Chapter 5

TIME AVERAGED BALANCE EQUATION

1.1   General balance equation

In the preceding chapter, the important definitions and basic relations between them have been given. We now apply them to the time averaging of the balance laws in the two-phase flow media. As it has been explained in the Section 1.1 of Chapter 4, it was necessary to introduce several sets of time intervals because of the discontinuous changes in the nature of fluid surrounding the point of average. Thus the domain of averaging has been divided into $[\Delta t]_S$ and $[\Delta t]_T$. During $[\Delta t]_T$, the standard balance equation (2-6) holds, since the fluid occupying the point x_0 can be considered as a continuum. However, in $[\Delta t]_S$ the interfacial balance equation, namely, the jump condition of the Section 1.2 of Chapter 2, is valid because the characteristics of the interface dominates in this time interval.

Our purpose here is to average the balance laws in time by properly assigning appropriate balance equations of the bulk fluid and of an interface. Now let us first proceed with an analysis in $[\Delta t]_T$ when the point of averaging is occupied by one of the phases and not by an interface. For time $t \in [\Delta t]_T = [\Delta t]_1 + [\Delta t]_2$, we consider the balance of a quantity ψ in the following form

$$B_V = \frac{\partial \rho \psi}{\partial t} + \nabla \cdot (\rho \psi \boldsymbol{v}) + \nabla \cdot \mathcal{J} - \rho \phi = 0. \tag{5-1}$$

Here $\mathcal{J}$ and ϕ represent the generalized tensor efflux and the source of ψ, respectively. Since it is multiplied by the density ρ, the quantity ψ is expressed as the quantity per unit mass. Thus the above equation itself is a mathematical statement of the balance of the quantity *in a unit volume*. This

is an important point to be remembered when we compare it to the surface balance equation in the course of the time averaging. In order to keep the volumetric origin of Eq.(5-1), the balance is denoted by B_V. Furthermore, we recall here that when Eq.(5-1) is applied for each phase, the subscripts that differentiate two fluids should appear with variables. For time $t \in [\Delta t]_S$, a different kind of balance equation should be used due to the special characteristics of an interface. Since the detailed derivation of the interfacial balance equation has been given in the Section 1.2 of Chapter 2, we simply recall those results. Thus, from Eq.(2-67), the balance of matter ψ at the interface becomes

$$
\begin{aligned}
B_S = \frac{1}{\delta} \bigg\{ &\frac{d_s}{dt} \psi_a + \psi_a \nabla_s \cdot v_i \\
&- \sum_{k=1}^{2} \left[\rho_k n_k \cdot (v_k - v_i) \psi_k + n_k \cdot \mathcal{J}_k \right] \\
&+ g_{\ln} A^{\alpha\beta} \left(t_\alpha^n \mathcal{J}_a^{l\bullet} \right)_{,\beta} - \phi_a \bigg\} = 0.
\end{aligned}
\tag{5-2}
$$

In order to obtain Eq.(5-2), we have divided Eq.(2-67) by the interfacial thickness δ. Consequently, the above equation is the balance of ψ in an unit volume of the region.

The averaged balance per volume can be obtained by integrating the proper balance equations in the time domain. Now let us express the balance equation in general by

$$
B = 0
\tag{5-3}
$$

where

$$
B = B_V = 0 \quad \text{for } t \in [\Delta t]_T
\tag{5-4}
$$

$$
B = B_S = 0 \quad \text{for } t \in [\Delta t]_S .
\tag{5-5}
$$

By taking a time average of B we have

$$
\frac{1}{\Delta t} \int_{[\Delta t]} B \, dt = 0.
\tag{5-6}
$$

Following the assumption previously made, we approximate the interfacial region with a singular surface by taking the limit $\delta \to 0$. Thus Eq.(5-6) becomes

$$\frac{1}{\Delta t} \lim_{\delta \to 0} \int_{[\Delta t]_r} B_V \, dt + \frac{1}{\Delta t} \lim_{\delta \to 0} \int_{[\Delta t]_S} B_S \, dt = 0. \tag{5-7}$$

The first part can be expressed in terms of the mean values defined in the Section 1.3 of Chapter 4, hence from Eq.(5-1) with Eqs.(4-25), (4-57) and (4-58) we obtain

$$\frac{1}{\Delta t} \lim_{\delta \to 0} \int_{[\Delta t]_T} B_V \, dt = \frac{\partial \overline{\rho \psi}}{\partial t} + \nabla \cdot \overline{\rho \psi v} + \nabla \cdot \overline{J} - \overline{\rho \phi}$$

$$+ \frac{1}{\Delta t} \sum_j \left\{ \frac{1}{v_{ni}} \sum_{k=1}^{2} \left[\boldsymbol{n}_k \cdot \rho_k \left(\boldsymbol{v}_k - \boldsymbol{v}_i \right) \psi_k + \boldsymbol{n}_k \cdot \boldsymbol{J}_k \right] \right\} = 0 \tag{5-8}$$

or in terms of the mixture properties

$$\frac{1}{\Delta t} \lim_{\delta \to 0} \int_{[\Delta t]_T} B_V \, dt = \frac{\partial \rho_m \psi_m}{\partial t} + \nabla \cdot \left(\rho_m \psi_m \boldsymbol{v}_m \right)$$

$$+ \nabla \cdot \left(\overline{J} + J^D + J^T \right) - \rho_m \phi_m \tag{5-9}$$

$$+ \frac{1}{\Delta t} \sum_j \left\{ \frac{1}{v_{ni}} \sum_{k=1}^{2} \left[\boldsymbol{n}_k \cdot \rho_k \left(\boldsymbol{v}_k - \boldsymbol{v}_i \right) \psi_k + \boldsymbol{n}_k \cdot \boldsymbol{J}_k \right] \right\} = 0$$

where the fundamental identity of the Section 1.7 of Chapter 4 has been used. From Eq.(4-2) with Eq.(4-1) the second part originating from interfaces becomes

$$\frac{1}{\Delta t} \lim_{\delta \to 0} \int_{[\Delta t]_S} B_S \, dt = \frac{1}{\Delta t} \sum_j \frac{1}{v_{ni}} \left\{ \frac{d_s}{dt} \left(\psi_a \right) + \psi_a \nabla_s \cdot \boldsymbol{v}_i - \phi_a \right.$$

$$\left. + g_{\ln} A^{\alpha\beta} \left(t_\alpha^n J_a^{l\cdot} \right)_{,\beta} - \sum_{k=1}^{2} \boldsymbol{n}_k \cdot \left[\rho_k \left(\boldsymbol{v}_k - \boldsymbol{v}_i \right) \psi_k + \boldsymbol{J}_k \right] \right\} = 0. \tag{5-10}$$

It is evident that the above equation is a time-averaged interfacial balance equation. In order to distinguish it from the local jump condition, we call it the *interfacial transfer condition* or the *macroscopic jump condition*.

In view of Eqs.(5-7), (5-9) and (5-10), we obtain a macroscopic balance equation for the mixture

$$\frac{\partial \rho_m \psi_m}{\partial t} + \nabla \cdot \left(\rho_m \psi_m \boldsymbol{v}_m \right) + \nabla \cdot \left(\overline{J} + J^D + J^T \right) - \rho_m \phi_m$$
$$+ \frac{1}{\Delta t} \sum_j \frac{1}{v_{ni}} \left\{ \frac{d_s}{dt} \left(\psi_a \right) + \psi_a \nabla_s \cdot \boldsymbol{v}_i - \phi_a \right\} \qquad (5\text{-}11)$$
$$+ \frac{1}{\Delta t} \sum_j \frac{1}{v_{ni}} g_{\ln} A^{\alpha\beta} \left(t_\alpha^n J_a^{l\bullet} \right)_{,\beta} = 0.$$

The terms given by $\overline{J}$, J^D and J^T represent the effluxes due to the average molecular diffusion, the macroscopic phase diffusions with respect to the mixture center of mass, and the statistical effects of the two-phase and turbulent fluctuations, whereas $\rho_m \phi_m$ is the mixture volumetric source. From the form of the balance equation, it is also possible to consider the interfacial terms as an additional source or sink.

It is generally accepted that the mass and momentum of the interface can be neglected. The surface energy, however, may not be insignificant because of the energy associated with the thermodynamic tension, namely, the surface tension. Thus, the first part of the interfacial term is important only in the energy balance equation. The surface line flux appears in the momentum and the energy balances, though the molecular diffusion transfers along an interface (namely the surface viscous stress and the surface heat flux) are neglected. This means that these line fluxes account for the effects of the surface tension only. When Eq.(5-11) is applied for the balance of mass, momentum and energy, appropriate forms corresponding to the simplified jump conditions of Eqs.(2-69), (2-72) and (2-73) should be used.

The averaged balance equations for each phase can be obtained by considering the function associated only with a particular phase, Eq.(4-8). Thus, in analogy with Eq.(5-9), we have

$$\frac{\partial \alpha_k \overline{\overline{\rho_k}} \widehat{\psi_k}}{\partial t} + \nabla \cdot \left(\alpha_k \overline{\overline{\rho_k}} \widehat{\psi_k} \widehat{\boldsymbol{v}_k} \right) + \nabla \cdot \left[\alpha_k \left(\overline{\overline{J_k}} + J_k^T \right) \right] - \alpha_k \overline{\overline{\rho_k}} \widehat{\phi_k}$$
$$+ \frac{1}{\Delta t} \sum_j \left\{ \frac{1}{v_{ni}} \left[\boldsymbol{n}_k \cdot \rho_k \left(\boldsymbol{v}_k - \boldsymbol{v}_i \right) \psi_k + \boldsymbol{n}_k \cdot J_k \right] \right\} = 0 \qquad (5\text{-}12)$$

where we have used the transformation (4-110) and the local instant general balance equation for the kth-phase, Eq.(2-6). For simplicity, let us define

$$I_k \equiv -\frac{1}{\Delta t} \sum_j \left\{ \frac{1}{v_{ni}} n_k \cdot \left[\rho_k \left(v_k - v_i \right) \psi_k + \mathcal{J}_k \right] \right\} \tag{5-13}$$

$$I_m \equiv -\frac{1}{\Delta t} \sum_j \left\{ \frac{1}{v_{ni}} \left[\frac{d_s \psi_a}{dt} + \psi_a \nabla_s \cdot v_i - \phi_a \right. \right.$$
$$+ g_{\ln} A^{\alpha\beta} \left(t_\alpha^n \mathcal{J}_a^{l\bullet} \right)_{,\beta} \right] \right\}. \tag{5-14}$$

And the mixture total flux is given by

$$\mathcal{J}_m \equiv \overline{\mathcal{J}} + \mathcal{J}^D + \mathcal{J}^T. \tag{5-15}$$

Here I_k and I_m represent the interfacial source for the kth-phase and for the mixture, respectively. With these definitions the *mixture general balance equation* (5-11) reduces to

$$\frac{\partial \rho_m \psi_m}{\partial t} + \nabla \cdot \left(\rho_m \psi_m v_m \right) = -\nabla \cdot \mathcal{J}_m + \rho_m \phi_m + I_m \tag{5-16}$$

whereas the *balance equation for the kth-phase* becomes

$$\frac{\partial \alpha_k \overline{\overline{\rho_k}} \widehat{\psi_k}}{\partial t} + \nabla \cdot \left(\alpha_k \overline{\overline{\rho_k}} \widehat{\psi_k} \widehat{v_k} \right) = -\nabla \cdot \left[\alpha_k \left(\overline{\overline{\mathcal{J}_k}} + \mathcal{J}_k^T \right) \right]$$
$$+ \alpha_k \overline{\overline{\rho_k}} \widehat{\phi_k} + I_k. \tag{5-17}$$

Furthermore, the interfacial transfer condition (5-10) can be rewritten as

$$\sum_{k=1}^{2} I_k - I_m = 0. \tag{5-18}$$

Each of these three macroscopic equations expresses the balance of matter ψ for the mixture, for the kth-phase, and at the interfaces, respectively. The mixture balance equation will be the foundation of the formulation of the drift-flux model. Furthermore, the phase balance equations and the interfacial transfer conditions are required for the two-fluid model formulation.

In view of Eqs.(5-16), (5-17) and (5-18), our fundamental purpose of averaging has been accomplished. Thus, the original two phases which are alternately occupying a point have been transformed into two co-existing continua. Moreover the hopelessly complicated two-phase and turbulent fluctuations have been smoothed out and their statistical macroscopic effects have been taken into account by the covariance (or turbulent flux) terms. In the next two sections we present balance equations of mass, momentum and energy for the *diffusion model* and for the *two-fluid model* separately.

1.2   Two-fluid model field equations

In this section, the macroscopic balance equation (5-17) and the interfacial transfer condition (5-18), which have been derived from the time averaging, are applied to the conservation laws of mass, momentum and energy. The choice of variables in these equations follows that of the local instant formulation of Chapter 2.

Mass Balance
In order to obtain mass balance equations, we set

$$\psi_k = 1, \quad \mathscr{J}_k = 0, \quad \phi_k = 0. \tag{2-7}$$

And in view of Eq.(2-69) we define

$$\Gamma_k \equiv I_k = -\frac{1}{\Delta t} \sum_j \left\{ \frac{1}{v_{ni}} \, \boldsymbol{n}_k \cdot \rho_k \left(\boldsymbol{v}_k - \boldsymbol{v}_i \right) \right\} \tag{5-19}$$

$$I_m = 0. \tag{5-20}$$

Then by substituting Eq.(2-7) into Eqs.(5-17) and (5-18) we get

$$\frac{\partial \alpha_k \overline{\overline{\rho_k}}}{\partial t} + \nabla \cdot \left(\alpha_k \overline{\overline{\rho_k}} \widehat{\boldsymbol{v}_k} \right) = \Gamma_k \quad k = 1 \text{ and } 2 \tag{5-21}$$

and

$$\sum_{k=1}^{2} \Gamma_k = 0. \tag{5-22}$$

Equation (5-21) is the continuity equation for each phase with the interfacial mass source Γ_k appearing on the right-hand side due to phase changes, whereas the second equation, Eq.(5-22), expresses the conservation of mass at the interfaces.

Momentum Balance

The macroscopic momentum balance can be obtained from Eqs.(5-13), (5-14) and (5-17) by setting

$$\psi_k = v_k, \quad \mathcal{J}_k = -\mathcal{T}_k = p_k I - \mathcal{C}_k, \quad \phi_k = g_k \tag{2-9}$$

and by defining the following terms in view of Eqs. (2-72) and (4-104)

$$M_k \equiv I_k = -\frac{1}{\Delta t} \sum_j \left\{ \frac{1}{v_{ni}} n_k \cdot \left[\rho_k \left(v_k - v_i \right) v_k - \mathcal{T}_k \right] \right\} \tag{5-23}$$

$$M_m \equiv I_m = \frac{1}{\Delta t} \sum_j \left\{ \frac{1}{v_{ni}} \left(t_\alpha A^{\alpha\beta} \sigma \right)_{,\beta} \right\} \tag{5-24}$$

$$\mathcal{C}_k^T \equiv -J_k^T = -\overline{\overline{\rho_k v_k' v_k'}}. \tag{5-25}$$

With these definitions we obtain from Eqs.(5-17) and (5-18)

$$\frac{\partial \alpha_k \overline{\overline{\rho_k}} \widehat{v_k}}{\partial t} + \nabla \cdot \left(\alpha_k \overline{\overline{\rho_k}} \widehat{v_k} \widehat{v_k} \right) = -\nabla \left(\alpha_k \overline{\overline{p_k}} \right)$$
$$+ \nabla \cdot \left[\alpha_k \left(\overline{\overline{\mathcal{C}_k}} + \mathcal{C}_k^T \right) \right] + \alpha_k \overline{\overline{\rho_k}} \widehat{g_k} + M_k \tag{5-26}$$

and

$$\sum_{k=1}^{2} M_k - M_m = 0. \tag{5-27}$$

Here the terms $\mathcal{C}_k^T$ and M_k denote the turbulent flux and the kth-phase momentum source form the interfacial transfer, respectively, whereas the term M_m is the mixture momentum source due to the surface tension effect.

Energy Balance

The energy balances for the macroscopic fields can be obtained from Eq.(5-17) by first setting

$$\psi_k = u_k + \frac{v_k^2}{2}, \quad J_k = q_k - T_k \cdot v_k, \quad \phi_k = g_k \cdot v_k + \frac{\dot{q}_k}{\rho_k} \quad (2\text{-}12)$$

and by defining following terms in view of Eqs.(5-13), (5-14) and (2-73)

$$E_k \equiv I_k$$

$$= -\frac{1}{\Delta t} \sum_j \left\{ \frac{1}{v_{ni}} \, n_k \cdot \left[\rho_k \left(v_k - v_i \right) \left(u_k + \frac{v_k^2}{2} \right) - T_k \cdot v_k + q_k \right] \right\} \quad (5\text{-}28)$$

$$E_m \equiv I_m = \frac{1}{\Delta t} \sum_j \left\{ \frac{1}{v_{ni}} \left[T_i \left\{ \frac{d_s}{dt} \left(\frac{d\sigma}{dT} \right) + \left(\frac{d\sigma}{dT} \right) \nabla_s \cdot v_i \right\} \right. \right.$$

$$+ \left(t_\alpha A^{\alpha\beta} \sigma \right)_{,\beta} \cdot v_i \right] \right\} \quad (5\text{-}29)$$

$$q_k^T \equiv J_k^T - \overline{\overline{T_k \cdot v_k'}} = \rho_k \overline{\left(u_k + \frac{v_k^2}{2} \right)' v_k'} - \overline{\overline{\mathcal{T}_k \cdot v_k'}} + \overline{\overline{p_k \cdot v_k'}} \quad (5\text{-}30)$$

$$\widehat{e_k} \equiv \widehat{u_k} + \frac{\widehat{\left(v_k' \right)^2}}{2}. \quad (5\text{-}31)$$

Thus, we have from Eqs.(5-17) and (5-18)

$$\frac{\partial}{\partial t} \left[\alpha_k \overline{\overline{\rho}}_k \left(\widehat{e_k} + \frac{\widehat{v_k}^2}{2} \right) \right] + \nabla \cdot \left[\alpha_k \overline{\overline{\rho}}_k \left(\widehat{e_k} + \frac{\widehat{v_k}^2}{2} \right) \widehat{v_k} \right]$$

$$= -\nabla \cdot \left[\alpha_k \left(\overline{\overline{q}}_k + q_k^T \right) \right] + \nabla \cdot \left(\alpha_k \overline{\overline{T}}_k \cdot \widehat{v_k} \right) \quad (5\text{-}32)$$

$$+ \alpha_k \overline{\overline{\rho}}_k \widehat{g}_k \cdot \widehat{v_k} + E_k$$

and

$$\sum_{k=1}^{2} E_k - E_m = 0 \tag{5-33}$$

where we have assumed

$$\boldsymbol{g}_k = \widehat{\boldsymbol{g}_k}. \tag{5-34}$$

We also note that the apparent internal energy $\widehat{e_k}$ consists of the standard thermal energy and the turbulent kinetic energy, see Eq.(5-31). The term E_k represents the interfacial supply of energy to the kth-phase, while E_m is the energy source for the mixture. This means that the energy can be stored at or released from interfaces. As it can be seen from the definition, the turbulent heat flux $\boldsymbol{q}_k^T$ takes account for the turbulent energy convection as well as for the turbulent work. For most two-phase flow problems, the internal heating $\dot{q}_k$ can be neglected.

The two-fluid model is based on the above *six field equations*, namely, two continuity, two momentum and two energy equations. The *interfacial transfer conditions* for mass, momentum and energy couple the transport processes of each phase. Since these nine equations basically express the conservation laws, they should be supplemented by various constitutive equations that specify molecular diffusions, turbulent transports, and interfacial transfer mechanisms as well as a relation between the thermodynamic state variables.

In solving problems, it is often useful to separate the mechanical and thermal effects in the total energy equation. Thus from the standard method of dotting the momentum equation by the velocity, we have the *mechanical energy equation*

$$\frac{\partial \left(\alpha_k \overline{\overline{\rho_k}} \frac{\widehat{v_k}^2}{2} \right)}{\partial t} + \nabla \cdot \left(\alpha_k \overline{\overline{\rho_k}} \frac{\widehat{v_k}^2}{2} \widehat{v_k} \right) = -\widehat{v_k} \cdot \nabla \left(\alpha_k \overline{\overline{p_k}} \right) \tag{5-35}$$

$$+ \widehat{v_k} \cdot \nabla \cdot \left[\alpha_k \left(\overline{\overline{\mathscr{T}_k}} + \mathscr{T}_k^T \right) \right] + \alpha_k \overline{\overline{\rho_k}} \boldsymbol{g}_k \cdot \widehat{v_k} + M_k \cdot \widehat{v_k} - \frac{\widehat{v_k}^2}{2} \Gamma_k.$$

Then by subtracting Eq.(5-35) from Eq.(5-32) the *internal energy equation* can be obtained, thus

$$\frac{\partial \alpha_k \overline{\overline{\rho_k}} \widehat{e_k}}{\partial t} + \nabla \cdot \left(\alpha_k \overline{\overline{\rho_k}} \widehat{e_k} \widehat{v_k} \right) = -\nabla \cdot \left(\alpha_k \overline{\overline{q_k}} \right)$$

$$-\nabla \cdot \left\{ \alpha_k \left(q_k^T + \mathcal{C}_k^T \cdot \widehat{v_k} \right) \right\} - \alpha_k \overline{\overline{p_k}} \nabla \cdot \widehat{v_k}$$

$$+\alpha_k \left(\overline{\overline{\mathcal{C}_k}} + \mathcal{C}_k^T \right) : \nabla \widehat{v_k} \tag{5-36}$$

$$+\left(\frac{\widehat{v_k}^2}{2} \Gamma_k - M_k \cdot \widehat{v_k} + E_k \right).$$

Here we recall that the virtual internal energy $\widehat{e_k}$ includes the turbulent kinetic energy in addition to the standard internal energy.

For two-phase flow analyses, the enthalpy energy equation is important and it is frequently used to solve various engineering problems. Thus, in parallel with Eq.(5-31), we introduce a virtual enthalpy $\widehat{h_k}$ defined by

$$\widehat{h_k} \equiv \widehat{i_k} + \frac{\widehat{(v_k')^2}}{2} = \widehat{e_k} + \frac{\overline{\overline{p_k}}}{\overline{\overline{\rho_k}}}. \tag{5-37}$$

By substituting Eq.(5-37) into Eq. (5-36) we obtain

$$\frac{\partial \alpha_k \overline{\overline{\rho_k}} \widehat{h_k}}{\partial t} + \nabla \cdot \left(\alpha_k \overline{\overline{\rho_k}} \widehat{h_k} \widehat{v_k} \right) = -\nabla \cdot \left(\alpha_k \overline{\overline{q_k}} \right)$$

$$-\nabla \cdot \left\{ \alpha_k \left(q_k^T + \mathcal{C}_k^T \cdot \widehat{v_k} \right) \right\} + \frac{D_k}{Dt} \left(\alpha_k \overline{\overline{p_k}} \right) \tag{5-38}$$

$$+\alpha_k \left(\overline{\overline{\mathcal{C}_k}} + \mathcal{C}_k^T \right) : \nabla \widehat{v_k} + \left(\frac{\widehat{v_k}^2}{2} \Gamma_k - M_k \cdot \widehat{v_k} + E_k \right)$$

where the substantial derivative D_k/Dt is taken by following the center of mass of kth-phase or moving with velocity $\widehat{v_k}$, thus $D_k/Dt = \partial/\partial t + \widehat{v_k} \cdot \nabla$. These thermal energy equations are extremely complicated due to the interactions between the mechanical terms from the turbulent fluctuations and the thermal terms. However, in many practical two-phase flow problems, the heat transfer and the phase change terms dominate the energy equations. In such a case, the above equations can be reduced to simple forms.

As it can be seen from Eq.(5-38), the interfacial transfer in the thermal energy equation has a special form which is expressed by a combination of the mass, momentum and energy transfer terms. Thus we define

$$\Lambda_k \equiv \frac{\widehat{v_k}^2 \Gamma_k}{2} - M_k \cdot \widehat{v_k} + E_k.$$ (5-39)

1.3 Diffusion (mixture) model field equations

The basic concept of the diffusion (mixture) model is to consider the mixture as a whole, therefore the field equations should be written for the balance of mixture mass, momentum and energy in terms of the mixture properties. These three macroscopic mixture conservation equations are then supplemented by a diffusion equation that takes account for the concentration changes.

Mixture Continuity and Diffusion Equations
From the mixture general balance equation, Eq.(5-16), with the definitions of ρ_m and v_m, we obtain the mixture continuity equation

$$\frac{\partial \rho_m}{\partial t} + \nabla \cdot \left(\rho_m v_m \right) = 0.$$ (5-40)

The above equation has exactly the same form as that for a continuum without internal discontinuities.

The diffusion equation, which expresses the changed in concentration α_1, can be derived from Eqs.(5-21) and (4-89)

$$\frac{\partial \alpha_1 \overline{\overline{\rho_1}}}{\partial t} + \nabla \cdot \left(\alpha_1 \overline{\overline{\rho_1}} v_m \right) = \Gamma_1 - \nabla \cdot \left(\alpha_1 \overline{\overline{\rho_1}} V_{1m} \right).$$ (5-41)

It has a mass source term Γ_1 that appears only after the continuity equation being averaged over the time interval because it accounts for the mass transfer at the interface. In addition, Eq.(5-41) has a diffusion term on the right-hand side, since the convective flux has been expressed by the mixture center of mass velocity v_m.

Mixture Momentum Equation
By applying the general balance equation (5-16) to the conservation of momentum we obtain

$$\frac{\partial \rho_m v_m}{\partial t} + \nabla \cdot \left(\rho_m v_m v_m \right) = -\nabla p_m + \nabla \cdot \left(\overline{\overline{\mathcal{T}}} + \mathcal{T}^T + \mathcal{T}^D \right)$$
$$+ \rho_m g_m + M_m$$ (5-42)

where we have

$$p_m = \sum_{k=1}^{2} \alpha_k \overline{\overline{p_k}}$$

$$\overline{\overline{\mathcal{T}}} = \sum_{k=1}^{2} \alpha_k \overline{\overline{\mathcal{T}_k}}$$

$$\mathcal{T}^T = -\sum_{k=1}^{2} \alpha_k \overline{\overline{\rho_k v_k' v_k'}} \tag{5-43}$$

$$\mathcal{T}^D = -\sum_{k=1}^{2} \alpha_k \overline{\rho_k} V_{km} V_{km}$$

$$g_m = \frac{\sum_{k=1}^{2} \alpha_k \overline{\rho_k} g_k}{\rho_m}.$$

Furthermore the interfacial momentum source M_m is given by Eq.(5-24). Three tensor fluxes $\overline{\overline{\mathcal{T}}}$, $\mathcal{T}^T$ and $\mathcal{T}^D$ represent the average viscous stress, the turbulent stress and the diffusion stress, respectively. It is evident that if the surface tension term is neglected, then there are not direct interfacial terms in the mixture momentum equation.

Mixture Total Energy Equation

The mixture energy equation can be obtained from Eq.(5-16) applied to the balance of the total energy, thus

$$\frac{\partial}{\partial t}\left\{\rho_m\left[e_m + \left(\frac{v^2}{2}\right)_m\right]\right\} + \nabla \cdot \left\{\rho_m\left[e_m + \left(\frac{v^2}{2}\right)_m\right]v_m\right\}$$

$$= -\nabla \cdot \left(\overline{q} + q^T + q^D\right) - \nabla \cdot \left(p_m v_m\right) + \nabla \cdot \left(\overline{\overline{\mathcal{T}}} \cdot v_m\right) \tag{5-44}$$

$$+\rho_m g_m \cdot v_m + \sum_{k=1}^{2} \alpha_k \overline{\rho_k} g_k \cdot V_{km} + E_m$$

where we have

$$\overline{q} = \sum_{k=1}^{2} \alpha_k \overline{\overline{q_k}} \tag{5-45}$$

$$q^T = \sum_{k=1}^{2} \alpha_k q_k^T = \sum_{k=1}^{2} \alpha_k \overline{\left\{ \overline{\rho_k \left(u_k + \frac{v_k^2}{2} \right)'} v_k' - \overline{\overline{T_k} \cdot v_k'} \right\}} \qquad (5\text{-}46)$$

$$q^D = J^D - \sum_{k=1}^{2} \alpha_k \overline{\overline{T_k}} \cdot V_{km}$$

$$= \sum_{k=1}^{2} \alpha_k \left\{ \overline{\overline{\rho_k}} \left(\widehat{e_k} + \frac{\widehat{v_k}^2}{2} \right) V_{km} - \overline{\overline{T_k}} \cdot V_{km} \right\}. \qquad (5\text{-}47)$$

And, by definition, we have following mixture properties

$$e_m = \frac{\displaystyle\sum_{k=1}^{2} \alpha_k \overline{\overline{\rho_k}} \widehat{e_k}}{\rho_m} = \frac{\displaystyle\sum_{k=1}^{2} \alpha_k \overline{\overline{\rho_k}} \left(\widehat{u_k} + \frac{\widehat{v_k'^2}}{2} \right)}{\rho_m} \qquad (5\text{-}48)$$

$$\left(\frac{v^2}{2} \right)_m = \frac{\displaystyle\sum_{k=1}^{2} \alpha_k \overline{\overline{\rho_k}} \frac{\widehat{v_k}^2}{2}}{\rho_m} = \frac{v_m^2}{2} + \frac{\displaystyle\sum_{k=1}^{2} \alpha_k \overline{\overline{\rho_k}} \frac{V_{km}^2}{2}}{\rho_m}. \qquad (5\text{-}49)$$

The interfacial energy source E_m is given by Eq.(5-29). The important special case is when the body force field is constant

$$g_k = \widehat{g_k} = g_m = g. \qquad (5\text{-}50)$$

Then the diffusion body work term becomes zero, thus

$$\sum_{k=1}^{2} \alpha_k \overline{\overline{\rho_k}} g_k \cdot V_{km} = 0 \qquad (5\text{-}51)$$

where we used the identity, Eq.(4-94).

Hence, under the standard condition of the constant body force field, the total mixture energy equation reduces to

$$\frac{\partial}{\partial t}\left\{\rho_m\left[e_m+\left(\frac{v^2}{2}\right)_m\right]\right\}+\nabla\cdot\left\{\rho_m\left[e_m+\left(\frac{v^2}{2}\right)_m\right]\boldsymbol{v}_m\right\}$$

$$=-\nabla\cdot\left(\overline{\boldsymbol{q}}+\boldsymbol{q}^T+\boldsymbol{q}^D\right)-\nabla\cdot\left(p_m\boldsymbol{v}_m\right)+\nabla\cdot\left(\overline{\overline{\mathscr{T}}}\cdot\boldsymbol{v}_m\right) \qquad (5\text{-}52)$$

$$+\rho_m\boldsymbol{g}_m\cdot\boldsymbol{v}_m+E_m.$$

It can be seen that the form of Eq.(5-52) is quite similar to the single-phase flow energy equation. The differences appear as additional heat fluxes, namely, the turbulent flux $\boldsymbol{q}^T$ and the diffusion flux $\boldsymbol{q}^D$, and the interfacial body source E_m. However the most interesting characteristic of the mixture can be found in the kinetic energy term, Eq.(5-49). We see from the equation that the total mixture kinetic energy consists of the kinetic energy of the center of mass plus the diffusion kinetic energies of both phases. It also should be remembered that the turbulent kinetic energy has been included in the virtual internal energy due to the great difficulties in separating it from the thermal effects. We also point out that if the surface tension effects are neglected, then the interfacial term does not appear in the mixture total energy equation (as in the case with the mixture momentum equation).

Mixture Thermal Energy Equation

In a single-phase flow, the separation of the mechanical and thermal energy can be carried out quite easily by subtracting the mechanical energy equation from the total energy balance. Exactly the same method could be used in the two-fluid model formulation, if we would include the turbulent kinetic energy in the virtual thermal energy as we have done in Eqs.(5-36) and (5-37). In the diffusion model formulation, however, it is further complicated by the existence of the *diffusion kinetic energy* transport. Consequently, there is no clear-cut method to obtain a corresponding thermal energy equation for the mixtures. In the following, we demonstrate two distinct methods which give quite different results.

The first method is to subtract the sum of the kinetic energy equations of both phases from the total energy equation (5-44). In this way, the diffusion kinetic energy can be eliminated. Thus, from Eqs.(5-35) and (5-44), we obtain

$$\frac{\partial\rho_m h_m}{\partial t}+\nabla\cdot\left(\rho_m h_m\boldsymbol{v}_m\right)=-\nabla\cdot\left(\overline{\boldsymbol{q}}+\boldsymbol{q}^T\right)$$

$$-\nabla\cdot\left(\sum_{k=1}^{2}\alpha_k\overline{\overline{\rho_k}}\widehat{h}_k\boldsymbol{V}_{km}\right)+\frac{D}{Dt}p_m+\sum_{k=1}^{2}\alpha_k\overline{\overline{\mathscr{T}_k}}:\nabla\widehat{\boldsymbol{v}_k} \qquad (5\text{-}53)$$

$$+\sum_{k=1}^{2} \Lambda_k + \sum_{k=1}^{2} \left\{ \boldsymbol{V}_{km} \cdot \nabla\left(\alpha_k \overline{\overline{p_k}}\right) - \widehat{\boldsymbol{v}_k} \cdot \nabla \cdot \left(\alpha_k \boldsymbol{\mathcal{C}}_k^T\right)\right\}.$$

Here from the definition, the mixture enthalpy h_m is given by

$$h_m \equiv \frac{\displaystyle\sum_{k=1}^{2} \alpha_k \overline{\overline{\rho_k}} \widehat{h_k}}{\rho_m} = \frac{\displaystyle\sum_{k=1}^{2} \alpha_k \overline{\overline{\rho_k}}\left(\widehat{i_k} + \frac{\widehat{v_k'^2}}{2}\right)}{\rho_m}. \tag{5-54}$$

The same equation (5-53) can also be obtained by adding the enthalpy equation of each phase, Eq.(5-38). The form of the equation is reasonably simple except the last term, but we should realize that the interfacial term $\sum_{k=1}^{2} \Lambda_k$ involves complicated exchanges between the total and the mechanical energies.

It is noted that by using the mixture kinetic energy equation in terms of the center of mass velocity $\boldsymbol{v}_m$, this difficulty in the interfacial term can be avoided. The resulting thermal energy equation, however, has additional terms from the diffusion kinetic energy. By subtracting the mixture mechanical energy equation, namely, the momentum equation (5-42) dotted by $\boldsymbol{v}_m$, from Eq.(5-52), we obtain

$$\frac{\partial \rho_m h_m}{\partial t} + \nabla \cdot \left(\rho_m h_m \boldsymbol{v}_m\right) = -\nabla \cdot \left(\overline{\boldsymbol{q}} + \boldsymbol{q}^T\right)$$
$$-\nabla \cdot \left(\sum_{k=1}^{2} \alpha_k \overline{\overline{\rho_k}} \widehat{h_k} \boldsymbol{V}_{km}\right) + \frac{Dp_m}{Dt}$$
$$-\left\{\rho_m \frac{D}{Dt}\left(\sum_{k=1}^{2} \frac{\alpha_k \overline{\overline{\rho_k}}}{\rho_m} \frac{V_{km}^2}{2}\right) + \nabla \cdot \sum_{k=1}^{2} \alpha_k \overline{\overline{\rho_k}} \frac{V_{km}^2}{2} \boldsymbol{V}_{km}\right\} \tag{5-55}$$
$$+\left(\overline{\overline{\boldsymbol{\mathcal{C}}}} + \boldsymbol{\mathcal{C}}^D\right) : \nabla \boldsymbol{v}_m + \left(E_m - \boldsymbol{M}_m \cdot \boldsymbol{v}_m\right) - \boldsymbol{v}_m \cdot \left(\nabla \cdot \boldsymbol{\mathcal{C}}^T\right)$$
$$+\nabla \cdot \left(\sum_{k=1}^{2} \alpha_k \overline{\overline{\boldsymbol{\mathcal{C}}_k}} \cdot \boldsymbol{V}_{km}\right).$$

In view of these two thermal energy equations, namely, Eqs.(5-53) and (5-55), it can be concluded that the mixture energy transfer is highly

complicated due to the diffusion of each phase with respect to the mass center. The form of the right-hand side of each equation suggests that if the effects of the mechanical terms originated from the diffusion are important, then the constitutive laws for the diffusion (or mixture) model cannot be simple. Thus, in such a case, the two-fluid model may be more suitable. However, in most two-phase problems with large heat additions, these mechanical effects from the diffusions are insignificant. The only important effect to be taken into account is the diffusion transport of thermal energy because of the large difference on the phase enthalpies, namely, the latent heat.

1.4   Singular case of v_{ni}=0 (quasi-stationary interface)

In the preceding analyses it has been assumed that the interfacial displacement velocity v_{ni} is non-zero, however in reality it can be zero at isolated singularities. For example, it happens when an interface is stationary or the motion of the interface is purely tangential to it. Since $v_{ni} = 0$ is an important singularity associated with all the interfacial terms in the balance equations such as I_k and I_m, we study it in some detail.

In connection with this singularity, we first introduce a surface area concentration per volume. By considering only one interface it can be given as

$$a_{ij} = \frac{1}{L_j} = \frac{1}{\Delta t} \lim_{\delta \to 0} \frac{2\varepsilon_j}{\delta} = \frac{1}{\Delta t} \left(\frac{1}{v_{ni}} \right)_j \qquad (5\text{-}56)$$

whereas the total area concentration is given by

$$a_i = \frac{1}{L_S} = \frac{1}{\Delta t} \lim_{\delta \to 0} \int_{[\Delta t]_s} \frac{1}{\delta} dt = \frac{1}{\Delta t} \sum_j \left(\frac{1}{v_{ni}} \right)_j$$

$$= \sum_j \frac{1}{L_j} = \sum_j \frac{1}{a_{ij}} \qquad (5\text{-}57)$$

The reciprocals of the area concentrations have the dimension of length and they are denoted by L_j and L_S for a single interface and for combined interfaces, respectively. a_{ij} is the surface area concentration for the jth-interface. We note here that the total interfacial length scale L_S has an important physical significance comparative to those of the molecular mean free path and the mixing length. Consequently all the interfacial terms appearing in the field equations, I_k and I_m, are expressed as an addition of

contributions from each interface with a_{ij} as a weighting factor. This fact is clearly demonstrated in Eqs.(5-13) and (5-14). Furthermore, the derivatives of the time fraction α_k are closely related to the area concentrations, as it can be seen from Eqs.(4-61) and (4-62). The importance of the interfacial area concentration a_i or the length scale L_S should be noted. a_i has the physical significance of the interfacial area per unit volume and it is the most important geometrical factor affecting the interfacial transfer. The inverse of a_i given by L_S is the internal length scale of the two-phase flow. This variable is discussed in detail in Chapter 10.

Now we return to the singular case of $v_{ni} = 0$. In view of Eqs.(5-56) and (5-57), it can be said that the transport length L_S becomes also singular in such a case and, thus it loses its physical significance. As a consequence all the interfacial terms in the balance equations, I_k and I_m, are also singular and the time fraction α_S or its derivative may suffer discontinuities. In order to cope with this difficulty, we first recall that α_S is the time fraction of the interfaces. We note here that from Eq.(4-14), the case of $v_{ni} \neq 0$ corresponds to $\alpha_S = 0$. Furthermore, if the normal velocity of an interface v_{ni} is zero, then it may stay at x_0 for some finite time. Thus we have

$$\alpha_S = \frac{\Delta t_S}{\Delta t} \geq 0 \qquad (5\text{-}58)$$

where Δt_S is the total time occupied by interfaces in the interval of Δt. And therefore

$$\Delta t = \Delta t_S + \sum_{k=1}^{2} \Delta t_k \qquad (5\text{-}59)$$

or in terms of the time fractions

$$1 = \alpha_S + \alpha_1 + \alpha_2. \qquad (5\text{-}60)$$

Now it is clear that we have two distinct cases of singularities, namely

1. $v_{ni} = 0$ and $\alpha_S = 0$;
2. $v_{ni} = 0$ and $\alpha_S > 0$.

As the definition of α_k shows, Case 1 does not bring discontinuities in α_k, but only in its derivatives in the microscopic sense. However, it has been explained in the Section 1.3 of Chapter 4 in connection to the *fundamental*

hypothesis on smoothness of mean values, these microscopic singularities should be neglected when macroscopic problems are concerned. Thus, unless an interface stays at a point for a finite time interval, the field is considered to be occupied by two continua with continuous interfacial transfer and source term I_k and I_m. Hence the singular surface of the interfacial origin appears in the macroscopic formulation only when $\alpha_g > 0$.

The above discussion also clearly indicates that the interfacial terms I_k and I_m given by Eq.(5-13) and Eq.(5-14) are not the constitutive relations to be used in the macroscopic formulation. These equations still retain all the details of the local instant variables which should not appear in the averaged formulation. Consequently, it is necessary to transform these equations in terms of the macroscopic variables.

We note that the macroscopic interface represented by Case 2 is most easily exemplified by the stationary interface such as a solid wall. Since for $\alpha_g > 0$ it is not possible to consider the average of the volumetric balance equation, the correct form of the macroscopic balance is simply the time average of the jump condition in the time interval of Δt. Thus we have

$$\frac{1}{\Delta t}\lim_{\delta \to 0} \int_{[\Delta t]_s} \left(B_s \delta\right) dt = 0. \tag{5-61}$$

Case 2 in normal two-phase flow corresponds to the discontinuity in α_k, and therefore, it can be treated as a concentration shock, see Eqs.(4-61) and (4-62). For most of the flow field it is assumed to be continuous. As the time-averaged macroscopic formulation is intended to be applied for such two-phase flows, these interfacial singularities can be neglected in most applications.

1.5   Macroscopic jump conditions

We have discussed the singularity related to a quasi-stationary interface in the preceding section. Now we study important singularities related to *macroscopic shock discontinuities* in the time averaged field. The essential part of the analysis can be developed in parallel with the Section 1.2 of Chapter 2 where the standard jump conditions at an interface have been derived.

In single-phase flows as well as in two-phase flows, the existence of regions where various properties suffer extremely large changes is well known. It can be exemplified by shock waves due to compressibility effects or by concentration shocks in mixtures. The unusually high gradients in these regions require special considerations on the constitutive laws in order to treat them as a part of continuum mechanics. However, as it has been
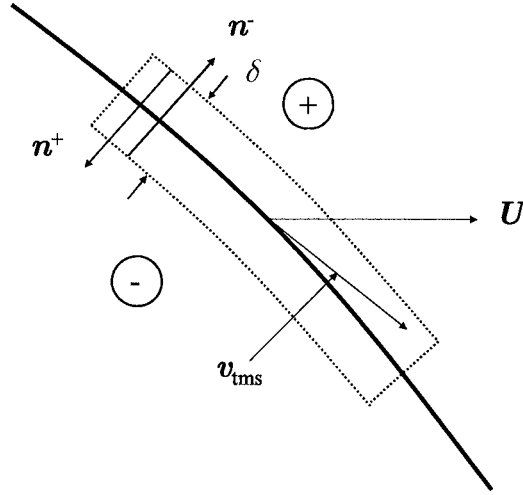
Figure 5-1. Macroscopic discontinuity (Ishii, 1975)

mentioned in the Section 1.2 of Chapter 2, for most practical flow problems replacements of these regions by surfaces of discontinuity with the jump conditions yield sufficiently accurate models. Hence in this section we derive macroscopic jump conditions which stand as balance equations at a surface of discontinuities in the averaged field. By considering the time-averaged macroscopic field as a continuum, the analysis of the Section of Chapter 2 can be directly applied here. The velocity of the surface U is defined in analogy with v_i of Eqs.(2-49) and (2-50), thus its normal component is the surface displacement velocity, whereas its tangential component is the mean mixture tangential velocity in the region with the thickness δ. By denoting each side of the region by + and -, we have from Eq.(2-64)

$$\frac{d_s}{dt}\left(\rho_{ma}\psi_{ms}\right) + \rho_{ma}\psi_{ms}\nabla_s \cdot U$$

$$= \sum_{+,-}\left\{\rho_m\psi_m\boldsymbol{n}\cdot\left(\boldsymbol{v}_m - U\right) + \boldsymbol{n}\cdot\mathcal{J}_m\right\} \tag{5-62}$$

$$-g_{\ln}A^{\alpha\beta}\left(t_\alpha^n\mathcal{J}_{ma}^{l\cdot}\right)_{,\beta} + \rho_{ma}\phi_{ms} + I_{ma}$$

where the summation stands for both sides of the region, the subscript a and s represent the mean values in the region as defined by Eqs.(2-45) to (2-54) and the surface derivatives have the standard significances. Equation (5-62) is a balance of ψ_m at the region of a shock. The left-hand side of the

equation accounts for the change of the matter ψ_m in the region, and each term on the right-hand side represents: the flux from the bulk fluid; the flux from the periphery with the thickness δ; the body source; and the interfacial source term.

It is evident that the balance equations similar to Eq.(5-62) can be obtained also for each of the two phases, thus

$$
\begin{aligned}
\frac{d_s}{dt} &\left\{ \left(\alpha_k \overline{\overline{\rho_k}} \right)_a \widehat{\psi_{ks}} \right\} + \left(\alpha_k \overline{\overline{\rho_k}} \right)_a \widehat{\psi_{ks}} \nabla_s \cdot U \\
&= \sum_{+,-} \left\{ \alpha_k \overline{\overline{\rho_k}} \widehat{\psi_k} \boldsymbol{n} \cdot \left(\widehat{\boldsymbol{v}_k} - \boldsymbol{U} \right) + \boldsymbol{n} \cdot \left[\alpha_k \left(\overline{\overline{\mathcal{J}_k}} + \mathcal{J}_k^T \right) \right] \right\} \\
&\quad - g_{\mathrm{ln}} A^{\alpha\beta} \left(t_\alpha^n \mathcal{J}_{ka}^{l\bullet} \right)_{,\beta} + \left(\alpha_k \overline{\overline{\rho_k}} \right)_a \widehat{\phi_{ks}} + I_{ka}.
\end{aligned}
\tag{5-63}
$$

From the definition of the mean values at the region it is easy to show that if each term in Eq.(5-63) is summed up for both phases, the resulting term becomes that of the mixture appearing in Eq.(5-62).

Since Eqs.(5-62) and (5-63) introduce new variables associated with the discontinuities, namely, the surface properties and the line fluxes, it is necessary to make some specific assumptions on these terms or to give sufficient constitutive laws. A simple result of practical importance can be obtained by considering the limit of $\delta \rightarrow 0$ and, furthermore, by neglecting the surface energy of shocks and the associated thermodynamic tension. Under these conditions, we have for the mixture

$$
\sum_{+,-} \left\{ \rho_m \psi_m \boldsymbol{n} \cdot \left(\boldsymbol{v}_m - \boldsymbol{U} \right) + \boldsymbol{n} \cdot \mathcal{J}_m \right\} + I_{ma} = 0.
\tag{5-64}
$$

And for each phase with $k = 1$ and 2

$$
\sum_{+,-} \left\{ \alpha_k \overline{\overline{\rho_k}} \widehat{\psi_k} \boldsymbol{n} \cdot \left(\widehat{\boldsymbol{v}_k} - \boldsymbol{U} \right) + \boldsymbol{n} \cdot \alpha_k \left(\overline{\overline{\mathcal{J}_k}} + \mathcal{J}_k^T \right) \right\} + I_{ka} = 0.
\tag{5-65}
$$

Here, we note the importance of the terms I_{ma} and I_{ka} that permit the exchange of mass, momentum and energy within the shock layers. It is incorrect to neglect these terms simply because they appear as volumetric sources. Depending on the constitutive laws expressing them, it is possible that they take a form of fluxes. Furthermore, from the physical points of view it is natural to have these interfacial transfer terms I_{ka} in the macroscopic jump conditions because of the highly non-equilibrium state of two-phase shock layers.

1.6 Summary of macroscopic field equations and jump conditions

The field equations for the mixture and for each phase were given by Eqs. (5-16) and (5-17)

$$\frac{\partial \rho_m \psi_m}{\partial t} + \nabla \cdot \left(\rho_m \psi_m \boldsymbol{v}_m \right) = -\nabla \cdot \mathcal{J}_m + \rho_m \phi_m + I_m \qquad (5\text{-}16)$$

and

$$\frac{\partial \alpha_k \overline{\overline{\rho_k}} \widehat{\psi_k}}{\partial t} + \nabla \cdot \left(\alpha_k \overline{\overline{\rho_k}} \widehat{\psi_k} \widehat{\boldsymbol{v}_k} \right) = -\nabla \cdot \left[\alpha_k \left(\overline{\overline{\mathcal{J}_k}} + \mathcal{J}_k^T \right) \right]$$
$$+ \alpha_k \overline{\overline{\rho_k}} \widehat{\phi_k} + I_k. \qquad (5\text{-}17)$$

The mixture total flux has been defined by

$$\mathcal{J}_m \equiv \overline{\mathcal{J}} + \mathcal{J}^D + \mathcal{J}^T \qquad (5\text{-}15)$$

with

$$\overline{\mathcal{J}} = \sum_{k=1}^{2} \alpha_k \overline{\overline{\mathcal{J}_k}} \qquad (4\text{-}24)$$

$$\mathcal{J}^D = \sum_{k=1}^{2} \alpha_k \overline{\overline{\rho_k}} \widehat{\psi_k} \boldsymbol{V}_{km} \qquad (4\text{-}103)$$

$$\mathcal{J}^T = \sum_{k=1}^{2} \alpha_k \mathcal{J}_k^T = \sum_{k=1}^{2} \alpha_k \overline{\rho_k \psi_k' \boldsymbol{v}_k'}. \qquad (4\text{-}105)$$

And the interfacial transfer condition was

$$I_m = \sum_{k=1}^{2} I_k. \qquad (5\text{-}18)$$

The macroscopic jump conditions at shock waves in their simplified forms
were

$$\sum_{+,-} \left\{ \rho_m \psi_m \boldsymbol{n} \cdot \left(\boldsymbol{v}_m - \boldsymbol{U} \right) + \boldsymbol{n} \cdot \mathcal{J}_m \right\} + I_{ma} = 0 \qquad (5\text{-}64)$$

and

$$\sum_{+,-} \left\{ \alpha_k \overline{\overline{\rho_k}} \widehat{\psi_k} \boldsymbol{n} \cdot \left(\widehat{\boldsymbol{v}_k} - \boldsymbol{U} \right) + \boldsymbol{n} \cdot \alpha_k \left(\overline{\overline{\mathcal{J}_k}} + \mathcal{J}_k^T \right) \right\} + I_{ka} = 0 \qquad (5\text{-}65)$$

where $\boldsymbol{n}$ (with + and -) is the outward unit normal vector at each side of the
surface, and $\boldsymbol{U}$ denotes shock surface velocity.

1.7   Alternative form of turbulent heat flux

The energy equations in the Sections 1.2 and 1.3 of Chapter 5 are derived
based on the definition of turbulent heat flux of Eq.(5-30). Here, an
alternative definition of the turbulent heat flux of Eq.(5-30)' may be possible
as

$$\boldsymbol{q}_k^T \equiv \rho_k \overline{\overline{\left[u_k' + \left(\frac{v_k^2}{2} \right)' \right] v_k'}} - \overline{\overline{\mathcal{C}_k \cdot v_k'}}. \qquad (5\text{-}30)'$$

Then, we can recast the stagnation internal energy equation, Eq.(5-32), the
internal energy equation, Eq.(5-36), and the stagnation enthalpy equation,
Eq.(5-38) as given by Eqs.(5-32)', (5-36)', and (5-38)', respectively.

$$\frac{\partial}{\partial t} \left[\alpha_k \overline{\overline{\rho}}_k \left(\widehat{e_k} + \frac{\widehat{v_k}^2}{2} \right) \right] + \nabla \cdot \left[\alpha_k \overline{\overline{\rho}}_k \left(\widehat{e_k} + \frac{\widehat{v_k}^2}{2} \right) \widehat{v_k} \right]$$

$$= -\nabla \cdot \left[\alpha_k \left(\overline{\overline{q_k}} + q_k^T \right) \right] - \nabla \cdot \left(\alpha_k \overline{\overline{p_k}} \widehat{v_k} \right) \qquad (5\text{-}32)'$$

$$+ \nabla \cdot \left[\alpha_k \left(\overline{\overline{\mathcal{C}_k}} + \mathcal{C}_k^T \right) \cdot \widehat{v_k} \right] + \alpha_k \overline{\overline{\rho}}_k \widehat{g_k} \cdot \widehat{v_k} + E_k$$

$$\frac{\partial \alpha_k \overline{\overline{\rho_k}} \widehat{e_k}}{\partial t} + \nabla \cdot \left(\alpha_k \overline{\overline{\rho_k}} \widehat{e_k} \widehat{v_k} \right) = -\nabla \cdot \left(\alpha_k \overline{\overline{q_k}} \right) - \nabla \cdot \left(\alpha_k q_k^T \right)$$

$$- \alpha_k \overline{\overline{p_k}} \nabla \cdot \widehat{v_k} + \alpha_k \left(\overline{\overline{\mathcal{T}_k}} + \mathcal{T}_k^T \right) : \nabla \widehat{v_k}$$

$$+ \left[\Gamma_k \widehat{h_{ki}} + \frac{\overline{\overline{q_{ki}''}}}{L_s} + W_{ki}^T + \left(M_k - \Gamma_k \widehat{v_{ki}} \right) \cdot \left(\widehat{v_{ki}} - \widehat{v_k} \right) \right] \tag{5-36'}$$

$$- p_{ki} \left[\frac{\partial \alpha_k}{\partial t} + \widehat{v_{ki}} \cdot \nabla \alpha_k \right]$$

$$\frac{\partial \alpha_k \overline{\overline{\rho_k}} \widehat{h_k}}{\partial t} + \nabla \cdot \left(\alpha_k \overline{\overline{\rho_k}} \widehat{h_k} \widehat{v_k} \right) = -\nabla \cdot \left(\alpha_k \overline{\overline{q_k}} \right) - \nabla \cdot \left(\alpha_k q_k^T \right)$$

$$+ \frac{D_k}{Dt} \left(\alpha_k \overline{\overline{p_k}} \right) + \alpha_k \left(\overline{\overline{\mathcal{T}_k}} + \mathcal{T}_k^T \right) : \nabla \widehat{v_k} \tag{5-38'}$$

$$+ \left(\frac{\widehat{v_k}^2}{2} \Gamma_k - M_k \cdot \widehat{v_k} + E_k \right).$$

We can also recast the total mixture energy equation, Eq.(5-44), and the mixture stagnation enthalpy equation, Eq.(5-53) as given by Eqs.(5-44)' and (5-53)', respectively.

$$\frac{\partial}{\partial t} \left\{ \rho_m \left[e_m + \left(\frac{v^2}{2} \right)_m \right] \right\} + \nabla \cdot \left\{ \rho_m \left[e_m + \left(\frac{v^2}{2} \right)_m v_m \right] \right\}$$

$$= -\nabla \cdot \left(\overline{q} + q^T + q^D \right) - \nabla \cdot \left(p_m v_m \right)$$

$$+ \nabla \cdot \left\{ \left(\overline{\mathcal{T}} + \mathcal{T}^T \right) \cdot v_m \right\} + \rho_m g_m \cdot v_m \tag{5-44'}$$

$$+ \sum_{k=1}^{2} \alpha_k \overline{\overline{\rho_k}} g_k \cdot V_{km} + E_m$$

where we have

$$q^T = \sum_{k=1}^{2} \alpha_k q_k^T = \sum_{k=1}^{2} \alpha_k \overline{\left[\overline{\rho_k \left\{ u'_k + \left(\frac{v_k^2}{2} \right)' \right\} v'_k} - \overline{\overline{\mathcal{T}_k} \cdot v'_k} \right]} \qquad (5\text{-}46)'$$

$$q^D = J^D - \sum_{k=1}^{2} \alpha_k \overline{\overline{T_k}} \cdot V_{km}$$

$$= \sum_{k=1}^{2} \alpha_k \left\{ \overline{\overline{\rho_k}} \left(\widehat{e_k} + \frac{\widehat{v_k}^2}{2} \right) V_{km} - \left(\overline{\overline{T_k}} + \mathcal{T}_k^T \right) \cdot V_{km} \right\} \qquad (5\text{-}47)'$$

$$\frac{\partial \rho_m h_m}{\partial t} + \nabla \cdot \left(\rho_m h_m v_m \right) = -\nabla \cdot \left(\overline{q} + q^T \right)$$

$$-\nabla \cdot \left(\sum_{k=1}^{2} \alpha_k \overline{\overline{\rho_k}} \widehat{h_k} V_{km} \right) + \frac{D}{Dt} p_m + \sum_{k=1}^{2} \alpha_k \left(\overline{\overline{\mathcal{T}_k}} + \mathcal{T}_k^T \right) : \nabla \widehat{v_k} \quad (5\text{-}53)'$$

$$+ \sum_{k=1}^{2} \Lambda_k + \sum_{k=1}^{2} \left\{ V_{km} \cdot \nabla \left(\alpha_k \overline{\overline{p_k}} \right) \right\}.$$

Correspondingly, Eqs.(5-52) and (5-55) can be recast as given by Eqs.(5-52)' and (5-55)', respectively.

$$\frac{\partial}{\partial t} \left\{ \rho_m \left[e_m + \left(\frac{v^2}{2} \right)_m \right] \right\} + \nabla \cdot \left\{ \rho_m \left[e_m + \left(\frac{v^2}{2} \right)_m \right] v_m \right\}$$

$$= -\nabla \cdot \left(\overline{q} + q^T + q^D \right) - \nabla \cdot \left(p_m v_m \right) \qquad (5\text{-}52)'$$

$$+ \nabla \cdot \left\{ \left(\overline{\mathcal{T}} + \mathcal{T}^T \right) \cdot v_m \right\} + \rho_m g_m \cdot v_m + E_m$$

$$\frac{\partial \rho_m h_m}{\partial t} + \nabla \cdot \left(\rho_m h_m v_m \right) = -\nabla \cdot \left(\overline{q} + q^T \right)$$

$$-\nabla \cdot \left(\sum_{k=1}^{2} \alpha_k \overline{\overline{\rho_k}} \widehat{h_k} V_{km} \right) + \frac{D p_m}{Dt} \qquad (5\text{-}55)'$$

$$-\left\{\rho_m \frac{D}{Dt}\left(\sum_{k=1}^{2} \frac{\alpha_k \overline{\overline{\rho_k}} V_{km}^2}{\rho_m} \frac{V_{km}^2}{2}\right) + \nabla \cdot \sum_{k=1}^{2} \alpha_k \overline{\overline{\rho_k}} \frac{V_{km}^2}{2} V_{km}\right\}$$

$$+\left(\overline{\overline{\mathcal{T}}} + \mathcal{T}^T + \mathcal{T}^D\right) : \nabla v_m$$

$$+\left(E_m - M_m \cdot v_m\right) + \nabla \cdot \left\{\sum_{k=1}^{2} \alpha_k \left(\overline{\overline{\mathcal{T}_k}} + \mathcal{T}^T\right) \cdot V_{km}\right\}.$$

With the alternative definition of the turbulent heat flux such as Eq.(5-30)', the energy equations become symmetrical about the stress tensor term. The energy equations with the definition of Eq.(5-30)' are identical with those with the definition of Eq.(5-30). However, the energy equations with the definition of Eq.(5-30)' may be controversial and misleading on the following grounds. For example, the apparent energy dissipation term due to the turbulent stress such as $\alpha_k \mathcal{T}_k^T : \nabla \widehat{v_k}$ appears in the internal energy equation of Eq.(5-36)'. Since this term is due to convection or turbulence, it may take a negative or positive value. Thus, the term due to turbulent work may not be regarded as the energy dissipation, which should invariably be positive. In order for the term due to turbulent work to be invariably positive, some additional constraints may be applied to the entropy inequality. Thus, the energy equations with the definition of Eq.(5-30)' are questionable to explain irreversible thermodynamics.