}^{3,w}\sum_{i=1}^{i_{\max}}\left(\mu_{iml}-\mu_{ilm}\right)s_{il}\,. \tag{5.89}$$

Here

$$DT_l^N=\alpha_l\rho_l\left(P_{k,l}+\delta_l\varepsilon_{\eta,l}+\varepsilon_l\right)+E_l^*+E_l'^*+\dot{q}_l'''+\sum_{i=1}^{i_{\max}}\mu_{iwl}\left(h_{iwl}-h_{il}\right)$$

$$+\sum_{\substack{m=1\\m\neq l}}^{l_{\max}}\left[\mu_{Mml}\left(h_{Ml}^\sigma-h_{Ml}\right)-\mu_{Mlm}\left(h_{Ml}^\sigma-h_{Ml}\right)+\sum_{n=1}^{n_{\max}}\mu_{nml}\left(h_{nm}-h_{nl}\right)\right]$$

$$+\frac{1}{2}\left[\begin{array}{l}\mu_{wl}\left(\mathbf{V}_{wl}-\mathbf{V}_l\right)^2-\mu_{lw}\left(\mathbf{V}_{lw}-\mathbf{V}_l\right)^2+\sum\limits_{m=1}^{3}\mu_{ml}\left(\mathbf{V}_m-\mathbf{V}_l\right)^2\\ \\ +\mu_{wl}\overline{\left(\mathbf{V}_{wl}'-\mathbf{V}_l'\right)^2}-\mu_{lw}\overline{\left(\mathbf{V}_{lw}'-\mathbf{V}_l'\right)^2}+\sum\limits_{m=1}^{3}\mu_{ml}\overline{\left(\mathbf{V}_m'-\mathbf{V}_l'\right)^2}\end{array}\right], \tag{5.90}$$

$$\gamma_v\alpha_l\rho_l\varepsilon_{\eta,l}=\alpha_l^e\gamma\cdot\left(\mathbf{T}_{\eta,l}:\nabla\cdot\mathbf{V}_l\right) \tag{5.91}$$

is the *irreversible dissipated power* caused by the viscous forces *due to deformation of the mean values of the velocities* in the space, and

$$\gamma_v\alpha_l\rho_l\varepsilon_l'=\alpha_l^e\gamma\cdot\left(\mathbf{T}_1':\nabla\cdot\mathbf{V}_l'\right) \tag{5.92}$$

is the *irreversibly dissipated power* in the viscous fluid due to *turbulent pulsations*, and

$$\gamma_v\alpha_l\rho_l P_{k,l}=\alpha_l^e\gamma\cdot\left(\mathbf{T}_l':\nabla\cdot\mathbf{V}_l\right)$$

is the power needed for production of turbulence. By modeling of the turbulence usually the last term is removed from the energy conservation equation and introduced as a generation term for the turbulent kinetic energy.

It is evident that the mass transfer between the velocity fields and between the fields and external sources causes additional entropy transport as a result of the different pulsation characteristics of the donor and receiver fields.

For simplicity's sake, averaging signs are omitted except in the turbulent diffusion term, which will be discussed next. The diffusion can also have *macroscopic* character, being caused by the macroscopic strokes between eddies with dimensions considerably larger than the molecular dimensions: turbulent diffusion. In a mixture at rest, *molecular* strokes represent the only mechanism driving diffusion. In real flows both mechanisms are observed. The higher the velocity of the flow, the higher the effect of turbulent diffusion.

To permit practical application of the entropy equation, it is necessary to define more accurately the term

$$\nabla \cdot \left[\alpha_l^e \rho_l \left(\overline{s_l' \mathbf{V}'_l} - \sum_{i=1}^{i_{\max}} \overline{s_{il}' \, D_{il}^l \nabla C_{il}'} \right) \gamma \right].$$

A possible assumption for this case is that the mechanism of entropy transport caused by fluctuations is a diffusion-like mechanism, which means that

$$\nabla \cdot \left[\alpha_l^e \rho_l \left(\overline{s_l' \mathbf{V}'_l} - \sum_{i=1}^{i_{\max}} \overline{s_{il}' \, D_{il}^l \nabla C_{il}'} \right) \gamma \right]$$

$$= -\frac{1}{T_l} \nabla \cdot \left[\alpha_l^e \rho_l \left(c_{pl} \frac{\nu_l^t}{\mathrm{Pr}_l^t} \nabla T_l \right) \gamma \right] - \nabla . \left[\alpha_l^e \rho_l \left(\sum_{i=1}^{i_{\max}} s_{il} \frac{\nu_l^t}{Sc_l^t} \nabla C_{il} \right) \gamma \right] \qquad (5.93)$$

where

$$\mathrm{Pr}_l^t = \rho_l c_{pl} \nu_l^t / \lambda_l^t \qquad (5.94)$$

is the turbulent *Prandtl* number and λ_l^t is the *turbulent coefficient of thermal conductivity* or *eddy conductivity*. Note that the thermal diffusion

$$\lambda_l = \rho_l c_{pl} \nu_l \, / \, \mathrm{Pr}_l \qquad (5.95)$$

is a thermodynamic property of the continuum l, and

$$\lambda_l^t = \rho_l c_{pl} \nu_l^t / \mathrm{Pr}_l^t \qquad (5.96)$$

is a mechanical property of the flowing field l. In channels,

$$\mathrm{Pr}_l^t \approx 0.7...0.9 \, , \qquad (5.97)$$

whereas for flow in jets, i.e., in *free turbulence*, the value is closer to 0.5 -see *Bird* et al. (1960),

$$\mathrm{Pr}_l^t \approx 0.25...2.5 \qquad (5.98)$$

for water, air and steam - see *Hammond* (1985)]. The turbulent *Schmidt* number is defined as

$$Sc_l^t = \nu_l^t / D_l^t \, . \qquad (5.99)$$

Here again the turbulent diffusion coefficient

$$D_l^t = \nu_l^t / Sc_l^t \qquad (5.100)$$

is a mechanical property of the flowing field l. As a result, the final form of the entropy equation is

$$\frac{\partial}{\partial \tau}\left(\alpha_l \rho_l s_l \gamma_v\right)+\nabla \cdot\left(\alpha_l^e \rho_l s_l \mathbf{V}_l \gamma\right)-\frac{1}{T_l} \nabla \cdot\left[\alpha_l^e \rho_l c_{pl}\left(\delta_l \frac{\nu_l}{\Pr_l}+\frac{\nu_l^t}{\Pr_l^t}\right) \gamma \nabla T_l\right]$$

$$-\nabla .\left\{\alpha_l^e \rho_l \gamma\left[\sum_{i=1}^{i_{\max}} s_{il}\left(\delta_l \frac{\nu_l}{Sc_l}+\frac{\nu_l^t}{Sc_l^t}\right) \nabla C_{il}\right]\right\}=\gamma_v\left[\frac{1}{T_l} DT_l^N+\sum_{\substack{m=1 \\ m \neq l}}^{3, w} \sum_{i=1}^{i_{\max}}\left(\mu_{iml}-\mu_{ilm}\right) s_{il}\right], \tag{5.101}$$

with this called the *conservative form*.

Keeping in mind that there is no net mass diffusively transported across a cross section perpendicular to the strongest concentration gradient

$$\sum_{i=1}^{i_{\max}}\left(D_{il}^* \nabla C_{il}\right)=0, \tag{5.102}$$

results in

$$D_{1l}^* \nabla C_{1l}=-\sum_{i=2}^{i_{\max}}\left(D_{il}^* \nabla C_{il}\right). \tag{5.103}$$

where the effective conductivity, and the diffusivity are

$$\lambda_l^*=\delta_l \lambda_l+\rho_l c_{pl} \frac{\nu_l^t}{\Pr_l^t}=\rho_l c_{pl}\left(\delta_l \frac{\nu_l}{\Pr_l}+\frac{\nu_l^t}{\Pr_l^t}\right), \tag{5.104}$$

$$D_{il}^*=\delta_l D_{il}+\frac{\nu_l^t}{Sc_l^t}=\delta_l \frac{\nu_l}{Sc_l}+\frac{\nu_l^t}{Sc_l^t}, \tag{5.105}$$

we obtain finally

$$\boxed{\begin{aligned}
&\frac{\partial}{\partial \tau}\left(\alpha_l \rho_l s_l \gamma_v\right)+\nabla \cdot\left\{\alpha_l^e \rho_l \gamma\left[s_l \mathbf{V}_l-\sum_{i=2}^{i_{\max}}\left(s_{il}-s_{1l}\right) D_{il}^* \nabla C_{il}\right]\right\} \\
&-\frac{1}{T_l} \nabla \cdot\left(\alpha_l^e \lambda_l^* \gamma \nabla T_l\right)=\gamma_v\left[\frac{1}{T_l} DT_l^N+\sum_{\substack{m=1 \\ m \neq l}}^{3, w} \sum_{i=1}^{i_{\max}}\left(\mu_{iml}-\mu_{ilm}\right) s_{il}\right]. \qquad (5.101\text{b})
\end{aligned}}$$

For a mixture consisting of several inert components and one no-inert component it is advisable to select subscript $i = 1 = M$ for the non-inert component and consider the mixture of the inert components as an ideal gas. In this case we have

$$... = \nabla\cdot\left[\alpha_l^e\rho_l\gamma\left(s_{nl}-s_{Ml}\right)D_{nl}^*\nabla C_{nl}\right]... \tag{5.101c}$$

This method is used in IVA6 computer code *Kolev* (1997b) developed by this author.

5.8 Local volume- and time-averaged internal energy equation

Following the same procedure as for the entropy equation we perform time averaging of Eq. (5.58). The result is

$$\frac{\partial}{\partial\tau}\left(\alpha_l\rho_l e_l\gamma_v\right)+\nabla\cdot\left(\alpha_l^e\rho_l e_l\mathbf{V}_l\gamma\right)+p_l\left[\frac{\partial}{\partial\tau}\left(\alpha_l\gamma_v\right)+\nabla\cdot\left(\alpha_l^e\mathbf{V}_l\gamma\right)\right]$$

$$-\nabla\cdot\left[\alpha_l^e\rho_l\left(\delta_l c_{pl}\frac{\nu_l^l}{\Pr_l^l}\nabla T_l+\overline{e_l'\mathbf{V}'_l}\right)\gamma\right]$$

$$-\nabla\cdot\left[\alpha_l^e\rho_l\left(\delta_l\sum_{i=1}^{i_{\max}}e_{il}D_{il}^l\nabla C_{il}+\sum_{i=1}^{i_{\max}}\overline{e_{il}'D_{il}^l\nabla C_{il}'}\right)\gamma\right]+\overline{p_l'\nabla\cdot\left(\alpha_l^e\mathbf{V}_l'\gamma\right)}=\gamma_v De_l^* \tag{5.106}$$

where

$$De_l^*=\alpha_l\rho_l\left(P_{k,l}+\delta_l\varepsilon_{\eta,l}+\varepsilon_l'\right)+\dot{q}'''$$

$$+\frac{1}{2}\left[\begin{array}{l}\mu_{wl}\left(\mathbf{V}_{wl}-\mathbf{V}_l\right)^2-\mu_{lw}\left(\mathbf{V}_{lw}-\mathbf{V}_l\right)^2+\sum\limits_{\substack{m=1\\m\neq l}}^{3}\mu_{ml}\left(\mathbf{V}_m-\mathbf{V}_l\right)^2\\[2ex]+\mu_{wl}\overline{\left(\mathbf{V}'_{wl}-\mathbf{V}'_l\right)^2}-\mu_{lw}\overline{\left(\mathbf{V}'_{lw}-\mathbf{V}'_l\right)^2}+\sum\limits_{\substack{m=1\\m\neq l}}^{3}\mu_{ml}\overline{\left(\mathbf{V}'_m-\mathbf{V}'_l\right)^2}\end{array}\right]$$

$$+\sum_{i=1}^{i_{\max}}\left(\mu_{iwl}h_{iwl}-\mu_{ilw}h_{il}\right)+\sum_{\substack{m=1\\m\neq l}}^{l_{\max}}\left[\mu_{Mml}h_{Ml}^{\sigma}+\sum_{n=1}^{n_{\max}}\left(\mu_{nml}h_{nm}-\mu_{nlm}h_{nl}\right)\right] \tag{5.107}$$

or introducing

$$\nabla\cdot\left[\alpha_l^e\rho_l\left(\overline{e_l'\mathbf{V}'_l}-\delta_l\sum_{i=1}^{i_{\max}}\overline{e_{il}'D_{il}^l\nabla C_{il}'}\right)\gamma\right]$$

$$= -\nabla \cdot \left[\alpha_l^e \rho_l \left(c_{pl} \frac{\nu_l^t}{\mathrm{Pr}_l^t} \nabla T_l + \sum_{i=1}^{i_{\max}} e_{il} \frac{\nu_l^t}{Sc_l^t} \nabla C_{il} \right) \gamma \right] \tag{5.108}$$

we obtain finally

$$\boxed{\begin{gathered} \frac{\partial}{\partial \tau}\left(\alpha_l \rho_l e_l \gamma_v\right) + \nabla \cdot \left(\alpha_l^e \rho_l e_l \mathbf{V}_l \gamma\right) + p_l \left[\frac{\partial}{\partial \tau}\left(\alpha_l \gamma_v\right) + \nabla \cdot \left(\alpha_l^e \mathbf{V}_l \gamma\right) \right] \\ -\nabla \cdot \left\{ \alpha_l^e \gamma \left[\lambda_l^* \nabla T_l + \rho_l \sum_{i=2}^{i_{\max}} \left(e_{il} - e_{1l}\right) D_{il}^* \nabla C_{il} \right] \right\} + \overline{p_l' \nabla \cdot \left(\alpha_l^e \mathbf{V}_l' \gamma\right)} = \gamma_v D e_l^* . \\ (5.109) \end{gathered}}$$

The expression defining the diffusion coefficient for the specific internal mixture energy is then

$$\nabla \cdot \left(\alpha_l^e \rho_l D_l^e \gamma \cdot \nabla e_l\right)$$

$$= \nabla \cdot \left\{ \alpha_l^e \rho_l \gamma \left[c_{pl} \left(\delta_l \frac{\nu_l}{\mathrm{Pr}_l} + \frac{\nu_l^t}{\mathrm{Pr}_l^t} \right) \nabla T_l + \sum_{i=2}^{i_{\max}} \left(e_{il} - e_{1l}\right) D_{il}^* \nabla C_{il} \right] \right\} \tag{5.110a}$$

which for ideal gas mixtures where the specific internal energy is not a function of pressure reduces to

$$\nabla \cdot \left(\alpha_l^e \rho_l D_l^e \gamma \cdot \nabla e_l\right) = \nabla \cdot \left\{ \alpha_l^e \rho_l \left[\frac{\lambda_l^*}{\rho_l c_{pl}} + \sum_{i=1}^{i_{\max}} e_{il} D_{il}^* / \left(\frac{\partial e_l}{\partial C_{il}} \right)_{p,T_l} \right] \gamma \nabla e_l \right\} \tag{5.110b}$$

where

$$D_l^e = \frac{\lambda_l^*}{\rho_l c_{pl}} + \sum_{i=1}^{i_{\max}} e_{il} D_{il}^* / \left(\frac{\partial e_l}{\partial C_{il}} \right)_{p,T_l} \tag{5.111}$$

This equation can be used to derive an alternative form for computation of the entropy diffusion coefficient

$$\nabla \cdot \left(\alpha_l^e \rho_l D_l^s \gamma \cdot \nabla s_l\right) = \left[\nabla \cdot \left(\alpha_l^e \rho_l D_l^e \gamma \cdot \nabla e_l\right) - \overline{p_l' \nabla \cdot \left(\alpha_l^e \mathbf{V}_l' \gamma\right)} \right] / T_l . \tag{5.112}$$

5.9 Local volume- and time-averaged specific enthalpy equation

Following the same procedure as for the entropy equation we perform time averaging of Eq. (5.55). The result is

$$
\begin{aligned}
&\frac{\partial}{\partial \tau}\left(\alpha_l \rho_l h_l \gamma_v\right) + \nabla \cdot \left(\alpha_l^e \rho_l \mathbf{V}_l h_l \gamma\right) - \left(\alpha_l \gamma_v \frac{\partial p_l}{\partial \tau} + \alpha_l^e \mathbf{V}_l \gamma \cdot \nabla p_l\right) \\
&-\nabla \cdot \left\{\alpha_l^e \gamma \left[\delta_l \lambda_l \nabla T_l - \rho_l \overline{\mathbf{V}_l' h_l'} + \delta_l \rho_l \sum_{i=1}^{i_{\max}} \left(h_{il} D_{il} \nabla C_{il}\right) + \rho_l \sum_{i=1}^{i_{\max}} \left(h_{il}' D_{il} \nabla C_{il}'\right)\right]\right\} \\
&-\alpha_l^e \overline{\mathbf{V}_l' \gamma \cdot \nabla p_l'} + \delta_l \left(\alpha_l^e \gamma \nabla p_l\right) \cdot \sum_{i=1}^{i_{\max}} D_{il}^l \nabla \ln C_{il} \\
&= \gamma_v D T_l^N + \gamma_v \sum_{\substack{m=1 \\ m \neq l}}^{3,w} \sum_{i=1}^{i_{\max}} \left(\mu_{iml} - \mu_{ilm}\right) h_{il} \qquad (5.113)
\end{aligned}
$$

Introducing

$$
\begin{aligned}
&\nabla \cdot \left\{\alpha_l^e \rho_l \left[\overline{\mathbf{V}_l' h_l'} - \sum_{i=1}^{i_{\max}} \left(h_{il}' D_{il} \nabla C_{il}'\right)\right] \gamma\right\} \\
&= -\nabla \cdot \left[\alpha_l^e \rho_l \left(\delta_l c_{pl} \frac{\nu_l^t}{\Pr_l^t} \nabla T_l + \sum_{i=1}^{i_{\max}} h_{il} \frac{\nu_l^t}{Sc_l^t} \nabla C_{il}\right) \gamma\right] \qquad (5.114)
\end{aligned}
$$

we obtain

$$
\boxed{
\begin{aligned}
&\frac{\partial}{\partial \tau}\left(\alpha_l \rho_l h_l \gamma_v\right) + \nabla \cdot \left(\alpha_l^e \rho_l \mathbf{V}_l h_l \gamma\right) - \left(\alpha_l \gamma_v \frac{\partial p_l}{\partial \tau} + \alpha_l^e \mathbf{V}_l \gamma \cdot \nabla p_l\right) \\
&-\nabla \cdot \left\{\alpha_l^e \left[\lambda_l^* \nabla T_l + \rho_l \sum_{i=2}^{i_{\max}} \left(h_{il} - h_{1l}\right) D_{il}^* \nabla C_{il}\right] \gamma\right\} - \alpha_l^e \overline{\mathbf{V}_l' \gamma \cdot \nabla p_l'} \\
&+\delta_l \left(\alpha_l^e \gamma \nabla p_l\right) \cdot \sum_{i=1}^{i_{\max}} D_{il}^l \nabla \ln C_{il} = \gamma_v D T_l^N + \gamma_v \sum_{\substack{m=1 \\ m \neq l}}^{3,w} \sum_{i=1}^{i_{\max}} \left(\mu_{iml} - \mu_{ilm}\right) h_{il} . \qquad (5.115)
\end{aligned}
}
$$

The non-conservative form is then

$$
\begin{aligned}
&\alpha_l \rho_l \gamma_v \frac{\partial h_l}{\partial \tau} + \alpha_l^e \rho_l \left(\mathbf{V}_l \gamma \cdot \nabla\right) h_l - \left(\alpha_l \gamma_v \frac{\partial p_l}{\partial \tau} + \alpha_l^e \mathbf{V}_l \gamma \cdot \nabla p_l\right) \\
&-\nabla \cdot \left\{\alpha_l^e \left[\lambda_l^* \nabla T_l + \rho_l \sum_{i=2}^{i_{\max}} \left(h_{il} - h_{1l}\right) D_{il}^* \nabla C_{il}\right] \gamma\right\} - \alpha_l^e \overline{\mathbf{V}_l' \gamma \cdot \nabla p_l'}
\end{aligned}
$$

$$+\delta_l\left(\alpha_l^e \gamma \nabla p_l\right)\cdot\sum_{i=1}^{i_{\max}} D_{il}^l \nabla \ln C_{il} = \gamma_v D T_l^N . \tag{5.115}$$

The definition equation for an enthalpy diffusion coefficient is then

$$\nabla\cdot\left(\alpha_l^e \rho_l D_l^h \gamma \nabla h_l\right) = \nabla\cdot\left\{\alpha_l^e \rho_l \left[\frac{\lambda_l^*}{\rho_l}\nabla T_l + \sum_{i=2}^{i_{\max}}\left(h_{il}-h_{1l}\right) D_{il}^* \nabla C_{il}\right]\gamma\right\}. \tag{5.116}$$

For mixtures of two ideal gases n and M we have

$$\nabla\cdot\left(\alpha_l^e \rho_l D_l^h \gamma\cdot\nabla h_l\right) = \nabla\cdot\left\{\alpha_l^e \rho_l \left[\frac{\lambda_l^*}{\rho_l}\nabla T_l + \left(h_{nl}-h_{Ml}\right) D_{nl}^* \nabla C_{nl}\right]\gamma\right\} \tag{5.117a}$$

and an equation of state in differential form

$$\nabla h_l = c_{pl}\nabla T_l + \left(h_{nl}-h_{Ml}\right)\nabla C_{nl},$$

which finally gives

$$\nabla\cdot\left(\alpha_l^e \rho_l D_l^h \gamma \nabla h_l\right) = \nabla\cdot\left\{\alpha_l^e \gamma\left[\lambda_l^*\left(1-Le_{il}\right)\nabla T + \rho_l D_{nl}^* \nabla h_l\right]\right\} \tag{5.117b}$$

where

$$Le_{il} = \frac{\rho_l c_{pl} D_{nl}^*}{\lambda_l^*}$$

is the *Lewis-Semenov* number. For a lot of binary gas mixtures $Le_{il} \approx 1$ and

$$\nabla\cdot\left(\alpha_l^e \rho_l D_l^h \gamma \nabla h_l\right) = \nabla\cdot\left(\alpha_l^e \rho_l D_{nl}^* \gamma \nabla h_l\right), \tag{5.117c}$$

which results in

$$D_l^h = D_{nl}^*,$$

Grigorieva and *Zorina* (1988) p. 267. This relation is widely used for simulation of diffusion in binary gas mixtures. If both components possess equal specific capacities at constant pressures, and therefore $h_{nl} \approx h_{Ml}$, we have

$$\nabla\cdot\left(\alpha_l^e \rho_l D_l^h \gamma\cdot\nabla h_l\right) = \nabla\cdot\left(\alpha_l^e \lambda_l^* \gamma \nabla T_l\right). \tag{5.117d}$$

This condition is fulfilled for many liquid mixtures and solutions. In this case the diffusion enthalpy transport looks like the *Fick*'s law and is totally controlled by the temperature gradient.

5.10 Non-conservative and semi-conservative forms of the entropy equation

The *non-conservative* form of the entropy equation is obtained by differentiating the first and second terms of the conservative form appropriately and comparing with the mass conservation equation. The result is

$$\rho_l \left[\alpha_l \gamma_v \frac{\partial s_l}{\partial \tau} + \left(\alpha_l^e \mathbf{V}_l \gamma \cdot \nabla \right) s_l \right]$$

$$-\frac{1}{T_l} \nabla \cdot \left(\alpha_l^e \lambda_l^* \gamma \nabla T \right) - \nabla . \left\{ \alpha_l^e \rho_l \gamma \left[\sum_{i=2}^{i_{\max}} \left(s_{il} - s_{1l} \right) D_{il}^* \nabla C_{il} \right] \right\}$$

$$= \gamma_v \left(\frac{1}{T_l} DT_l^N + \sum_{\substack{m=1 \\ m \neq l}}^{l_{\max},w} \sum_{i=1}^{i_{\max}} \left(\mu_{iml} - \mu_{ilm} \right) s_{il} - \mu_l s_l \right) \equiv \gamma_v Ds_l^{N\,\prime}. \qquad (5.118)$$

The superscript N stands to remember that the RHS is for the non-conservative form of the energy conservation equation written in entropy form. *Note* that in addition to the enthalpy source terms divided by the field temperature, new terms arise. In fact, these denote the difference between the sum of the mass source per unit time and mixture volume multiplied by the corresponding specific component entropies and the product of the specific field entropy and the field mass source density.

$$\gamma_v \left[\sum_{\substack{m=1 \\ m \neq l}}^{l_{\max},w} \sum_{i=1}^{i_{\max}} \left(\mu_{iml} - \mu_{ilm} \right) s_{il} - s_l \sum_{\substack{m=1 \\ m \neq l}}^{l_{\max},w} \sum_{i=1}^{i_{\max}} \left(\mu_{iml} - \mu_{ilm} \right) \right]. \qquad (5.119)$$

Splitting the mass source term into *sources* and *sinks*

$$\mu_l = \sum_{\substack{m=1 \\ m \neq l}}^{l_{\max},w} \sum_{i=1}^{i_{\max}} \left(\mu_{iml} - \mu_{ilm} \right) = \mu_l^+ - \mu_l^- \qquad (5.120)$$

where

$$\mu_l^+ = \sum_{\substack{m=1 \\ m \neq l}}^{l_{\max},w} \sum_{i=1}^{i_{\max}} \mu_{iml} \geq 0, \qquad (5.121)$$

$$\mu_l^- = \sum_{\substack{m=1 \\ m \neq l}}^{l_{\max},w} \sum_{i=1}^{i_{\max}} \mu_{ilm} \geq 0, \qquad (5.122)$$

$$\mu_l^+ s_l \geq 0, \qquad (5.123)$$

$$\mu_l^- s_l \geq 0 , \tag{5.124}$$

one then obtains the *final semi-conservative* form for the entropy equation

$$\rho_l \left[\alpha_l \gamma_v \frac{\partial s_l}{\partial \tau} + \left(\alpha_l^e \mathbf{V}_l \gamma \cdot \nabla \right) s_l \right] - \frac{1}{T_l} \nabla \cdot \left(\alpha_l^e \lambda_l^* \gamma \nabla T \right)$$

$$- \nabla . \left\{ \alpha_l^e \rho_l \gamma \left[\sum_{i=2}^{i_{\max}} \left(s_{il} - s_{1l} \right) D_{il}^* \nabla C_{il} \right] \right\} + \gamma_v \mu_l^+ s_l = \gamma_v D s_l , \tag{5.125}$$

in which

$$D s_l = \frac{1}{T_l} D T_l^N + \sum_{\substack{m=1 \\ m \neq l}}^{3,w} \sum_{i=1}^{i_{\max}} \left(\mu_{iml} - \mu_{ilm} \right) s_{il} - \mu_l s_l + \mu_l^+ s_l$$

$$= \frac{1}{T_l} D T_l^N + \sum_{\substack{m=1 \\ m \neq l}}^{3,w} \sum_{i=1}^{i_{\max}} \left(\mu_{iml} - \mu_{ilm} \right) s_{il} + \mu_l^- s_l$$

$$= \frac{1}{T_l} D T_l^N + \gamma_v \left\{ \sum_{\substack{m=1 \\ m \neq l}}^{3,w} \left[\mu_{lm} s_l + \sum_{i=1}^{i_{\max}} \left(\mu_{iml} - \mu_{ilm} \right) s_{il} \right] \right\} \tag{5.126}$$

The three forms of the entropy equation, conservative (5.110b), non-conservative (5.118), and semi-conservative (5.125) are mathematically identical.

The introduction of the semi-conservative form is perfectly suited to numerical integration because it ensures proper initialization of the value for the entropy in a computational cell in which a previously non-existent field is just in the course of origination.

5.11 Comments on the source terms in the mixture entropy equation

The following terms in the semi-conservative entropy equation (5.125),

$$D s_l = ... + \gamma_v \left\{ \sum_{\substack{m=1 \\ m \neq l}}^{3,w} \left[\mu_{lm} s_l + \sum_{i=1}^{i_{\max}} \left(\mu_{iml} - \mu_{ilm} \right) s_{il} \right] \right\}$$

$$+\frac{\gamma_v}{T_l}\left\{\sum_{i=1}^{i_{\max}}\mu_{iwl}\left(h_{iwl}-h_{il}\right)+\sum_{m=1}^{3}\left[\mu_{Mml}\left(h_{Ml}^{\sigma}-h_{Ml}\right)+\sum_{n=1}^{n_{\max}}\mu_{nml}\left(h_{nm}-h_{nl}\right)\right]\right\}, \quad (5.127)$$

are discussed in some detail in this section in order to facilitate their practical application. For the wall source terms, that is, for injection from the wall into the flow and suction from the flow into the wall one can write

$$\mu_{iwl}=C_{iwl}\mu_{wl}\,, \quad (5.128)$$

$$\mu_{ilw}=C_{il}\mu_{lw}\,, \quad (5.129)$$

and therefore

$$Ds_l = ... +\gamma_v\mu_{wl}\sum_{i=1}^{i_{\max}}C_{iwl}\left[s_{il}+\left(h_{iwl}-h_{il}\right)/T_l\right]+\gamma_v\sum_{\substack{m=1\\ m\neq l}}^{l_{\max}}\left\{\mu_{lm}s_l+\sum_{i=1}^{i_{\max}}\left(\mu_{iml}-\mu_{ilm}\right)s_{il}\right\}$$

$$+\frac{\gamma_v}{T_l}\sum_{m=1}^{3}\left[\mu_{Mml}\left(h_{Ml}^{\sigma}-h_{Ml}\right)+\sum_{n=1}^{n_{\max}}\mu_{nml}\left(h_{nm}-h_{nl}\right)\right]. \quad (5.130)$$

Similar relationships as Eqs. (5.128) and (5.129) are valid for entrainment from field 2 to 3 and deposition from field 3 to 2, that is for *lm* = 23, 32. Note that, say, for steam condensation from multi-component gas mixtures, *lm* = 12, 13, and for evaporation, *lm* = 21, 31, the following then applies: $\mu_{ilm}\neq\mu_{lm}C_{il}$. For practical applications it is convenient to group all inert and non-inert components in pseudo-two-component mixtures inside the field *l* designated simply with *n* and *M*, respectively.

The most important mass transfer mechanisms in the three velocity fields flow will now be taken into account in accordance with the following assumptions:

a) No solution of gas into field 2 and/or 3;
b) No gas dissolution from field 2 and/or 3;
c) Evaporation from field 2 and/or 3 into the gas field 1 is allowed;
d) Condensation of the component *M* from the gas field onto the interface of fields 2 and/or 3 is allowed;
e) Injection from the wall into all of the fields is allowed;
f) Suction from all of the fields through the wall is allowed.

The mass transfer terms are written in the following form:

$$\mu_{nlm}=\left|\begin{array}{cccc}0 & 0 & 0 & \mu_{n1w}=C_{n1}\mu_{1w}\\ 0 & 0 & \mu_{n23}=C_{n2}\mu_{23} & \mu_{n2w}=C_{n2}\mu_{2w}\\ 0 & \mu_{n32}=C_{n3}\mu_{32} & 0 & \mu_{n3w}=C_{n3}\mu_{3w}\\ \mu_{nw1}=C_{nw1}\mu_{w1} & \mu_{nw2}=C_{nw2}\mu_{w2} & \mu_{nw3}=C_{nw3}\mu_{w3} & 0\end{array}\right|, \quad (5.131)$$

$$\mu_{Mlm} = \begin{vmatrix} 0 & \mu_{M12} = \mu_{12} & \mu_{M13} = \mu_{13} & \mu_{M1w} = C_{M1}\mu_{1w} \\ \mu_{M21} = \mu_{21} & 0 & \mu_{M23} = C_{M2}\mu_{23} & \mu_{M2w} = C_{M2}\mu_{2w} \\ \mu_{M31} = \mu_{31} & \mu_{M32} = C_{M3}\mu_{32} & 0 & \mu_{M3w} = C_{M3}\mu_{3w} \\ \mu_{Mw1} = C_{Mw1}\mu_{w1} & \mu_{Mw2} = C_{Mw2}\mu_{w2} & \mu_{Mw3} = C_{Mw3}\mu_{w3} & 0 \end{vmatrix}. \tag{5.132}$$

Except for the diagonal elements, the zeros in Eq. (5.132) result from assumptions a) and b). Assumptions c) and d) give rise to the terms

$$\mu_{Mlm} = \begin{vmatrix} 0 & \mu_{M12} = \mu_{12} & \mu_{M13} = \mu_{13} & \ldots \\ \mu_{M21} = \mu_{21} & 0 & \ldots & \ldots \\ \mu_{M31} = \mu_{31} & \ldots & 0 & \ldots \\ \ldots & \ldots & \ldots & 0 \end{vmatrix} \tag{5.133}$$

in the above equation.

Figures 5.2 and 5.3 illustrate the l-field side interface properties for the three fields under consideration.

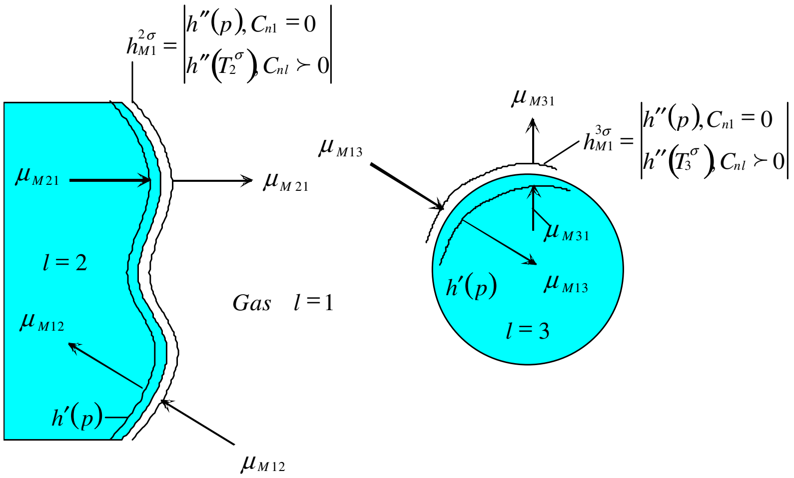

Fig. 5.2 Evaporation and condensation mass transfer. Interface properties

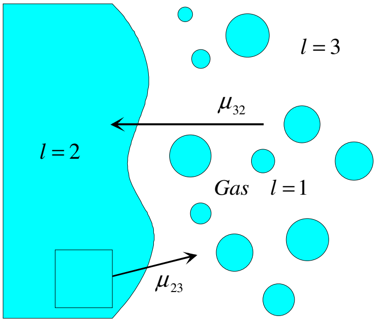

Fig. 5.3 Entrainment and deposition mass transfer

Taking into account Eqs. (5.131) and (5.132), the specific form for the source terms is:

$$Ds_1 = \dot{q}_1'''/T_1$$

$$+\gamma_v \mu_{w1}\left\{\left(1 - C_{nw1}\right)\left[s_{M1} + \left(h_{Mw1} - h_{M1}\right)/T_1\right] + C_{nw1}\left[s_{n1} + \left(h_{nw1} - h_{n1}\right)/T_1\right]\right\}$$

$$+\gamma_v \begin{bmatrix} \mu_{21}\left[s_{M1} + \left(h_{M1}^{2\sigma} - h_{M1}\right)/T_1\right] - \mu_{12}C_{n1}\left(s_{M1} - s_{n1}\right) \\ \\ \mu_{31}\left[s_{M1} + \left(h_{M1}^{3\sigma} - h_{M1}\right)/T_1\right] - \mu_{13}C_{n1}\left(s_{M1} - s_{n1}\right) \end{bmatrix} + \alpha_1\rho_1\left(\delta_1 P_{k1}^{\tau} + \varepsilon_1\right)/T_1$$

$$+\frac{1}{2}\left[\mu_{w1}\left(\mathbf{V}_{w1} - \mathbf{V}_1\right)^2 - \mu_{1w}\left(\mathbf{V}_{1w} - \mathbf{V}_1\right)^2 + \sum_{m=2,3}\mu_{m1}\left(\mathbf{V}_m - \mathbf{V}_1\right)^2\right]/T_1$$

$$+\frac{1}{2}\left[\mu_{w1}\overline{\left(\mathbf{V}_{w1}' - \mathbf{V}_1'\right)^2} - \mu_{1w}\overline{\left(\mathbf{V}_{1w}' - \mathbf{V}_1'\right)^2} + \sum_{m=2,3}\mu_{m1}\overline{\left(\mathbf{V}_m' - \mathbf{V}_1'\right)^2}\right]/T_1, \quad (5.134)$$

$$Ds_2 = \dot{q}_2'''/T_2$$

$$+\gamma_v \mu_{w2}\left\{\left(1 - C_{nw2}\right)\left[s_{M2} + \left(h_{Mw2} - h_{M2}\right)/T_2\right] + C_{nw2}\left[s_{n2} + \left(h_{nw2} - h_{n2}\right)/T_2\right]\right\}$$

$$+\gamma_v \mu_{32}\left\{\left(1 - C_{n3}\right)\left[s_{M2} + \left(h_{M3} - h_{M2}\right)/T_2\right] + C_{n3}\left[s_{n2} + \left(h_{n3} - h_{n2}\right)/T_2\right]\right\}$$

$$+\gamma_v\left\{\mu_{12}\left[s_{M2} + \left(h_{M2}^{\sigma} - h_{M2}\right)/T_2\right] - \mu_{21}C_{n2}\left(s_{M2} - s_{n2}\right)\right\} + \alpha_2\rho_2\left(\delta_2 P_{k2}^{\tau} + \varepsilon_2\right)/T_2$$

$$+\frac{1}{2}\left[\mu_{w2}\left(\mathbf{V}_{w2} - \mathbf{V}_2\right)^2 - \mu_{2w}\left(\mathbf{V}_{2w} - \mathbf{V}_2\right)^2 + \sum_{m=1,3}\mu_{m2}\left(\mathbf{V}_m - \mathbf{V}_2\right)^2\right]/T_2$$

$$+\frac{1}{2}\left[\mu_{w2}\overline{\left(\mathbf{V}'_{w2}-\mathbf{V}'_{2}\right)^{2}}-\mu_{2w}\overline{\left(\mathbf{V}'_{2w}-\mathbf{V}'_{2}\right)^{2}}+\sum_{m=1,3}\mu_{m2}\overline{\left(\mathbf{V}'_{m}-\mathbf{V}'_{2}\right)^{2}}\right]/T_{2}, \quad (5.135)$$

$$Ds_{3}=\dot{q}_{3}'''/T_{3}$$

$$+\gamma_{v}\mu_{w3}\left\{\left(1-C_{nw3}\right)\left[s_{M3}+\left(h_{Mw3}-h_{M3}\right)/T_{3}\right]+C_{nw3}\left[s_{n3}+\left(h_{nw3}-h_{n3}\right)/T_{3}\right]\right\}$$

$$+\gamma_{v}\mu_{23}\left\{\left(1-C_{n2}\right)\left[s_{M3}+\left(h_{M2}-h_{M3}\right)/T_{3}\right]+C_{n2}\left[s_{n3}+\left(h_{n2}-h_{n3}\right)/T_{3}\right]\right\}$$

$$+\gamma_{v}\left\{\mu_{13}\left[s_{M3}+\left(h_{M3}^{\sigma}-h_{M3}\right)/T_{3}\right]-\mu_{31}C_{n3}\left(s_{M3}-s_{n3}\right)\right\}+\alpha_{3}\rho_{3}\left(\delta_{3}P_{k3}^{\tau}+\varepsilon_{3}\right)/T_{3}$$

$$+\frac{1}{2}\left[\mu_{w3}\left(\mathbf{V}_{w3}-\mathbf{V}_{3}\right)^{2}-\mu_{3w}\left(\mathbf{V}_{3w}-\mathbf{V}_{3}\right)^{2}+\sum_{m=1,2}\mu_{m3}\left(\mathbf{V}_{m}-\mathbf{V}_{3}\right)^{2}\right]/T_{3}$$

$$+\frac{1}{2}\left[\mu_{w3}\overline{\left(\mathbf{V}'_{w3}-\mathbf{V}'_{3}\right)^{2}}-\mu_{3w}\overline{\left(\mathbf{V}'_{3w}-\mathbf{V}'_{3}\right)^{2}}+\sum_{m=1,2}\mu_{m3}\overline{\left(\mathbf{V}'_{m}-\mathbf{V}'_{3}\right)^{2}}\right]/T_{3}. \quad (5.136)$$

The above equations can be simplified by taking into account

$$s_{iwl}=s_{il}+\left(h_{iwl}-h_{il}\right)/T_{l}, \quad (5.137)$$

$$s_{wl}=\sum_{i=1}^{i_{\max}}C_{iwl}s_{iwl}, \quad (5.138)$$

$$s_{il}=s_{im}+\left(h_{il}-h_{im}\right)/T_{m}, \quad (5.139)$$

$$s_{l}=\sum_{i=1}^{i_{\max}}C_{il}s_{il}, \quad (5.140)$$

$$s_{Ml}^{\sigma}=s_{Ml}+\left(h_{Ml}^{\sigma}-h_{Ml}\right)/T_{l}, \quad (5.141)$$

for $l = 2,3$ and $m = 3,2$ respectively.

$$Ds_{1}=\ldots+\gamma_{v}\mu_{w1}\left\{\left(1-C_{nw1}\right)\left[s_{M1}+\left(h_{Mw1}-h_{M1}\right)/T_{1}\right]+C_{nw1}\left[s_{n1}+\left(h_{nw1}-h_{n1}\right)/T_{1}\right]\right\}$$

$$+\gamma_{v}\left[\begin{array}{l}\left(\mu_{21}+\mu_{31}\right)s_{M1}+\left[\mu_{21}\left(h_{M1}^{2\sigma}-h_{M1}\right)+\mu_{31}\left(h_{M1}^{3\sigma}-h_{M1}\right)\right]/T_{1}\\ \\ -\left(\mu_{12}+\mu_{13}\right)C_{n1}\left(s_{M1}-s_{n1}\right)\end{array}\right]+\ldots, \quad (5.142)$$

$$Ds_{2}=\ldots+\gamma_{v}\left[\mu_{w2}s_{w2}+\mu_{32}s_{3}+\mu_{12}s'\left(p\right)\right]+\ldots, \quad (5.143)$$

$$Ds_3 = ... + \gamma_v \left[\mu_{w3} s_{w3} + \mu_{23} s_2 + \mu_{13} s'(p) \right] + ... \tag{5.144}$$

Note that the mass transfer terms can give rise to entropy change even if mass leaves the field with entropy at the interface not equal to the intrinsic average field entropy. There is an additional source of entropy change if the non-inert component leaves the field with entropy at the interface not equal to the intrinsic average field entropy as a result of evaporation or condensation.

For evaporation only within the closed control volume one obtains

$$\left(\mu_{12} + \mu_{13}\right) s_1 = \mu_{21} \left[s_{M1} + \left(h''\left(T_2^\sigma\right) - h_{M1} \right) / T_1 \right] + \mu_{31} \left[s_{M1} + \left(h''\left(T_3^\sigma\right) - h_{M1} \right) / T_1 \right] \tag{5.145}$$

or

$$s_1 = \left\{ \mu_{21} \left[s_{M1} + \left(h''\left(T_2^\sigma\right) - h_{M1} \right) / T_1 \right] + \mu_{31} \left[s_{M1} + \left(h''\left(T_3^\sigma\right) - h_{M1} \right) / T_1 \right] \right\} / \left(\mu_{12} + \mu_{13}\right) . \tag{5.146}$$

For condensation and deposition the following is obtained for the specific entropy of the second velocity field

$$s_2 = \left[\mu_{32} s_3 + \mu_{12} s'(p) \right] / \left(\mu_{12} + \mu_{32} \right) . \tag{5.147}$$

For condensation and entrainment the following is obtained for the specific entropy of the third velocity field

$$s_3 = \left[\mu_{23} s_2 + \mu_{13} s'(p) \right] / \left(\mu_{13} + \mu_{23} \right) . \tag{5.148}$$

A frequently used simplification of the energy jump condition for computing the resulting evaporation or condensation is

$$\dot{q}'''_{m\sigma l} + \dot{q}'''_{l\sigma m} + \mu^{\tau}_{Ml} \left(h^\sigma_{Mm} - h^\sigma_{Ml} \right) = 0 , \tag{5.149}$$

or if $-\left(\dot{q}'''_{m\sigma l} + \dot{q}'''_{l\sigma m} \right) / \left(h^\sigma_{Mm} - h^\sigma_{Ml} \right) > 0$, then

$$\mu_{Mml} = -\left(\dot{q}'''_{m\sigma l} + \dot{q}'''_{l\sigma m} \right) / \left(h^\sigma_{Mm} - h^\sigma_{Ml} \right) \quad \text{and} \quad \mu_{Mlm} = 0 , \tag{5.150}$$

else

$$\mu_{Mlm} = \left(\dot{q}'''_{m\sigma l} + \dot{q}'''_{l\sigma m} \right) / \left(h^\sigma_{Ml} - h^\sigma_{Mm} \right) \quad \text{and} \quad \mu_{Mml} = 0 . \tag{5.151}$$

5.12 Viscous dissipation

Now we will discuss three important terms reflecting the irreversible part of the dissipation of the mechanical energy. The *irreversibly dissipated power* in the viscous fluid due to *turbulent pulsations* and due to *change of the mean velocity* in space is

$$\gamma_v \alpha_l \rho_l \varepsilon_l = \gamma_v \alpha_l \rho_l \left(\varepsilon_l' + \varepsilon_{\eta,l} \right) = \alpha_l^e \gamma \cdot \left[\left(\mathbf{T}_l' : \nabla \cdot \mathbf{V}_l' \right) + \left(\mathbf{T}_{\eta,l} : \nabla \cdot \mathbf{V}_l \right) \right]. \quad (5.152)$$

These components can not be returned back as a mechanical energy of the flow. They express quantitatively the transfer of mechanical in thermal energy in the field *l*. In a notation common for Cartesian and cylindrical coordinates the irreversibly dissipated power in the viscous fluid due to turbulent pulsations is expressed as follows

$$\frac{\varepsilon_l'}{\nu_l} = 2\left\{ \gamma_r \overline{\left(\frac{\partial u_l'}{\partial r} \right)^2} + \gamma_\theta \overline{\left[\frac{1}{r^\kappa} \left(\frac{\partial v_l'}{\partial \theta} + \kappa u_l' \right) \right]^2} + \gamma_z \overline{\left(\frac{\partial w_l'}{\partial z} \right)^2} \right\}$$

$$+ \overline{\left[\frac{\partial v_l'}{\partial r} + \frac{1}{r^\kappa} \left(\frac{\partial u_l'}{\partial \theta} - \kappa v_l' \right) \right] \left[\gamma_r \frac{\partial v_l'}{\partial r} + \gamma_\theta \frac{1}{r^\kappa} \left(\frac{\partial u_l'}{\partial \theta} - \kappa v_l' \right) \right]}$$

$$+ \overline{\left[\frac{\partial w_l'}{\partial r} + \frac{\partial u_l'}{\partial z} \right] \left[\gamma_r \frac{\partial w_l'}{\partial r} + \gamma_z \frac{\partial u_l'}{\partial z} \right]} + \overline{\left[\frac{1}{r^\kappa} \frac{\partial w_l'}{\partial \theta} + \frac{\partial v_l'}{\partial z} \right] \left[\gamma_\theta \frac{1}{r^\kappa} \frac{\partial w_l'}{\partial \theta} + \gamma_z \frac{\partial v_l'}{\partial z} \right]}$$

$$- \frac{2}{3} \overline{\left[\frac{\partial u_l'}{\partial r} + \frac{1}{r^\kappa} \left(\frac{\partial v_l'}{\partial \theta} + \kappa u_l' \right) + \frac{\partial w_l'}{\partial z} \right] \left[\gamma_r \frac{\partial u_l'}{\partial r} + \gamma_\theta \frac{1}{r^\kappa} \left(\frac{\partial v_l'}{\partial \theta} + \kappa u_l' \right) + \gamma_z \frac{\partial w_l'}{\partial z} \right]} \ge 0.$$

(5.153)

All terms in the right-hand side of this equation are time averages. Similarly, the irreversibly dissipated power in the viscous fluid due to deformation of the mean velocity field in space is expressed as follows

$$\gamma_v \alpha_l \rho_l \varepsilon_{\eta,l} = \alpha_l^e \gamma \cdot \left(\mathbf{T}_{\eta,l} : \nabla \cdot \mathbf{V}_l \right)$$

$$= \alpha_l^e \rho_l \nu_l \left(\begin{array}{c} 2\left\{ \gamma_r \left(\dfrac{\partial u_l}{\partial r} \right)^2 + \gamma_\theta \left[\dfrac{1}{r^\kappa} \left(\dfrac{\partial v_l}{\partial \theta} + \kappa u_l \right) \right]^2 + \gamma_z \left(\dfrac{\partial w_l}{\partial z} \right)^2 \right\} \\ \\ -\dfrac{2}{3} (\nabla . \mathbf{V}_l)(\gamma \nabla . \mathbf{V}_l) + \tilde{S}_{k,l}^2 \end{array} \right), \quad (5.154)$$

where

$$\gamma \nabla . \mathbf{V}_l = \gamma_r \frac{\partial u_l}{\partial r} + \gamma_\theta \frac{1}{r^\kappa} \left(\frac{\partial v_l}{\partial \theta} + \kappa u_l \right) + \gamma_z \frac{\partial w_l}{\partial z}, \quad (5.155)$$

$$\nabla.\mathbf{V}_l = \frac{\partial u_l}{\partial r} + \frac{1}{r^\kappa}\left(\frac{\partial v_l}{\partial \theta} + \kappa u_l\right) + \frac{\partial w_l}{\partial z}, \tag{5.156}$$

$$\tilde{S}_{k,l}^2 = \left[\frac{\partial v_l}{\partial r} + \frac{1}{r^\kappa}\left(\frac{\partial u_l}{\partial \theta} - \kappa v_l\right)\right]\left[\gamma_r \frac{\partial v_l}{\partial r} + \gamma_\theta \frac{1}{r^\kappa}\left(\frac{\partial u_l}{\partial \theta} - \kappa v_l\right)\right]$$

$$+\left(\frac{\partial w_l}{\partial r} + \frac{\partial u_l}{\partial z}\right)\left(\gamma_r \frac{\partial w_l}{\partial r} + \gamma_z \frac{\partial u_l}{\partial z}\right)$$

$$+\left(\frac{1}{r^\kappa}\frac{\partial w_l}{\partial \theta} + \frac{\partial v_l}{\partial z}\right)\left(\gamma_\theta \frac{1}{r^\kappa}\frac{\partial w_l}{\partial \theta} + \gamma_z \frac{\partial v_l}{\partial z}\right). \tag{5.157}$$

Here the *Stokes* hypothesis is used. For single-phase flow, $\alpha_l = 1$, in free three-dimensional space, $\gamma = 1$, the above equation then reducing to the form obtained for the first time by *Rayleigh*. Note that in a turbulent pipe flow in the viscous boundary layer $\varepsilon_l' = 0$ and $\varepsilon_{\eta,l} > 0$. Outside the boundary layer for relatively flat velocity profiles $\varepsilon_l' > 0$ and $\varepsilon_{\eta,l} \to 0$

The specific irreversibly dissipated power per unit viscous fluid mass due to turbulent pulsations

$$\varepsilon_l = \varepsilon_{\eta,l} + \varepsilon_l' \qquad (5.158]$$

is used as important dependent variable characterizing the turbulence in the field. It is subject of model description. This power is considered to be constantly removed from the specific turbulent kinetic energy per unit mass of the flow field defined as follows

$$k_l = \frac{1}{2}\left(u_l'^2 + v_l'^2 + w_l'^2\right). \tag{5.159}$$

This is the second dependent variable for the velocity field which is also a subject of modeling.

In fact, Eq. (5.152) is the definition equation for the viscous dissipation rate, ε_l of the turbulent kinetic energy k_l. Here it is evident that ε_l is

(a) a non-negative quadratic form, $\varepsilon_l \geq 0$,

(b) its mathematical description does not depend on the rotation of the coordinate system, and

(c) it contains no derivatives of the viscosity,

compare with *Zierep* (1983) for single phase flow.

The term

$$\gamma_v \alpha_l \rho_l P_{k,l} = \alpha_l^e \gamma \cdot \left(\mathbf{T}_l' : \nabla \cdot \mathbf{V}_l\right) = \alpha_l^e \left[\nabla\gamma \cdot \left(\mathbf{T}' \cdot \mathbf{V}_l\right) - \mathbf{V}_l \cdot \left(\nabla\gamma \cdot \mathbf{T}'\right)\right]$$

$$= \alpha_l^e \left[\begin{array}{l} \tau'_{xx}\gamma_x \dfrac{\partial u}{\partial x} + \tau'_{yy}\gamma_y \dfrac{\partial v}{\partial y} + \tau'_{zz}\gamma_z \dfrac{\partial w}{\partial z} \\ \\ +\tau'_{xy}\left(\gamma_y \dfrac{\partial u}{\partial y} + \gamma_x \dfrac{\partial v}{\partial x}\right) + \tau'_{zx}\left(\gamma_z \dfrac{\partial u}{\partial z} + \gamma_x \dfrac{\partial w}{\partial x}\right) + \tau'_{zy}\left(\gamma_z \dfrac{\partial v}{\partial z} + \gamma_y \dfrac{\partial w}{\partial y}\right) \end{array} \right]. \quad (5.160)$$

is considered to be a generation of turbulent kinetic energy, a turbulence source term. It is removed from the energy conservation and introduced as a source term in the balance equation for the turbulent kinetic energy. Inserting the *Reynolds* stresses by using the *Boussinesq* (1877) hypothesis results in common notation for Cartesian and cylindrical coordinates

$$\gamma_v \overline{P_{k,l}} := \gamma_v \frac{\alpha_l P_{k,l}}{\alpha_l^e \nu_l^t} = 2\left\{\gamma_r \left(\frac{\partial u_l}{\partial r}\right)^2 + \gamma_\theta \left[\frac{1}{r^\kappa}\left(\frac{\partial v_l}{\partial \theta} + \kappa u_l\right)\right]^2 + \gamma_z \left(\frac{\partial w_l}{\partial z}\right)^2\right\}$$

$$-\frac{2}{3}(\nabla.\mathbf{V}_l)(\gamma\nabla.\mathbf{V}_l) + \tilde{S}_{k,l}^2. \quad (5.161)$$

Compare this expression with Eqs. (5.153) and (5.154) and recognize the difference.

An alternative notation of the Eq. (5.161) is given for isotropic turbulence

$$\alpha_l^e \gamma\left(\mathbf{T}' : \nabla \mathbf{V}_l\right) = -\alpha_l^e \rho_l \frac{2}{3} k_l \gamma\nabla.\mathbf{V}_l + \alpha_l^e \rho_l \nu_l^t \tilde{S}_{k,l}^2. \quad (5.162)$$

Nothing that the pressure pulsation caused the eddies is

$$p' = \rho_l V_l'^2 = \rho_l \frac{2}{3} k_l \quad (5.163)$$

the term

$$\alpha_l \rho_l \frac{2}{3} k_l \gamma\nabla.\mathbf{V}_l \equiv p\mathrm{d}Vol\text{-work} \quad (5.164)$$

is immediately recognized as the mechanical expansion or compression *p*d*Vol*-work.

For the case of steady-state single-phase, $\alpha_l = 1$, incompressible ($\nabla \mathbf{V}_l = 0$), isentropic, and developed flow, $P_{k,l} + \varepsilon'_l = 0$, with equal velocity gradients in all directions, *Taylor* (1935) noticed that

$$\varepsilon_l \approx 12\nu_l \left(\frac{\partial w_l}{\partial z}\right)^2. \quad (5.165)$$

The modeling of turbulence in multi-phase flows constitutes an exciting challenge for theoreticians and experimental scientists. We collect useful information to this subject in Volume 3 of this monograph.

Problem 1: Compute the power dissipation in *laminar* flow inside a pipe.

Solution to problem 1: For axially symmetric flow in a pipe the Eqs. (5.163) and (5.152) reduce to

$$-\alpha_l^e \rho_l \varepsilon_{\eta,l} = \frac{1}{Vol}\int\limits_{Vol} \alpha_l^e \left(\mathbf{T}_{\eta,l} : \nabla \mathbf{V}_l\right) dVol = \frac{4}{\pi D_h^2 \Delta z}\int\limits_0^{\Delta z}\int\limits_0^{R_h} \alpha_l^e \left(\mathbf{T}_{\eta,l} : \nabla \mathbf{V}_l\right) 2\pi r\, dr\, dz$$

$$= \int\limits_0^1\int\limits_0^1 \alpha_l^e \left(\mathbf{T}_{\eta,l} : \nabla \mathbf{V}_l\right) d\left(r/R_h\right)^2 d\left(z/\Delta z\right) \tag{5.166}$$

$$-\alpha_l^e \rho_l \varepsilon_l' = \frac{1}{Vol}\int\limits_{Vol} \alpha_l^e \left(\mathbf{T}_l' : \nabla \mathbf{V}_l'\right) dVol = \int\limits_0^1\int\limits_0^1 \alpha_l^e \left(\mathbf{T}_l' : \nabla \mathbf{V}_l'\right) d\left(r/R_h\right)^2 d\left(z/\Delta z\right). \tag{5.167}$$

For a single-phase flow Eq. (5.166) reduces to

$$\rho_l \varepsilon_{\eta,l} = \int\limits_0^1 \left(\frac{dw}{dr}\right)^2 d\left(r/R_h\right)^2 . \tag{5.168}$$

As an illustration of how to estimate the above integral, laminar flow in a pipe in line with the *Hagen-Poiseuille* law will now be considered, with the velocity distribution

$$w\left(r\right) = -\frac{dp}{dz}\frac{1}{4\eta}\left(R_h^2 - r^2\right), \tag{5.169}$$

$$\rho \varepsilon_k = \left(\frac{dp}{dz}\right)^2 \frac{D_h^2}{32\eta}. \tag{5.170}$$

Bearing in mind that

$$\frac{dp}{dz} = 32\eta \overline{w} / D_h^2 , \tag{5.171}$$

one then obtains

$$\rho \varepsilon_k = \overline{w}\frac{dp}{dz} , \tag{5.172}$$

i.e., the *frictional pressure loss per unit mixture volume multiplied by the averaged flow velocity gives the irreversible part of the dissipated energy due to friction per unit time and unit flow volume*. There are a number of industrial processes where this component is important, e.g., heating of liquid in a circuit due to heat dissipation from pumping, and gas flow in very long pipes.

Problem 2: Compute the power dissipation in *turbulent* flow inside a pipe.

Solution to problem 2: The predominant cross section averaged velocity is $\overline{w}$. The *irreversible dissipated power* per unit flow volume caused by the viscous forces is $\rho\left(\varepsilon_\eta + \varepsilon'\right)$. The *irreversible dissipated power* per unit flow volume caused by the viscous forces *due to deformation of the mean values of the velocities* in the space is $\rho\varepsilon_\eta = \left(\mathbf{T}_\eta : \nabla \cdot \mathbf{V}\right)$. In case of turbulence flow the second component, the *irreversibly dissipated power* per unit flow volume in the viscous fluid due to *turbulent pulsations* is $\rho\varepsilon' = \left(\mathbf{T}' : \nabla \cdot \mathbf{V}'\right)$. The friction force per unit flow volume can be computed in this case using correlations based on the macroscopic flow,

$$f_w = \frac{\lambda_{fr}}{D_{hyd}} \frac{1}{2} \rho \overline{w}^2 . \tag{5.173}$$

The power per unit flow volume needed to overcome this force is $f_w \overline{w}$. Therefore

$$f_w w = \rho\left(P_k + \varepsilon_\eta + \varepsilon'\right) = \left(\mathbf{T}' : \nabla \cdot \mathbf{V}\right) + \left(\mathbf{T}_\eta : \nabla \cdot \mathbf{V}\right) + \left(\mathbf{T}' : \nabla \cdot \mathbf{V}'\right). \tag{5.174}$$

With other words, in turbulent flow there are two components of the mechanical energy dissipation: the viscous dissipation mainly in the viscous sub-layer where the velocity gradient possesses a maximum and the dissipation due to disappearing of microscopic eddies. In the flow considered here the following simplification can be used

$$\mathbf{T}_\eta : \nabla \cdot \mathbf{V} \approx \rho\nu \left(\frac{d\overline{w}}{dy}\right)^2 , \tag{5.175}$$

$$\left(\mathbf{T}' : \nabla \cdot \mathbf{V}'\right) \approx 0 . \tag{5.176}$$

Within the laminar sub-layer, $y^+ \le 5$, there is no turbulence energy dissipation, $\mathbf{T}' : \nabla \cdot \mathbf{V}' = 0$. In this region the velocity is linear function of the wall distance $w^+ = y^+$ or $w = y \frac{\overline{w}^2}{\nu} \frac{\lambda_{fr}}{8}$, $\frac{dw}{dy} = \frac{\overline{w}^2}{\nu} \frac{\lambda_{fr}}{8}$ and consequently

$$\mathbf{T}_\eta : \nabla \cdot \mathbf{V} \approx \rho \frac{\overline{w}^4}{\nu} \left(\frac{\lambda_{fr}}{8}\right)^2 . \tag{5.177}$$

The ratio of the viscous boundary layer volume to the total flow volume is

$$\frac{\Pi \Delta z y_{\lim}}{F_{flow} \Delta z} = \frac{4 y_{\lim}}{D_h} . \tag{5.178}$$

Here Π is the wetted perimeter and F_{flow} is the flow cross section. The *irreversible dissipated power* per unit flow *volume* caused by the viscous forces *due to deformation of the mean values of the velocities* in the space is then approximately

$$\rho\varepsilon_\eta = \frac{\Pi\Delta z}{F_{flow}\Delta z}\int_0^{y_{\lim}}\left(\mathbf{T}:\nabla\cdot\mathbf{V}\right)dy = \frac{4y_{\lim}}{D_h}\rho\frac{\overline{w}^4}{\nu}\left(\frac{\lambda_{fr}}{8}\right)^2 . \tag{5.179}$$

From $f_w w = \rho\left(P_k + \varepsilon_\eta + \varepsilon\right)$ we compute *irreversibly dissipated power* per unit flow volume in the viscous fluid due to *turbulent pulsations*

$$\rho P_k = f_w w - \rho\varepsilon_\eta - \rho\varepsilon' \tag{5.180}$$

or

$$\rho P_k = \frac{\lambda_{fr}}{D_h}\frac{1}{2}\rho\overline{w}^3\left(1 - y_{\lim}^{+}\sqrt{\frac{\lambda_{fr}}{8}}\right), \tag{5.181}$$

compare with *Chandesris* et al. (2005). In Volume 3 I will extend this method to multiphase flows.

5.13 Temperature equation

The purpose of this section is to rewrite the entropy equation in terms of the field temperature and system pressure. It will be shown that the temperature and pressure changes do not depend on the absolute values of the specific component entropies, and therefore on the selection of the reference temperature and pressure to define the zero specific entropies. Important differences between mixtures of perfect and non-perfect gases will also be demonstrated.

In Chapter 3 the relationship between the field temperature, T_l, and the field properties $\left(s_l, C_{il}, p\right)$, Eq. (3.106), is found to be

$$c_{pl}\frac{dT_l}{T_l} - \overline{R}_l\frac{dp_l}{p_l} = ds_l - \sum_{i=2}^{i_{\max}}\left(\frac{\partial s_l}{\partial C_{il}}\right)_{p,T_l,all\_C's\_except\_C_{il}} dC_{il}, \tag{5.182}$$

where

$$\left(\frac{\partial s}{\partial C_i}\right)_{p,T,all\_C's\_except\_C_i} = s_{il} - s_{1l} + \Delta s_{il}^{np} . \tag{5.183}$$

One of the mass concentrations, arbitrarily numbered with subscript 1, C_{1l}, depends on all others and is computed as all others are known,

$$C_{1l}=1-\sum_{i=2}^{i_{\max}}C_{il}\,. \tag{5.184}$$

Equation (3.86) consists of two parts. For the case of a mixture consisting of ideal gases the second part is equal to zero,

$$\Delta s_{il}^{np}=0\,, \tag{5.185}$$

this also demonstrating the meaning of the subscript *np*, which stands for non-perfect fluid.

The non-conservative form of the entropy equation, Eq. (5.118), is

$$\rho_l\left[\alpha_l\gamma_v\frac{\partial s_l}{\partial\tau}+\left(\alpha_l^e\mathbf{V}_l\gamma\cdot\nabla\right)s_l\right]-\frac{1}{T_l}\nabla\cdot\left(\alpha_l^e\lambda_l^*\gamma\nabla T_l\right)-\nabla.\left\{\alpha_l^e\rho_l\gamma\left[\sum_{i=1}^{i_{\max}}s_{il}D_{il}^*\nabla C_{il}\right]\right\}$$

$$=\gamma_v\left[\frac{1}{T_l}DT_l^N+\sum_{i=1}^{i_{\max}}\mu_{il}\left(s_{il}-s_l\right)\right], \tag{5.186}$$

The non-conservative form of the mass conservation for each component inside the velocity field, Eq. (1.95), is

$$\alpha_l\rho_l\left(\gamma_v\frac{\partial C_{il}}{\partial\tau}+\mathbf{V}_l\gamma\nabla C_{il}\right)-\nabla\left(\alpha_l\rho_lD_{il}^*\gamma\nabla C_{il}\right)=\gamma_v\left(\mu_{il}-C_{il}\mu_l\right). \tag{5.187}$$

The non-conservative form of the entropy equation in terms of temperature and pressure is obtained by multiplying the $i_{\max}-1$ mass conservation equations (5.187) by $s_{il}-s_{1l}+\Delta s_{il}^{np}$ and subtracting them from the equation (5.186). The result is simplified by using

$$\sum_{i=1}^{i_{\max}}\mu_{il}\left(s_{il}-s_l\right)-\sum_{i=2}^{i_{\max}}\left(s_{il}-s_{1l}+\Delta s_{il}^{np}\right)\left(\mu_{il}-C_{il}\mu_l\right)=-\sum_{i=2}^{i_{\max}}\Delta s_{il}^{np}\left(\mu_{il}-C_{il}\mu_l\right), \tag{5.188}$$

namely

$$\rho_l\left[\alpha_l\gamma_v\frac{\partial s_l}{\partial\tau}+\left(\alpha_l^e\mathbf{V}_l\gamma\cdot\nabla\right)s_l\right]-\rho_l\sum_{i=2}^{i_{\max}}\left(s_{il}-s_{1l}+\Delta s_{il}^{np}\right)\left(\alpha_l\gamma_v\frac{\partial C_{il}}{\partial\tau}+\alpha_l^e\mathbf{V}_l\gamma\nabla C_{il}\right)$$

$$-\frac{1}{T_l}\nabla\cdot\left[\alpha_l^e\lambda_l^*\gamma\nabla T_l\right]-\nabla.\left[\alpha_l^e\gamma\left(\sum_{i=1}^{i_{\max}}s_{il}\rho_lD_{il}^*\nabla C_{il}\right)\right]$$

$$+\sum_{i=2}^{i_{\max}}\left(s_{il}-s_{1l}+\Delta s_{il}^{np}\right)\nabla\left(\alpha_l^e\rho_lD_{il}^*\gamma\nabla C_{il}\right)=\gamma_v\left[\frac{1}{T_l}DT_l^N-\sum_{i=2}^{i_{\max}}\Delta s_{il}^{np}\left(\mu_{il}-C_{il}\mu_l\right)\right]. \tag{5.189}$$

Further simplification is obtained by using

$$\rho_l\left[\alpha_l\gamma_v\frac{\partial s_l}{\partial\tau}+\left(\alpha_l^e\mathbf{V}_l\gamma\cdot\nabla\right)s_l\right]$$

$$-\rho_l\sum_{i=2}^{i_{\max}}\left(\frac{\partial s_l}{\partial C_{il}}\right)_{p,T_l,all\_C's\_except\_C_{il}}\left(\alpha_l\gamma_v\frac{\partial C_{il}}{\partial\tau}+\alpha_l^e\mathbf{V}_l\gamma\nabla C_{il}\right)$$

$$=\left\{\rho_l c_{pl}\left[\alpha_l\gamma_v\frac{\partial T_l}{\partial\tau}+\left(\alpha_l^e\mathbf{V}_l\gamma\cdot\nabla\right)T_l\right]-\frac{\rho_l\bar{R}_lT_l}{p}\left[\alpha_l\gamma_v\frac{\partial p}{\partial\tau}+\left(\alpha_l^e\mathbf{V}_l\gamma\cdot\nabla\right)p\right]\right\}/T_l,\tag{5.190}$$

where Eq. (3.121) is

$$\frac{\rho_l\bar{R}_lT_l}{p}=\left[1-\rho_l\left(\frac{\partial h_l}{\partial p}\right)_{T_l,all\_C's}\right].\tag{5.191}$$

The last two terms of the left-hand side are simplified by using Eq. (5.103)

$$\nabla.\left[\alpha_l^e\gamma\left(\sum_{i=1}^{i_{\max}}s_{il}\rho_lD_{il}^*\nabla C_{il}\right)\right]-\sum_{i=2}^{i_{\max}}\left(s_{il}-s_{1l}+\Delta s_{il}^{np}\right)\nabla\left(\alpha_l^e\rho_lD_{il}^*\gamma\nabla C_{il}\right)$$

$$=\nabla.\left[\alpha_l^e\gamma\left(\sum_{i=2}^{i_{\max}}\left(s_{il}-s_{1l}\right)\rho_lD_{il}^*\nabla C_{il}\right)\right]-\sum_{i=2}^{i_{\max}}\left(s_{il}-s_{1l}+\Delta s_{il}^{np}\right)\nabla\left(\alpha_l^e\rho_lD_{il}^*\gamma\nabla C_{il}\right)$$

$$=\alpha_l^e\rho_l\gamma\sum_{i=2}^{i_{\max}}\left(D_{il}^*\nabla C_{il}\right)\nabla\left(s_{il}-s_{1l}\right)-\sum_{i=2}^{i_{\max}}\Delta s_{il}^{np}\nabla\left(\alpha_l^e\rho_lD_{il}^*\gamma\nabla C_{il}\right)\tag{5.192}$$

Neglecting the second order terms

$$\alpha_l^e\rho_l\gamma\sum_{i=2}^{i_{\max}}\left(D_{il}^*\nabla C_{il}\right)\nabla\left(s_{il}-s_{1l}\right),\tag{5.193}$$

we obtain the form below that is very convenient for practical applications

$$\rho_lc_{pl}\left[\alpha_l\gamma_v\frac{\partial T_l}{\partial\tau}+\left(\alpha_l^e\mathbf{V}_l\gamma\cdot\nabla\right)T_l\right]$$

$$-\nabla\cdot\left(\alpha_l^e\lambda_l^*\gamma\nabla T\right)-\left[1-\rho_l\left(\frac{\partial h_l}{\partial p}\right)_{T_l,all\_C's}\right]\left[\alpha_l\gamma_v\frac{\partial p}{\partial\tau}+\left(\alpha_l^e\mathbf{V}_l\gamma\cdot\nabla\right)p\right]$$

$$\boxed{+T_l\sum_{i=2}^{i_{\max}}\Delta s_{il}^{np}\nabla\left(\alpha_l^e\rho_l D_{il}^*\gamma\nabla C_{il}\right)=\gamma_v\left[DT_l^N-T_l\sum_{i=2}^{i_{\max}}\Delta s_{il}^{np}\left(\mu_{il}-C_{il}\mu_l\right)\right].\quad(5.194)}$$

This is the entropy equation rewritten in terms of temperature and pressure. For perfect gas mixtures, the following is obtained

$$\rho_l c_{pl}\left[\alpha_l\gamma_v\frac{\partial T_l}{\partial\tau}+\left(\alpha_l^e\mathbf{V}_l\gamma\cdot\nabla\right)T_l\right]-\nabla\cdot\left(\alpha_l^e\lambda_l^*\gamma\nabla T\right)$$

$$-\left[\alpha_l\gamma_v\frac{\partial p}{\partial\tau}+\left(\alpha_l^e\mathbf{V}_l\gamma\cdot\nabla\right)p\right]=\gamma_v DT_l^N. \qquad (5.195)$$

Conclusions:

a) The temperature change caused by the injection into the velocity field depends on the difference between the specific enthalpy of the donor and the specific enthalpy of the velocity field. It is important to note that this is an *enthalpy difference* but not, say, differences in the specific internal energies, entropies, etc.

b) Equation (5.194) does not contain any specific entropies. As a result, the temperature change described by Eq. (5.194) does not depend on the reference temperature and pressure for computation of the specific entropies for the specific components.

c) Consider diffusion in a gas mixture consisting of non-perfect gases in adiabatic closed space. The initial state is characterized by spatially uniform temperature. At nearly constant system pressure Eq. (5.194) reduces to

$$\gamma_v\rho_l c_{pl}\frac{\partial T_l}{\partial\tau}\approx -T_l\sum_{i=2}^{i_{\max}}\Delta s_{il}^{np}\nabla\left(\rho_l D_{il}^*\gamma\nabla C_{il}\right), \qquad (5.196)$$

which demonstrates that a temporal temperature change takes place at the locations of considerable diffusion. Bad numerical resolution can amplify this effect, leading to considerable local error in the numerical analysis.

d) Injection of non-perfect gas components into a volume initially filled with perfect gas can also give rise to behavior different from that of injection of a perfect gas component, due to the differences in the temperature and pressure equations describing both cases. This will be demonstrated in a simple case in the next section.

5.14 Second law of the thermodynamics

The entropy equation reflects very interesting physical phenomena. It is evident that velocity gradients in continuum of viscous fluid cause energy dissipation, $\varepsilon_{\eta,l}+\varepsilon_l'\geq 0$, and may generate turbulent kinetic energy $P_{k,l}\geq 0$. The turbulent kinetic energy increases the turbulent viscosity according to the *Prandtl-Kolmogorov* law, and helps to reduce the velocity gradients. The irreversible dissipation of kinetic energy caused by the turbulent pulsation increases the specific internal energy of the continuum field, $\varepsilon_l' \geq 0$. This dissipation decreases the specific turbulent kinetic energy directly. The same action is caused by the direct viscous dissipation $\varepsilon_{\eta,l}$.

If the equation is applied to a single velocity field in a closed system without interaction with external mass, momentum or energy sources, the change in the specific entropy of the system will be non-negative, as the sum of the dissipation terms, $\varepsilon_{\eta,l} + \varepsilon_l'$, is non-negative. This expresses the *second law of thermodynamics*. The second law tells us in what direction a process will develop in nature for closed and isolated systems.

The process will proceed in a direction such that the entropy of the system always increases, or at best stays the same, $\varepsilon_{\eta,l} + \varepsilon_l' = 0$, - entropy principle.

This information is not contained in the first law of thermodynamics. It results only after combining the three conservation principles (mass, momentum and energy) and introducing a *Legendre* transformation in the form of a *Gibbs* equation. In a way, it is a general expression of these conservation principles.

The entropy equation is not only very informative, but as already mentioned, it is very convenient for numerical integration because of its *simplicity* compared to the primitive form of the energy principle. This is the reason why the *specific entropies* of the velocity fields together with the concentrations of the inert component C_{nl} were chosen for use as *components of the dependent variables* vector as already mentioned in *Kolev* (1994a). This unique combination of the dependent variables *simply minimizes the computational effort* associated with numerical integration and therefore makes the computer code *faster* and the analysis *cheaper*. It also makes the computer code architecture simple and allows the inclusion of more physical phenomena within a general flow model.

I call the flow modeling concept which makes use of the specific entropies of the velocity fields as components of the dependent variables vector the *entropy concept*.

5.15 Mixture volume conservation equation

Any numerical method in fluid mechanics should provide correct coupling between pressure changes and velocity changes. There are different ways of achieving this. One of these is faster than the others. Probably the fastest of these methods uses a specially derived equation, referred to as here the *mixture volume conservation equation*, MVCE. The MVCE is a linear combination of the mass conservation equations. The purpose of this section is to derive the analytical form of the MVCE, to discuss the physical meaning of each separate term and finally to show the reasons that make this equation so appropriate for use in constructing numerical schemes for complicated multi-phase flows.

The MVCE was obtained as follows:

(a) The mass conservation equations (1.62) were differentiated using the chain rule.
(b) Each equation was divided by the associated density. The resulting equations are dimensionless, m^3/m^3, and reflect the volume change balance for each velocity field per unit time and per unit mixture volume.

$$\gamma_v \frac{\partial \alpha_l}{\partial \tau} + \alpha_l \frac{\partial \gamma_v}{\partial \tau} + \frac{1}{\rho_l}\left[\alpha_l \gamma_v \frac{\partial \rho_l}{\partial \tau} + \left(\alpha_l \mathbf{V}_l \gamma \cdot \nabla\right)\rho_l\right] + \nabla \cdot \left(\alpha_l \mathbf{V}_l \gamma\right) = \gamma_v \frac{\mu_l}{\rho_l} \qquad (5.197)$$

(c) The volume conservation equations obtained in this way were added and the fact that

$$\sum_{l=1}^{3} \alpha_l = 1 \qquad (5.198)$$

and

$$\sum_{l=1}^{3} d\alpha_l = 0 \qquad (5.199)$$

was used to cancel the sum of the time derivatives of the volume concentrations.

$$\sum_{l=1}^{l_{\max}} \frac{1}{\rho_l}\left[\alpha_l \gamma_v \frac{\partial \rho_l}{\partial \tau} + \left(\alpha_l \mathbf{V}_l \gamma \cdot \nabla\right)\rho_l\right] + \nabla \cdot \sum_{l=1}^{l_{\max}} \left(\alpha_l \mathbf{V}_l \gamma\right) = \gamma_v \sum_{l=1}^{l_{\max}} \frac{\mu_l}{\rho_l} - \frac{\partial \gamma_v}{\partial \tau} \qquad (5.200)$$

(d) The density derivatives were substituted using the differential form of the equation of state for each velocity field (3.137)

$$d\rho_l = \frac{dp_l}{a_l^2} + \left(\frac{\partial \rho_l}{\partial s_l}\right)_{p,all\_C_l's} ds_l + \sum_{i=2}^{i_{\max}} \left(\frac{\partial \rho_l}{\partial C_{li}}\right)_{p,s,all\_C_l's\_except\_C_{li}} dC_{li}\,. \qquad (5.201)$$

The result is

$$\gamma_v \left(\sum_{l=1}^{l_{\max}} \frac{\alpha_l}{\rho_l a_l^2} \frac{\partial p_l}{\partial \tau}\right) + \sum_{l=1}^{l_{\max}} \left[\frac{\alpha_l}{\rho_l a_l^2}\left(\mathbf{V}_l \gamma \cdot \nabla\right) p_l\right] + \nabla \cdot \sum_{l=1}^{l_{\max}} \left(\alpha_l \mathbf{V}_l \gamma\right)$$

$$= \sum_{l=1}^{l_{\max}} \frac{1}{\rho_l} \left\{ \gamma_v \mu_l - \frac{1}{\rho_l} \left\{ \begin{array}{l} \left(\dfrac{\partial \rho_l}{\partial s_l} \right)_{p, all\_C_l' s} \rho_l \left[\alpha_l \gamma_v \dfrac{\partial s_l}{\partial \tau} + \left(\alpha_l \mathbf{V}_l \gamma \cdot \nabla \right) s_l \right] \\ + \sum\limits_{i=2}^{i_{\max}} \left(\dfrac{\partial \rho_l}{\partial C_{li}} \right)_{p,s,all\_C's\_except\_C_i} \rho_l \left[\alpha_l \gamma_v \dfrac{\partial C_{li}}{\partial \tau} + \left(\alpha_l \mathbf{V}_l \gamma \cdot \nabla \right) C_{li} \right] \end{array} \right\} \right\}$$

$$- \frac{\partial \gamma_v}{\partial \tau} \tag{5.202}$$

(e) The concentration equations (1.96) in Chapter 1 and the non-conservative form of the entropy equation (5.118) in this Chapter are compared with the LHS of Eq. (5.202). Making the substitution

$$\rho_l \left[\alpha_l \gamma_v \frac{\partial C_{il}}{\partial \tau} + \left(\alpha_l^e \mathbf{V}_l \gamma . \nabla \right) C_{il} \right] = DC_{il}^N , \tag{5.203}$$

$$\rho_l \left[\alpha_l \gamma_v \frac{\partial s_l}{\partial \tau} + \left(\alpha_l^e \mathbf{V}_l \gamma . \nabla \right) s_l \right] = Ds_l^N , \tag{5.204}$$

where

$$\overline{DC_{il}^N} = \nabla \left(\alpha_l \rho_l D_{il}^* \gamma \nabla C_{il} \right) + \gamma_v \left(\mu_{il} - C_{il} \mu_l \right) , \tag{5.205}$$

$$\overline{Ds_l^N} = \frac{1}{T_l} \nabla \cdot \left(\alpha_l^e \lambda_l^* \gamma \nabla T_l \right) + \nabla . \left\{ \alpha_l^e \rho_l \gamma \left[\sum_{i=1}^{i_{\max}} s_{il} D_{il}^* \nabla C_{il} \right] \right\}$$

$$+ \gamma_v \left[\frac{1}{T_l} DT_l^N + \sum_{i=1}^{i_{\max}} \mu_{il} \left(s_{il} - s_l \right) \right] , \tag{5.206}$$

we obtain the final form for the MVCE

$$\gamma_v \left(\sum_{l=1}^{l_{\max}} \frac{\alpha_l}{\rho_l a_l^2} \frac{\partial p_l}{\partial \tau} \right) + \sum_{l=1}^{l_{\max}} \left[\frac{\alpha_l}{\rho_l a_l^2} \left(\mathbf{V}_l \gamma \cdot \nabla \right) p_l \right] + \nabla \cdot \sum_{l=1}^{l_{\max}} \left(\alpha_l \mathbf{V}_l \gamma \right) = \sum_{l=1}^{l_{\max}} D\alpha_l - \frac{\partial \gamma_v}{\partial \tau}$$

which for negligible differences in the field pressures is

$$\boxed{\frac{\gamma_v}{\rho a^2} \frac{\partial p}{\partial \tau} + \sum_{l=1}^{l_{\max}} \frac{\alpha_l}{\rho_l a_l^2} \left(\mathbf{V}_l \gamma \cdot \nabla \right) p + \nabla \cdot \sum_{l=1}^{l_{\max}} \left(\alpha_l \mathbf{V}_l \gamma \right) = \sum_{l=1}^{l_{\max}} D\alpha_l - \frac{\partial \gamma_v}{\partial \tau} , \qquad (5.207)}$$

or in scalar form for practical application in Cartesian and cylindrical coordinates

$$\frac{\gamma_v}{\rho a^2} \frac{\partial p}{\partial \tau} + \sum_{l=1}^{3} \frac{\alpha_l}{\rho_l a_l^2} \left(u_l \gamma_r \frac{\partial p}{\partial r} + v_l \gamma_\theta \frac{\partial p}{\partial \theta} + w_l \gamma_z \frac{\partial p}{\partial z} \right)$$

$$+\frac{\partial}{\partial r}\left(\alpha_l u_l \gamma_r\right)+\frac{1}{r^\kappa}\frac{\partial}{\partial \theta}\left(r^\kappa \alpha_l v_l \gamma_\theta\right)+\frac{\partial}{\partial z}\left(\alpha_l w_l \gamma_z\right)=\sum_{l=1}^{3} D\alpha_l-\frac{\partial \gamma_v}{\partial \tau} \tag{5.208}$$

where

$$D\alpha_l=\frac{1}{\rho_l}\left\{\gamma_v\mu_l-\frac{1}{\rho_l}\left[\left(\frac{\partial \rho_l}{\partial s_l}\right)_{p,all\_C_{li}'s}\overline{Ds_l^N}+\sum_{i=2}^{i_{\max}}\left(\frac{\partial \rho_l}{\partial C_{li}}\right)_{p,s,all\_C_{li}'s\_except\_C_{l1}}\overline{DC_{il}^N}\right]\right\} \tag{5.209}$$

Replacing the derivatives of the mixture density with the Eqs. (110) and (111) obtained in *Kolev* (1991), one obtains

$$D\alpha_l=\gamma_v\frac{\mu_l}{\rho_l}-\frac{1}{\rho_l^2}\left[\begin{array}{l}\left(\frac{\partial \rho_l}{\partial T_l}\right)_{p,all\_C's}\frac{T_l}{c_{pl}}\left[\overline{Ds_l^N}-\sum_{i=2}^{i_{\max}}\left(\frac{\partial s_l}{\partial C_{il}}\right)_{p,T_l,all\_C's\_except\_C_{il}}\overline{DC_{il}^N}\right]\\ +\sum_{i=2}^{i_{\max}}\left(\frac{\partial \rho_l}{\partial C_{il}}\right)_{p,T_l,all\_C's\_except\_C_{il}}\overline{DC_{il}^N}\end{array}\right]. \tag{5.210}$$

Further simplification is obtained by using Eqs. (5.205) and (5.206), subsequently the chain rules and neglecting the second order term

$$\alpha_l\rho_l\gamma T_l\sum_{i=2}^{i_{\max}}\nabla\left(D_{il}^*\nabla C_{il}\right)\nabla\left(s_{il}-s_{1l}\right). \tag{5.211}$$

The result is

$$T_l\left[\overline{Ds_l^N}-\sum_{i=2}^{i_{\max}}\left(\frac{\partial s_l}{\partial C_{il}}\right)_{p,T_l,all\_C's\_except\_C_{il}}\overline{DC_{il}^N}\right]$$

$$\approx\nabla\cdot\left(\alpha_l^e\lambda_l^*\gamma\nabla T\right)+\gamma_v DT_l^N-T_l\sum_{i=2}^{i_{\max}}\Delta s_{il}^{np}\left[\nabla\left(\alpha_l^e\rho_l D_{il}^*\gamma\nabla C_{il}\right)+\gamma_v\left(\mu_{il}-C_{il}\mu_l\right)\right], \tag{5.212}$$

For perfect gas mixtures the following alone is obtained

$$T_l\left[\overline{Ds_l^N}-\sum_{i=2}^{i_{\max}}\left(\frac{\partial s_l}{\partial C_{il}}\right)_{p,T_l,all\_C's\_except\_C_{il}}\overline{DC_{il}^N}\right]\approx\nabla\cdot\left(\alpha_l^e\lambda_l^*\gamma\nabla T\right)+\gamma_v\overline{DT_l^N} \tag{5.213}$$

a is the *sonic velocity* in a homogeneous multi-phase mixture and is defined as follows

$$\frac{1}{\rho a^2} = \sum_{l=1}^{3} \frac{\alpha_l}{\rho_l a_l^2} = \frac{1}{p} \sum_{l=1}^{3} \frac{\alpha_l}{\kappa_l} = \frac{1}{\kappa p}, \tag{5.214}$$

and

$$\rho = \sum_{l=1}^{3} \alpha_l \rho_l \tag{5.215}$$

is the mixture density. Equation (5.207) was already derived in *Kolev* (1986) and published in *Kolev* (1987) p.100.

The MVCE equation can be directly discretized and incorporated into the numerical scheme. Another possibility is to follow the same scheme as for deriving the MVCE analytically but starting with already discretized mass conservation equations. The coupling finally obtained is then *strictly consistent* with the discretized form of the mass conservation equations.

Alternative forms of the MVCE can also be used, e.g.

$$\frac{\gamma_v}{\kappa p} \frac{\partial p}{\partial \tau} + \sum_{l=1}^{3} \frac{\alpha_l}{\kappa_l p} \mathbf{V}_l \gamma . \nabla p + \nabla . \left(\sum_{l=1}^{3} \alpha_l \mathbf{V}_l \gamma \right) = \sum_{l=1}^{3} D\alpha_l - \frac{\partial \gamma_v}{\partial \tau}, \tag{5.216}$$

or certain integrated forms

$$\frac{\gamma_v}{\kappa} \frac{\partial}{\partial \tau} \ln p + \sum_{l=1}^{3} \frac{\alpha_l}{\kappa_l} \mathbf{V}_l \gamma . \nabla \ln p + \nabla . \left(\sum_{l=1}^{3} \alpha_l \mathbf{V}_l \gamma \right) = \sum_{l=1}^{3} D\alpha_l - \frac{\partial \gamma_v}{\partial \tau}, \tag{5.217}$$

where

$$\kappa = \rho a^2 / p, \tag{5.218}$$

$$\kappa_l = \rho_l a_l^2 / p \tag{5.219}$$

are the mixture isentropic exponent and the isentropic exponent of each particular velocity field, respectively.

For completeness of the theory the MVCE equation valid in the case of steady-state non-compressible flow will also be given

$$\nabla . \left(\sum_{l=1}^{3} \alpha_l \mathbf{V}_l \gamma \right) = \nabla . \left(\mathbf{J} \gamma \right) = \sum_{l=1}^{3} D\alpha_l, \tag{5.220}$$

where

$$\mathbf{J} = \sum_{l=1}^{3} \alpha_l \mathbf{V}_l = \sum_{l=1}^{3} j_l \tag{5.221}$$

is the *volumetric mixture flow rate* in *$m^3/(m^2 s)$*. If diffusion is neglected and no mass exchange takes place between the velocity fields or between the flow and external sources, this gives

$$\nabla . \left(\mathbf{J} \gamma \right) = 0 \tag{5.222}$$

or

$$\mathbf{J}\gamma = const\,. \tag{5.223}$$

The MVCE has the remarkable feature that it couples the temporal pressure change through the compressibility $1/\left(\rho a^2\right)$ with

a) the convective specific volume change $\nabla.\left(\sum_{l=1}^{3}\alpha_l \mathbf{V}_l \gamma\right)$ for the control volume;

b) the change in the specific volume of the mixture associated with the net specific volume change for the mixture due to the mass sources $\gamma_v \sum_{l=1}^{3} \mu_l / \rho_l$;

c) the density change due to the spatial pressure, entropy and concentration changes for the associated velocity field.

Another specific property of Eq. (5.207) should be emphasized. The second term on the left-hand side represents the dimensionless changes in the density. This fact allows one to use *up-wind* discretization even for the pressure terms (*donor-cell* concept), because one in fact discretizes the dimensionless density change within the interval $\Delta r, \Delta\theta, \Delta z$.

The above features of this equation make it very suitable for coupling with the momentum equations in order to derive an equation for the mixtures which is similar to the *Poisson* equation for single-phase flow.

For the case of negligible diffusion the right-hand side of the MVCE contains no differential terms:

$$D\alpha_l = \frac{\gamma_v}{\rho_l}\left\{\mu_l - \left[\frac{\partial\rho_l}{\partial s_l}\left(Ds_l - \mu_l^+ s_l\right) + \sum_{i=1}^{i_{\max}} \frac{\partial\rho_l}{\partial C_{li}}\left(\mu_{li} - \mu_{li}^+ C_{li}\right)\right] / \rho_l\right\}. \tag{5.224}$$

This means that during numerical integration the influence of the changes of entropies and concentrations on the pressure field can be taken into account in a single step only (without outer iterations). The computer code architecture is thus extremely simplified, speeding up the numerical integration and therefore making it cheaper. This is an important feature of the entropy concept presented here and used in the IVA computer code development compared to the concepts of other computer codes, e.g. TRAC *Liles* et al. (1978, 1981), COBRA-TF *Kelly* and *Kohrt* (1983), COBRA/TRAC *Thurgood* et al. (1983) and AFDM *Bohl* et al. (1988).

The right-hand side of the pressure equation, Eq. (5.207), does not contain any specific entropy. As a result, the pressure change described by Eq. (5.207) is not dependent on the reference temperature and pressure for computation of the specific entropies for the specific components.

Comparing Eqs. (5.212) and (5.213) it is evident that if systems in which at least one of the gas components deviates from the perfect gas behavior are approximated as consisting of perfect gasses, an entropy imbalance of about

$$-\sum_{i=2}^{i_{\max}} \Delta s_{il}^{np}\left[\nabla\left(\alpha_l^e \rho_l D_{il}^* \gamma \nabla C_{il}\right) + \gamma_v\left(\mu_{il} - C_{il}\mu_l\right)\right] \tag{5.225}$$

is introduced. This is a very surprising result. I call this result the *non-perfect gas paradox*.

5.16 Linearized form of the source term for the temperature equation

The source terms with fluctuation components neglected

$$DT_l^N = \alpha_l \rho_l \left(\delta_l P_{\eta,l}^{\tau} + \varepsilon_l \right) + \dot{q}''' + \sum_{i=1}^{i_{\max}} \mu_{iwl} \left(h_{iwl} - h_{il} \right)$$

$$+ \sum_{m=1}^{3} \left[\mu_{Mml} \left(h_{Ml}^{\sigma} - h_{Ml} \right) + \sum_{n=1}^{n_{\max}} \mu_{nml} \left(h_{nm} - h_{nl} \right) \right] \quad (5.226)$$

will be next rewritten for each velocity field in a form that allows the use of implicit integration schemes. The conditions governing heat and mass transfer can change during the time step, thereby influencing the averaged rate for the transported quantity. This feedback effect during a single time step may be crucial in the case of a number of applications associated with strong heat and mass transfer processes. The first work known to this author formalizing source terms is those by *Solbrig* et al. published in 1977. *Solbrig* et al. considered mass and energy equations in a closed system for two single component phases. The meta-stable state of the phases was not allowed in their work. Instead the pressure depending mass sources are defined adjusting the state of each phase to the saturation with the changing pressure. But even the meta-stable state is the driving force for spontaneous evaporation and condensation, and therefore has to be taken into account as we do in our analysis.

The following definitions and assumptions are used here:

$$c_{pw2} = \sum_{i=1}^{i_{\max}} C_{iw2} c_{piw2} , \quad (5.227)$$

$$c_{pw3} = \sum_{i=1}^{i_{\max}} C_{iw3} c_{piw3} , \quad (5.228)$$

$$c_{p2} = \sum_{i=1}^{i_{\max}} C_{i2} c_{pi2} , \quad (5.229)$$

$$c_{p3} = \sum_{i=1}^{i_{\max}} C_{i3} c_{pi3} , \quad (5.230)$$

$$h_{M1}^{2\sigma} - h_{M1} \approx c_{pM1} \left(T_{M1}^{2\sigma} - T_1 \right) \quad \text{and} \quad p_{M1}^{2\sigma} \approx p_{M1} , \quad (5.231)$$

$$h_{M1}^{3\sigma} - h_{M1} \approx c_{pM1}\left(T_{M1}^{3\sigma} - T_1\right) \quad \text{and} \quad p_{M1}^{3\sigma} \approx p_{M1}, \tag{5.232}$$

$$h_{M2}^{1\sigma} - h_{M2} \approx c_{pM2}\left(T_2^{1\sigma} - T_2\right), \tag{5.233}$$

$$h_{M3}^{1\sigma} - h_{M3} \approx c_{pM3}\left(T_3^{1\sigma} - T_3\right), \tag{5.234}$$

$$C_{M2}\left(h_{M2} - h_{M3}\right) + \sum_{n=1}^{n_{\max}} C_{n2}\left(h_{n2} - h_{n3}\right) \approx c_{p2}\left(T_2 - T_3\right), \tag{5.235}$$

$$C_{M3}\left(h_{M3} - h_{M2}\right) + \sum_{n=1}^{n_{\max}} C_{n3}\left(h_{n3} - h_{n2}\right) \approx c_{p3}\left(T_3 - T_2\right), \tag{5.236}$$

$$\sum_{i=1}^{i_{\max}} C_{i2}\left(h_{iw2} - h_{i2}\right) \approx c_{pw2}\left(T_w - T_2\right), \tag{5.237}$$

$$\sum_{i=1}^{i_{\max}} C_{i3}\left(h_{iw3} - h_{i3}\right) \approx c_{pw3}\left(T_w - T_3\right). \tag{5.238}$$

It is assumed that the properties of the mass leaving the velocity field are equal to the properties of this donor field. Here I introduce the product of the effective heat transfer coefficient and the interfacial area density and designate this by $\chi_l^{m\sigma}$. The subscript l designates the location inside the velocity field l and the superscript $m\sigma$ designates the location at the interface σ dividing field m from field l. Superscripts are only used if the interfacial heat transfer is associated with mass transfer. If there is heat transfer only, the linearized interaction coefficient is assigned the subscript ml only, this indicating the interface at which the heat transfer takes place. These rules are valid also for the wall. Actually, the wall is treated as an additional field. The result is

$$DT_1^N = \alpha_1\rho_1\left(\delta_1 P_{k1}^\tau + \varepsilon_1\right) + \chi_1^{w\sigma}\left(T_1^{w\sigma} - T_1\right) + \left(\mu_{21}^w + \mu_{31}^w\right)c_{pM1}\left(T_{M1}^{w\sigma} - T_1\right)$$

$$+\chi_{w1}\left(T_w - T_1\right) + \chi_{21}\left(T_2 - T_1\right) + \chi_{31}\left(T_3 - T_1\right) + \chi_1^{2\sigma}\left(T_1^{2\sigma} - T_1\right) + \chi_1^{3\sigma}\left(T_1^{3\sigma} - T_1\right)$$

$$+\sum_{i=1}^{i_{\max}} \mu_{iw1}\left(h_{iw1} - h_{i1}\right) + c_{pM1}\left[\mu_{21}\left(T_1^{2\sigma} - T_1\right) + \mu_{31}\left(T_1^{3\sigma} - T_1\right)\right], \tag{5.239}$$

$$DT_2^N = \alpha_2\rho_2\left(\delta_2 P_{k2}^\tau + \varepsilon_2\right) + \chi_2^{w\sigma}\left(T_2^{w\sigma} - T_2\right) + \mu_{12}^w c_{pM2}\left(T_2^{w\sigma} - T_2\right)$$

$$+\left(\chi_{w2} + \mu_{w2}c_{pw2}\right)\left(T_w - T_2\right) + \left(\chi_{32} + \mu_{32}c_{p3}\right)\left(T_3 - T_2\right) - \chi_{21}\left(T_2 - T_1\right)$$

$$+\chi_2^{1\sigma}\left(T_2^{1\sigma} - T_2\right) + \mu_{12}c_{pM2}\left(T_2^{1\sigma} - T_2\right), \tag{5.240}$$

$$DT_3^N = \alpha_3\rho_3\left(\delta_3 P_{k3}^\tau + \varepsilon_3\right) + \chi_3^{w\sigma}\left(T_3^{w\sigma} - T_3\right) + \mu_{13}^w c_{pM3}\left(T_3^{w\sigma} - T_3\right)$$

$$+\left(\chi_{w3} + \mu_{w3} c_{pw3}\right)\left(T_w - T_3\right) - \left(\chi_{32} + \mu_{23} c_{p2}\right)\left(T_3 - T_2\right) - \chi_{31}\left(T_3 - T_1\right)$$

$$+\chi_3^{1\sigma}\left(T_3^{1\sigma} - T_3\right) + \mu_{13} c_{pM3}\left(T_3^{1\sigma} - T_3\right). \tag{5.241}$$

The energy jump condition at the interfaces yields the following for the *condensation* sources

$$\mu_{12} = \psi_{12}\frac{\chi_2^{1\sigma}\left(T_2^{1\sigma} - T_2\right) + \chi_1^{2\sigma}\left(T_1^{2\sigma} - T_1\right)}{h_{M1}^{2\sigma} - h_{M2}^{1\sigma}} \ge 0, \tag{5.242}$$

$$\mu_{13} = \psi_{13}\frac{\chi_3^{1\sigma}\left(T_3^{1\sigma} - T_3\right) + \chi_1^{3\sigma}\left(T_1^{3\sigma} - T_1\right)}{h_{M1}^{3\sigma} - h_{M3}^{1\sigma}} \ge 0, \tag{5.243}$$

for $C_{M1} > 0$. Here the integer switches

$$\psi_{12} = \frac{1}{2}\left\{1 + sign\left[\chi_2^{1\sigma}\left(T_2^{1\sigma} - T_2\right) + \chi_1^{2\sigma}\left(T_1^{2\sigma} - T_1\right)\right]\right\}, \tag{5.244}$$

$$\psi_{13} = \frac{1}{2}\left\{1 + sign\left[\chi_3^{1\sigma}\left(T_3^{1\sigma} - T_3\right) + \chi_1^{3\sigma}\left(T_1^{3\sigma} - T_1\right)\right]\right\} \tag{5.245}$$

guarantee that the mass sources are non-negative. For $C_{M1} = 0$ we have $\mu_{12} = 0$, and $\mu_{13} = 0$ because there is nothing to condense. The energy jump condition at the interfaces yields the following for the *evaporation* sources:

$$\mu_{21} = -\left(1 - \psi_{12}\right)\frac{\chi_2^{1\sigma}\left(T_2^{1\sigma} - T_2\right) + \chi_1^{2\sigma}\left(T_1^{2\sigma} - T_1\right)}{h_{M1}^{2\sigma} - h_{M2}^{1\sigma}} \ge 0, \text{ for } C_{M2} > 0, \tag{5.246}$$

$$\mu_{31} = -\left(1 - \psi_{13}\right)\frac{\chi_3^{1\sigma}\left(T_3^{1\sigma} - T_3\right) + \chi_1^{3\sigma}\left(T_1^{3\sigma} - T_1\right)}{h_{M1}^{2\sigma} - h_{M3}^{1\sigma}} \ge 0, \text{ for } C_{M3} > 0. \tag{5.247}$$

For $C_{M2} = 0$ we have $\mu_{21} = 0$ because there is nothing to evaporate. Similarly for $C_{M3} = 0$ we have $\mu_{31} = 0$.

The mass transfer at heated or cooled walls is defined similarly:

Condensation:

$$\mu_{12}^w = \psi_{12}^w f_{cond \to film}\frac{\chi_w^{1\sigma}\left(T_w^{1\sigma} - T_w\right) + \chi_1^{w\sigma}\left(T_1^{w\sigma} - T_1\right)}{h_{M1}^{2\sigma} - h_{M2}^{1\sigma}} \ge 0, \tag{5.248}$$

$$\mu_{13}^{w} = \psi_{13}^{w}\left(1 - f_{cond \to film}\right)\frac{\chi_{w}^{1\sigma}\left(T_{w}^{1\sigma} - T_{w}\right) + \chi_{1}^{w\sigma}\left(T_{1}^{w\sigma} - T_{1}\right)}{h_{M1}^{3\sigma} - h_{M3}^{1\sigma}} \ge 0 . \qquad (5.249)$$

Here we introduce the factor $f_{cond \to film}$ which determines how much of the condensed vapor is going into the film. For $f_{cond \to film} = 1$ we have film condensation at the wall. For $f_{cond \to film} = 0$ we have droplet condensation at the wall. The decision which of the mechanisms is active depends on the wetability of the surface and its orientation in space.

Evaporation:

$$\mu_{21}^{w} = -\psi_{21}^{w}\frac{\chi_{w}^{2\sigma}\left(T_{w}^{2\sigma} - T_{w}\right) + \chi_{2}^{w\sigma}\left(T_{2}^{w\sigma} - T_{2}\right)}{h_{M1}^{2\sigma} - h_{M2}^{1\sigma}}$$

$$= -\psi_{21}^{w}\frac{\chi_{w}^{2\sigma}\left[T'(p) - T_{w}\right] + \chi_{2}^{w\sigma}\left[T'(p) - T_{2}\right]}{h''(p) - h'(p)} \ge 0 , \text{ for } C_{M2} > 0, \qquad (5.250)$$

$$\mu_{31}^{w} = -\psi_{31}^{w}\frac{\chi_{w}^{3\sigma}\left(T_{w}^{3\sigma} - T_{w}\right) + \chi_{3}^{w\sigma}\left(T_{3}^{w\sigma} - T_{3}\right)}{h_{M1}^{3\sigma} - h_{M3}^{1\sigma}}$$

$$= -\psi_{31}^{w}\frac{\chi_{w}^{3\sigma}\left[T'(p) - T_{w}\right] + \chi_{3}^{w\sigma}\left[T'(p) - T_{3}\right]}{h''(p) - h'(p)} \ge 0 , \text{ for } C_{M3} > 0 . \qquad (5.251)$$

In deriving Eqs. (5.231) and (5.232) the following assumptions are made

$$T_{w}^{2\sigma}, T_{2}^{w\sigma}, T_{w}^{3\sigma}, T_{3}^{w\sigma} = T'(p), \qquad (5.252)$$

$$h_{M1}^{2\sigma}, h_{M1}^{3\sigma} = h''(p), \qquad (5.253)$$

and

$$h_{M2}^{1\sigma}, h_{M3}^{1\sigma} = h'(p). \qquad (5.254)$$

Here again the integer switches

$$\psi_{21}^{w} = \frac{1}{2}\left\{1 - sign\left(\chi_{w}^{2\sigma}\left[T'(p) - T_{w}\right] + \chi_{2}^{w\sigma}\left[T'(p) - T_{2}\right]\right)\right\}, \qquad (5.255)$$

$$\psi_{31}^{w} = \frac{1}{2}\left\{1 - sign\left(\chi_{w}^{3\sigma}\left[T'(p) - T_{w}\right] + \chi_{3}^{w\sigma}\left[T'(p) - T_{3}\right]\right)\right\}, \qquad (5.256)$$

$$\psi_{12}^{w} = \frac{1}{2}\left\{1 + sign\left[\chi_{w}^{1\sigma}\left(T_{w}^{1\sigma} - T_{w}\right) + \chi_{1}^{w\sigma}\left(T_{1}^{w\sigma} - T_{1}\right)\right]\right\}, \qquad (5.257)$$

and conditions for film condensation otherwise $\psi_{12}^{w} = 0$,

$$\psi_{13}^{w} = \frac{1}{2}\left\{1 + sign\left[\chi_{w}^{1\sigma}\left(T_{w}^{1\sigma} - T_{w}\right) + \chi_{1}^{w\sigma}\left(T_{1}^{w\sigma} - T_{1}\right)\right]\right\} \tag{5.258}$$

and conditions for droplet condensation otherwise $\psi_{13}^{w} = 0$, guarantee that the mass sources are non-negative.

Substituting for the evaporation and condensation mass sources one obtains

$$\begin{aligned}
DT_{1}^{N} &= \alpha_{1}\rho_{1}\left(\delta_{1}P_{k1}^{\tau} + \varepsilon_{1}\right) + \chi_{1}^{w\sigma}\left(T_{1}^{w\sigma} - T_{1}\right) \\
&- \begin{pmatrix} \psi_{21}^{w}\left\{\chi_{w}^{2\sigma}\left[T'(p) - T_{w}\right] + \chi_{2}^{w\sigma}\left[T'(p) - T_{2}\right]\right\} \\ +\psi_{31}^{w}\left\{\chi_{w}^{3\sigma}\left[T'(p) - T_{w}\right] + \chi_{3}^{w\sigma}\left[T'(p) - T_{3}\right]\right\} \end{pmatrix} \frac{c_{pM1}}{h''(p) - h'(p)}\left(T_{1}^{w\sigma} - T_{1}\right) \\
&+ \chi_{w1}\left(T_{w} - T_{1}\right) + \chi_{21}\left(T_{2} - T_{1}\right) + \chi_{31}\left(T_{3} - T_{1}\right) + \sum_{i=1}^{i_{\max}} \mu_{iw1}\left(h_{iw1} - h_{i1}\right) \\
&+ \chi_{1}^{2\sigma}\left(T_{1}^{2\sigma} - T_{1}\right) - \left(1 - \psi_{12}\right)\left[\chi_{2}^{1\sigma}\left(T_{2}^{1\sigma} - T_{2}\right) + \chi_{1}^{2\sigma}\left(T_{1}^{2\sigma} - T_{1}\right)\right]\frac{c_{pM1}\left(T_{1}^{2\sigma} - T_{1}\right)}{h_{M1}^{2\sigma} - h_{M2}^{1\sigma}} \\
&+ \chi_{1}^{3\sigma}\left(T_{1}^{3\sigma} - T_{1}\right) - \left(1 - \psi_{13}\right)\left[\chi_{3}^{1\sigma}\left(T_{3}^{1\sigma} - T_{3}\right) + \chi_{1}^{3\sigma}\left(T_{1}^{3\sigma} - T_{1}\right)\right]\frac{c_{pM1}\left(T_{1}^{3\sigma} - T_{1}\right)}{h_{M1}^{3\sigma} - h_{M3}^{1\sigma}},
\end{aligned} \tag{5.259}$$

$$\begin{aligned}
DT_{2}^{N} &= \alpha_{2}\rho_{2}\left(\delta_{2}P_{k2}^{\tau} + \varepsilon_{2}\right) + \chi_{2}^{w\sigma}\left(T_{2}^{w\sigma} - T_{2}\right) \\
&+ \psi_{12}^{w} f_{cond\rightarrow film}\left[\chi_{w}^{1\sigma}\left(T_{w}^{1\sigma} - T_{w}\right) + \chi_{1}^{w\sigma}\left(T_{1}^{w\sigma} - T_{1}\right)\right]\frac{c_{pM2}}{h_{M1}^{2\sigma} - h_{M2}^{1\sigma}}\left(T_{2}^{w\sigma} - T_{2}\right) \\
&+ \left(\chi_{w2} + \mu_{w2}c_{pw2}\right)\left(T_{w} - T_{2}\right) + \left(\chi_{32} + \mu_{32}c_{p3}\right)\left(T_{3} - T_{2}\right) - \chi_{21}\left(T_{2} - T_{1}\right) \\
&+ \chi_{2}^{1\sigma}\left(T_{2}^{1\sigma} - T_{2}\right) + \psi_{12}\left[\chi_{2}^{1\sigma}\left(T_{2}^{1\sigma} - T_{2}\right) + \chi_{1}^{2\sigma}\left(T_{1}^{2\sigma} - T_{1}\right)\right]\frac{c_{pM2}\left(T_{2}^{1\sigma} - T_{2}\right)}{h_{M1}^{2\sigma} - h_{M2}^{1\sigma}},
\end{aligned} \tag{5.260}$$

$$
\begin{aligned}
DT_3^N &= \alpha_3\rho_3\left(\delta_3 P_{k3}^{\tau} + \varepsilon_3\right) + \chi_3^{w\sigma}\left(T_3^{w\sigma} - T_3\right) \\
&+\psi_{13}^{w}\left(1 - f_{cond\to film}\right)\left[\chi_w^{1\sigma}\left(T_w^{1\sigma} - T_w\right) + \chi_1^{w\sigma}\left(T_1^{w\sigma} - T_1\right)\right]\frac{c_{pM3}}{h_{M1}^{3\sigma} - h_{M3}^{1\sigma}}\left(T_3^{w\sigma} - T_3\right) \\
&+\left(\chi_{w3} + \mu_{w3}c_{pw3}\right)\left(T_w - T_3\right) - \left(\chi_{32} + \mu_{23}c_{p2}\right)\left(T_3 - T_2\right) - \chi_{31}\left(T_3 - T_1\right) \\
&+\chi_3^{1\sigma}\left(T_3^{1\sigma} - T_3\right) + \psi_{13}\left[\chi_3^{1\sigma}\left(T_3^{1\sigma} - T_3\right) + \chi_1^{3\sigma}\left(T_1^{3\sigma} - T_1\right)\right]\frac{c_{pM3}\left(T_3^{1\sigma} - T_3\right)}{h_{M1}^{3\sigma} - h_{M3}^{1\sigma}} .
\end{aligned}
\tag{5.261}
$$

The above expressions can be rewritten in the compact form

$$
DT_l^N = c_l^T - \sum_{k=1}^{3} a_{lk}^{*T} T_k
\tag{5.262}
$$

where

$$
\begin{aligned}
c_1^T &= \alpha_1\rho_1\left(\delta_1 P_{k1}^{\tau} + \varepsilon_1\right) + \sum_{i=1}^{i_{\max}} \mu_{iw1}\left(h_{iw1} - h_{i1}\right) + \chi_{w1}T_w \\
&+\chi_1^{w\sigma}T_1^{w\sigma} - \left(\begin{matrix}\left[\psi_{21}^{w}\left(\chi_w^{2\sigma} + \chi_2^{w\sigma}\right) + \psi_{31}^{w}\left(\chi_w^{3\sigma} + \chi_3^{w\sigma}\right)\right]T'\left(p\right) \\ \\ -\left(\psi_{21}^{w}\chi_w^{2\sigma} + \psi_{31}^{w}\chi_w^{3\sigma}\right)T_w\end{matrix}\right)\frac{c_{pM1}}{h''\left(p\right) - h'\left(p\right)}T_1^{w\sigma} \\
&+\left[\chi_1^{2\sigma} - \frac{\left(1 - \psi_{12}\right)c_{pM1}}{h_{M1}^{2\sigma} - h_{M2}^{1\sigma}}\left(\chi_2^{1\sigma}T_2^{1\sigma} + \chi_1^{2\sigma}T_1^{2\sigma}\right)\right]T_1^{2\sigma} \\
&+\left[\chi_1^{3\sigma} - \frac{\left(1 - \psi_{13}\right)c_{pM1}}{h_{M1}^{3\sigma} - h_{M3}^{1\sigma}}\left(\chi_3^{1\sigma}T_3^{1\sigma} + \chi_1^{3\sigma}T_1^{3\sigma}\right)\right]T_1^{3\sigma} ,
\end{aligned}
\tag{5.263}
$$

$$
\begin{aligned}
a_{11}^{*T} &= +\chi_1^{w\sigma} + \chi_{21} + \chi_{31} + \chi_1^{2\sigma} + \chi_1^{3\sigma} + \chi_{w1} \\
&-\left(\begin{matrix}\psi_{21}^{w}\left\{\chi_w^{2\sigma}\left[T'\left(p\right) - T_w\right] + \chi_2^{w\sigma}\left[T'\left(p\right) - T_2\right]\right\} \\ \\ +\psi_{31}^{w}\left\{\chi_w^{3\sigma}\left[T'\left(p\right) - T_w\right] + \chi_3^{w\sigma}\left[T'\left(p\right) - T_3\right]\right\}\end{matrix}\right)\frac{c_{pM1}}{h''\left(p\right) - h'\left(p\right)}
\end{aligned}
$$

$$-\frac{\chi_2^{1\sigma}\left(1-\psi_{12}\right)c_{pM1}}{h_{M1}^{2\sigma}-h_{M2}^{1\sigma}}\left(T_2^{1\sigma}-T_2\right)+\frac{\chi_1^{2\sigma}\left(1-\psi_{12}\right)c_{pM1}}{h_{M1}^{2\sigma}-h_{M2}^{1\sigma}}\left(T_1-2T_1^{2\sigma}\right)$$

$$-\frac{\chi_3^{1\sigma}\left(1-\psi_{13}\right)c_{pM1}}{h_{M1}^{3\sigma}-h_{M3}^{1\sigma}}\left(T_3^{1\sigma}-T_3\right)+\frac{\chi_1^{3\sigma}\left(1-\psi_{13}\right)c_{pM1}}{h_{M1}^{3\sigma}-h_{M3}^{1\sigma}}\left(T_1-2T_1^{3\sigma}\right), \tag{5.264}$$

$$a_{12}^{*T}=-\chi_{21}-\frac{\chi_2^{1\sigma}\left(1-\psi_{12}\right)c_{pM1}}{h_{M1}^{2\sigma}-h_{M2}^{1\sigma}}T_1^{2\sigma}-\frac{\psi_{21}^{w}\chi_2^{w\sigma}c_{pM1}}{h''\left(p\right)-h'\left(p\right)}T_1^{w\sigma}, \tag{5.265}$$

$$a_{13}^{*T}=-\chi_{31}-\frac{\chi_3^{1\sigma}\left(1-\psi_{13}\right)c_{pM1}}{h_{M1}^{3\sigma}-h_{M3}^{1\sigma}}T_1^{3\sigma}-\frac{\psi_{31}^{w}\chi_3^{w\sigma}c_{pM1}}{h''\left(p\right)-h'\left(p\right)}T_1^{w\sigma}, \tag{5.266}$$

$$c_2^T=\alpha_2\rho_2\left(\delta_2P_{k2}^{\tau}+\varepsilon_2\right)+\chi_2^{w\sigma}T_2^{w\sigma}+\chi_2^{1\sigma}T_2^{1\sigma}+\left(\chi_{w2}+\mu_{w2}c_{pw2}\right)T_w$$

$$+\left\{\begin{array}{l}\psi_{12}^{w}f_{cond\to film}\left[\chi_w^{1\sigma}\left(T_w^{1\sigma}-T_w\right)+\chi_1^{w\sigma}T_1^{w\sigma}\right]T_2^{w\sigma}\\ \\ +\psi_{12}\left[\chi_2^{1\sigma}T_2^{1\sigma}+\chi_1^{2\sigma}T_1^{2\sigma}\right]T_2^{1\sigma}\end{array}\right\}\frac{c_{pM2}}{h_{M1}^{2\sigma}-h_{M2}^{1\sigma}}, \tag{5.267}$$

$$a_{21}^{*T}=\left(\psi_{12}^{w}f_{cond\to film}\chi_1^{w\sigma}T_2^{w\sigma}+\psi_{12}\chi_1^{2\sigma}T_2^{1\sigma}\right)\frac{c_{pM2}}{h_{M1}^{2\sigma}-h_{M2}^{1\sigma}}-\chi_{21}, \tag{5.268}$$

$$a_{22}^{*T}=\chi_2^{w\sigma}+\chi_2^{1\sigma}+\chi_{w2}+\mu_{w2}c_{pw2}+\chi_{32}+\mu_{32}c_{p3}+\chi_{21}$$

$$+\left\{\begin{array}{l}\psi_{12}^{w}f_{cond\to film}\left[\chi_w^{1\sigma}\left(T_w^{1\sigma}-T_w\right)+\chi_1^{w\sigma}\left(T_1^{w\sigma}-T_1\right)\right]\\ \\ +\psi_{12}\left[\chi_2^{1\sigma}\left(2T_2^{1\sigma}-T_2\right)+\chi_1^{2\sigma}\left(T_1^{2\sigma}-T_1\right)\right]\end{array}\right\}\frac{c_{pM2}}{h_{M1}^{2\sigma}-h_{M2}^{1\sigma}}, \tag{5.269}$$

$$a_{23}^{*T}=-\chi_{32}-\mu_{32}c_{p3}, \tag{5.270}$$

$$c_3^T=\alpha_3\rho_3\left(\delta_3P_{k3}^{\tau}+\varepsilon_3\right)+\chi_3^{w\sigma}T_3^{w\sigma}+\chi_3^{1\sigma}T_3^{1\sigma}+\left(\chi_{w3}+\mu_{w3}c_{pw3}\right)T_w$$

$$+\left\{\begin{array}{l}\psi_{13}^{w}\left(1-f_{cond\to film}\right)\left[\chi_w^{1\sigma}\left(T_w^{1\sigma}-T_w\right)+\chi_1^{w\sigma}T_1^{w\sigma}\right]T_3^{w\sigma}\\ \\ +\psi_{13}\left(\chi_3^{1\sigma}T_3^{1\sigma}+\chi_1^{3\sigma}T_1^{3\sigma}\right)T_3^{1\sigma}\end{array}\right\}\frac{c_{pM3}}{h_{M1}^{3\sigma}-h_{M3}^{1\sigma}}, \tag{5.271}$$

$$a_{31}^{*T}=\left[\psi_{13}^{w}\left(1-f_{cond\to film}\right)\chi_1^{w\sigma}T_3^{w\sigma}+\psi_{13}\chi_1^{3\sigma}T_3^{1\sigma}\right]\frac{c_{pM3}}{h_{M1}^{3\sigma}-h_{M3}^{1\sigma}}-\chi_{31}, \tag{5.272}$$

$$a_{32}^{*T} = -\chi_{32} - \mu_{23} c_{p2} , \tag{5.273}$$

$$a_{33}^{*T} = \chi_3^{w\sigma} + \chi_3^{1\sigma} + \chi_{w3} + \mu_{w3} c_{pw3} + \chi_{32} + \mu_{23} c_{p2} + \chi_{31}$$

$$+ \left\{ \begin{array}{l} \psi_{13}^{w} \left(1 - f_{cond \to film}\right) \left[\chi_w^{1\sigma} \left(T_w^{1\sigma} - T_w\right) + \chi_1^{w\sigma} \left(T_1^{w\sigma} - T_1\right) \right] \\ \\ + \psi_{13} \left[\chi_3^{1\sigma} \left(2 T_3^{1\sigma} - T_3\right) + \chi_1^{3\sigma} \left(T_1^{3\sigma} - T_1\right) \right] \end{array} \right\} \frac{c_{pM3}}{h_{M1}^{3\sigma} - h_{M3}^{1\sigma}} , \tag{5.274}$$

5.17 Interface conditions

Steam only: For the case of steam only in the gas field, i.e. $C_{M1} = 1$, one has

$$T_3^{1\sigma} = T_2^{1\sigma} = T_1^{2\sigma} = T_1^{3\sigma} = T'(p) \approx T'(p_a) + \frac{dT'}{dp}(p - p_a)$$

$$\approx T'(p_a) + \frac{dT'}{dp} \frac{dp}{d\tau} \Delta\tau , \tag{5.275}$$

$$h_{M3}^{1\sigma} = h_{M2}^{1\sigma} = h'(p) , \tag{5.276}$$

$$h_{M1}^{2\sigma} = h_{M1}^{3\sigma} = h''(p) . \tag{5.277}$$

Here p_a is the reference pressure for the previous time step. Note that the pressure p can change during the time interval considered, which can reduce or even stop the condensation and promote evaporation, for example.

Flashing: For the case of spontaneous evaporation of the water, e.g. from the second velocity field,

$$T_2 > \left(1 + \frac{\chi_1^{2\sigma}}{\chi_2^{1\sigma}}\right) T'(p) - \frac{\chi_1^{2\sigma}}{\chi_2^{1\sigma}} T_1 \tag{5.278}$$

one has

$$T_2^{1\sigma} = T_1^{2\sigma} = T'(p) \approx T'(p_a) + \frac{dT'}{dp}(p - p_a) , \tag{5.279}$$

$$h_{M1}^{2\sigma} = h''(p) . \tag{5.280}$$

Similarly, for the case of spontaneous evaporation of the water from the third velocity field,

$$T_3 > \left(1+\frac{\chi_1^{3\sigma}}{\chi_3^{1\sigma}}\right)T'(p)-\frac{\chi_1^{3\sigma}}{\chi_3^{1\sigma}}T_1 \tag{5.281}$$

one has

$$T_3^{1\sigma} = T_1^{3\sigma} = T'(p) \approx T'(p_a)+\frac{dT'}{dp}(p - p_a), \tag{5.282}$$

$$h_{M1}^{3\sigma} = h''(p). \tag{5.283}$$

Boiling at the wall: If boiling conditions are in force at the wall one has

$$T_{M1}^{w\sigma} = T'(p) \approx T'(p_a)+\frac{dT'}{dp}(p - p_a). \tag{5.284}$$

Non-condensibles present in the gas field: This case is much more complicated than the single component case, especially for diffusion-controlled interfacial mass transfer.

The liquid side interface temperature during condensation processes is the saturation temperature at the local partial steam pressure

$$T_3^{1\sigma} = T_2^{1\sigma} = T'(p_{M1}) = T'(p_{M1a})+\frac{dT'}{dp}(p_{M1} - p_{M1a}). \tag{5.285}$$

5.18 Lumped parameter volumes

If in a practical application a good mixing at any time within a control volume can be considered as a good approximation, the energy conservation equations in any of their variants simplify considerable. All convection and diffusion terms disappear. What remains are the time derivatives and the source terms. We summarize the results of this section for this particular case in order to make easy practical applications. Thus, we have for the entropy, specific internal energy, the temperature and the specific enthalpy equations the following result:

$$\rho_l \alpha_l \frac{ds_l}{d\tau} = \frac{1}{T_l} DT_l^N + \sum_{i=1}^{i_{\max}} \mu_{il}\left(s_{il} - s_l\right) \qquad \text{for} \quad \alpha_l \ge 0, \tag{5.286}$$

$$\frac{d}{d\tau}\left(\alpha_l \rho_l e_l \gamma_v\right) + p_l \frac{d}{d\tau}\left(\alpha_l \gamma_v\right) = \gamma_v De_l^*, \tag{5.287}$$

$$\rho_l c_{pl} \alpha_l \frac{dT_l}{d\tau} - \left[1 - \rho_l \left(\frac{\partial h_l}{\partial p}\right)_{T_l, all\_C's}\right] \alpha_l \frac{dp}{d\tau}$$

$$= DT_l^N - T_l \sum_{i=2}^{i_{\max}} \Delta s_{il}^{np} \left(\mu_{il} - C_{il}\mu_l \right), \tag{5.288}$$

$$\frac{d}{d\tau}\left(\alpha_l \rho_l h_l \gamma_v\right) - \alpha_l \gamma_v \frac{dp_l}{d\tau} = \gamma_v DT_l^N + \gamma_v \sum_{\substack{m=1 \\ m \neq l}}^{3,w} \sum_{i=1}^{i_{\max}} \left(\mu_{iml} - \mu_{ilm}\right) h_{il} . \tag{5.289}$$

The volume conservation equation divided by the volumetric porosity for this case reduces to

$$\frac{1}{\rho a^2}\frac{dp}{d\tau} = \sum_{l=1}^{l_{\max}} D\alpha_l - \frac{d}{d\tau}\ln\gamma_v , \tag{5.290}$$

where

$$D\alpha_l = \frac{\mu_l}{\rho_l} - \frac{1}{\rho_l^2}\left[\begin{array}{l} \left(\dfrac{\partial \rho_l}{\partial s_l}\right)_{p,all\_C_{li}'s} \left[\dfrac{1}{T_l} DT_l^N + \displaystyle\sum_{i=1}^{i_{\max}} \mu_{il}\left(s_{il} - s_l\right)\right] \\ \\ + \displaystyle\sum_{i=2}^{i_{\max}} \left(\dfrac{\partial \rho_l}{\partial C_{li}}\right)_{p,s,all\_C_{li}'s\_except\_C_{l1}} \left(\mu_{il} - C_{il}\mu_l\right) \end{array}\right] . \tag{5.291}$$

5.19 Steady state

Now we consider a steady state flows. Neglecting the time derivatives we obtain the following different forms of the energy conservation.

$$\rho_l \left(\alpha_l^e \mathbf{V}_l \gamma \cdot \nabla\right) s_l - \frac{1}{T_l}\nabla\cdot\left(\alpha_l^e \lambda_l^* \gamma \nabla T\right) - \nabla . \left\{ \alpha_l^e \rho_l \gamma \left[\sum_{i=2}^{i_{\max}} \left(s_{il} - s_{1l}\right) D_{il}^* \nabla C_{il} \right] \right\}$$

$$= \gamma_v \left[\frac{1}{T_l} DT_l^N + \sum_{\substack{m=1 \\ m \neq l}}^{3,w} \sum_{i=1}^{i_{\max}} \left(\mu_{iml} - \mu_{ilm}\right) s_{il} - \mu_l s_l \right], \tag{5.292}$$

$$\nabla\cdot\left(\alpha_l^e \rho_l e_l \mathbf{V}_l \gamma\right) + p_l \nabla\cdot\left(\alpha_l^e \mathbf{V}_l \gamma\right) - \nabla\cdot\left\{ \alpha_l^e \gamma \left[\lambda_l^* \nabla T_l + \rho_l \sum_{i=2}^{i_{\max}} \left(e_{il} - e_{1l}\right) D_{il}^* \nabla C_{il} \right] \right\}$$

$$+ \overline{p_l' \nabla\cdot\left(\alpha_l^e \mathbf{V}_l' \gamma\right)} = \gamma_v De_l^* , \tag{5.293}$$

$$\rho_l c_{pl} \left(\alpha_l^e \mathbf{V}_l \gamma \cdot \nabla \right) T_l - \left[1 - \rho_l \left(\frac{\partial h_l}{\partial p} \right)_{T_l, all\_C's} \right] \left(\alpha_l^e \mathbf{V}_l \gamma \cdot \nabla \right) p - \nabla \cdot \left(\alpha_l^e \lambda_l^* \gamma \nabla T \right)$$

$$+ T_l \sum_{i=2}^{i_{\max}} \Delta s_{il}^{np} \nabla \left(\alpha_l^e \rho_l D_{il}^* \gamma \nabla C_{il} \right) = \gamma_v \left[DT_l^N - T_l \sum_{i=2}^{i_{\max}} \Delta s_{il}^{np} \left(\mu_{il} - C_{il} \mu_l \right) \right], \quad (5.294)$$

$$\alpha_l^e \rho_l \left(\mathbf{V}_l \gamma \cdot \nabla \right) h_l - \alpha_l^e \mathbf{V}_l \gamma \cdot \nabla p_l - \nabla \cdot \left[\alpha_l^e \gamma \lambda_l^* \nabla T_l \right]$$

$$- \nabla \cdot \left[\alpha_l^e \gamma \rho_l \sum_{i=2}^{i_{\max}} \left(h_{il} - h_{1l} \right) D_{il}^* \nabla C_{il} \right] - \alpha_l^e \overline{\mathbf{V}_l' \gamma \cdot \nabla p_l'}$$

$$+ \delta_l \left(\alpha_l^e \gamma \nabla p_l \right) \cdot \sum_{i=1}^{i_{\max}} D_{il}^l \nabla \ln C_{il} = \gamma_v DT_l^N . \quad (5.295)$$

For single phase single component flows without mass transfer trough the external sources we obtain and neglecting second order terms including conduction we obtain the well known forms:

$$\rho \left(\mathbf{V} \gamma \cdot \nabla \right) s = \gamma_v \frac{1}{T} DT^N , \quad (5.296)$$

$$\nabla \cdot \left(\rho e \mathbf{V} \gamma \right) + p \nabla \cdot \left(\mathbf{V} \gamma \right) = \gamma_v De^* , \quad (5.297)$$

$$\rho c_p \left(\mathbf{V} \gamma \cdot \nabla \right) T - \left[1 - \rho \left(\frac{\partial h}{\partial p} \right)_T \right] \left(\mathbf{V} \gamma \cdot \nabla \right) p = \gamma_v DT^N , \quad (5.298)$$

$$\rho \left(\mathbf{V} \gamma \cdot \nabla \right) h - \mathbf{V} \gamma \cdot \nabla p = \gamma_v DT^N , \quad (5.299)$$

where

$$DT^N = De^* = \rho \left(P_k + \varepsilon \right) + \dot{q}''' . \quad (5.300)$$

Again note the simplicity of the entropy notation of the conservation of energy

$$\left(\mathbf{V} \gamma \cdot \nabla \right) s = \gamma_v P_\eta / T + \dot{q}''' / \rho . \quad (5.301)$$

Remember that in a adiabatic pipe flow in which $\dot{q}''' = 0$, the friction dissipation causes entropy production due to

$$P_\eta = \frac{\lambda_{fr}}{D_h} \frac{1}{2} \overline{w}^3 y_{\lim}^+ \sqrt{\frac{\lambda_{fr}}{8}} > 0 . \quad (5.302)$$

This is in the technology very important if one has to do with expansion of gases in long pipes. Without taking this term into account the gas may “freeze in the computation” which dies not happen in the reality.

Problem: Write the conservation equation for a pipe single-phase single-component flow without mass transfer.

Solution: The mass momentum and energy conservation equations are:

$$\frac{d}{dz}\left(\rho w \gamma_z\right) = 0 \text{ or } \frac{1}{w}\frac{dw}{dz} + \frac{1}{\rho}\frac{d\rho}{dz} = -\frac{1}{\gamma_z}\frac{d\gamma_z}{dz}, \tag{5.303}$$

$$\frac{1}{2}\frac{dw^2}{dz} + \frac{1}{\rho}\frac{dp}{dz} + \left(g_z + \frac{\lambda_{fr}}{D_h}\frac{1}{2}w^2\right)\frac{\gamma_v}{\gamma_z} = 0, \tag{5.304}$$

$$\frac{ds}{dz} = \frac{\gamma_v}{\gamma_z}\frac{\lambda_{fr}}{D_h}\frac{1}{2}w^2 y_{\lim}^{+}\sqrt{\frac{\lambda_{fr}}{8}}\Big/ T + \dot{q}'''\big/\left(\rho w \gamma_z\right) = s_z. \tag{5.305}$$

Problem: Assume the flow is a perfect gas and rewrite the above system in terms of temperature and pressure.

Solution: Having in mind $\rho = \frac{p}{RT}$, $\kappa = c_p \big/ \left(c_p - R\right)$, $a^2 = \kappa RT$ and $s = c_p \ln\frac{T}{T_0} - R\ln\frac{p}{p_0}$ we obtain

$$\frac{1}{w}\frac{dw}{dz} + \frac{1}{p}\frac{dp}{dz} - \frac{1}{T}\frac{dT}{dz} = -\frac{1}{\gamma_z}\frac{d\gamma_z}{dz}, \tag{5.306}$$

$$\frac{1}{2}\frac{dw^2}{dz} + \frac{RT}{p}\frac{dp}{dz} = -\left(g_z + \frac{\lambda_{fr}}{D_h}\frac{1}{2}w^2\right)\frac{\gamma_v}{\gamma_z}, \tag{5.307}$$

$$\frac{1}{T}\frac{dT}{dz} - \frac{R}{c_p p}\frac{dp}{dz} = \frac{s_z}{c_p}. \tag{5.308}$$

Solving with respect to the derivatives we finally obtain:

$$\frac{dp}{dz} = -\frac{\rho w^2\left(\frac{s_z}{c_p} - \frac{1}{\gamma_z}\frac{d\gamma_z}{dz}\right) + \rho\left(g_z + \frac{\lambda_{fr}}{D_h}\frac{1}{2}w^2\right)\frac{\gamma_v}{\gamma_z}}{1 - \frac{w^2}{a^2}}, \tag{5.309}$$

$$\frac{1}{w}\frac{dw}{dz}=\frac{s_z}{c_p}-\frac{1}{\gamma_z}\frac{d\gamma_z}{dz}-\frac{1}{\kappa p}\frac{dp}{dz}=\frac{\dfrac{s_z}{c_p}-\dfrac{1}{\gamma_z}\dfrac{d\gamma_z}{dz}+\dfrac{1}{a^2}\left(g_z+\dfrac{\lambda_{fr}}{D_h}\dfrac{1}{2}w^2\right)\dfrac{\gamma_v}{\gamma_z}}{1-\dfrac{w^2}{a^2}}, \tag{5.310}$$

$$\frac{dT}{dz}=\frac{T}{c_p}\left(s_z+\frac{R}{p}\frac{dp}{dz}\right). \tag{5.311}$$

The obtained system of non-homogeneous non-linear ordinary differential equation indicates important behavior immediately. For constant pipe cross section $\gamma_z = const$, the nominator of the pressure gradient is positive. For sub-critical flow, $w < a$, the pressure gradient is therefore negative. Consequently, the velocity gradient in the second equation is positive. If the pipe is long enough for a given pressure difference acting at the both ends and the velocity approach the sound velocity at the exit of the pipe, $w \to a$, the pressure gradient tends to minus infinity. We call such flow *critical single phase flow*. Because the multi-phase flows are compressible flows they obey also such behavior in pipes. Finding the conditions for the critical flow will be one of the tasks solved in the next chapters. We learn on this example haw to proceed in multiphase flows to.

Note the difference to the solution repeated in many gas-dynamics text books, *Albring* (1970), *Oswatitsch* (1952), *Shapiro* (1953), by using the energy conservation for adiabatic flow neglecting the gravitation and the friction component in the energy equation

$$\rho w\gamma_z\frac{d}{dz}\left(h+\frac{1}{2}w^2\right)+\cancel{\gamma_v\rho w g_z}=\cancel{\gamma_v\dot{q}_l'''}+\gamma_v\cancel{\frac{\lambda_{fr}}{D_h}\frac{1}{2}w^2 y_{\lim}^{+}\sqrt{\frac{\lambda_{fr}}{8}}}. \tag{5.312}$$

In this case the energy conservation for perfect fluid simplifies to

$$c_p\frac{dT}{dz}=-\frac{1}{2}\frac{dw^2}{dz} \text{ or } \frac{1}{T}\frac{dT}{dz}=-(\kappa-1)M^2\frac{1}{w}\frac{dw}{dz}, \tag{5.313}$$

and allows to write the definition of the mach number, $M^2=\dfrac{w^2}{\kappa RT}$, and the mass conservation equations in the following forms

$$\frac{1}{w}\frac{dw}{dz}=\frac{1}{\left[2+(\kappa-1)M^2\right]M^2}\frac{dM^2}{dz}, \tag{5.314}$$

$$\frac{1}{p}\frac{dp}{dz}=-\frac{1+(\kappa-1)M^2}{\left[2+(\kappa-1)M^2\right]M^2}\frac{dM^2}{dz}, \tag{5.315}$$

respectively. This allows in the rearranged momentum equation for separation of the variables

$$\frac{1-M^2}{\left(1+\frac{\kappa-1}{2}M^2\right)M^4}dM^2=-\frac{\lambda_{fr}}{D_h}\kappa dz\,, \tag{5.316}$$

Albring (1970) p. 315, and for integration it analytically for constant friction coefficient

$$\frac{(\kappa+1)}{2\kappa}\ln\frac{\left(\frac{2}{M_1^2}+\kappa-1\right)}{\left(\frac{2}{M_0^2}+\kappa-1\right)}+\frac{1}{\kappa}\left(\frac{1}{M_0^2}-\frac{1}{M_1^2}\right)=-\frac{\lambda_{fr}}{D_h}\Delta z\,. \tag{5.317}$$

For critical flow at the exit $M_1=1$ the results simplifies to

$$\frac{(\kappa+1)}{2\kappa}\ln\left[1-\frac{2}{1+\kappa}\left(1-\frac{1}{M_0^2}\right)\right]+\frac{1}{\kappa}\left(1-\frac{1}{M_0^2}\right)=\frac{\lambda_{fr}}{D_h}\Delta z\,, \tag{5.318}$$

which is Eq. 21.48 in *Albring* (1970) p. 315. For frictionless flow the above equation is satisfied only for $M_0=1$.

5.20 Final remarks

It should be emphasized that in the temperature equation, just as in the energy equation, in the enthalpy equation and in the internal energy equations, the specific enthalpy occurs in the mass transfer terms. In the entropy equations the interfacial mass source terms are associated with specific entropies.

The most important result of this chapter is the rigorous derivation of the entropy equation, which reflects the second law of thermodynamics for multiphase systems consisting of several chemical components which are conditionally divided into three velocity fields. It was shown that the use of specific entropy, introduced by *Clausius* and recognized by *Gibbs* as a very important quantity more than one hundred years ago, provides the simplest method for modern description and modeling of complicated flow systems. The experience gained by the author of this work in the development of the various versions of the IVA computer code, *Kolev* (1985-1995), which are based on the entropy concept allows for the recommendation of the local volume and time average entropy equation for general use in multi-phase flow dynamics.

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