# 13 Numerical methods for multi-phase flow in curvilinear coordinate systems

*This chapter presents a numerical solution method for multi-phase flow analysis based on local volume and time averaged conservation equations. The emphasis of this development was to create a computer code architecture that absorb all the constitutive physics and functionality from the past 25years development of the three fluid multi-component IVA-entropy concept for multi-phase flows into a boundary fitted orthogonal coordinate framework. Collocated discretization for the momentum equations is used followed by weighted averaging for the staggered grids resulting in analytical expressions for the normal velocities. Using the entropy concept analytical reduction to a pressure-velocity coupling is found. The performance of the method is demonstrated by comparison of two cases for which experimental results and numerical solution with the previous method are available. The agreement demonstrates the success of this development.*

## 13.1 Introduction

We extend now the method described in the previous chapter to more arbitrary geometry. Instead of considering Cartesian or cylindrical geometry only, we will consider an integration space called a *block* in which the computational finite volumes fit inside the block so that the outermost faces of the external layer of the finite volumes create the face of the block. Similarly, bodies immersed into this space have external faces identical with the faces of the environmental computational cells. Such blocks can be inter-connected. With this technology multi-phase flows in arbitrary interfaces can be conveniently handled.

For understanding the material presented in this section I strongly recommend going over Appendixes 1 and 2 before continuing reading.

Before starting with the description of the new method let us summarize briefly the state of the art in this field.

In the last ten years the numerical modeling of single-phase flow in boundary fitted coordinates is becoming standard in the industry. This is not the case with the numerical modeling of multiphase flows. There are some providers of single-phase-computer codes claming that their codes can simulate multi-phase flows. Taking close looks of the solution methods of these codes reveals that existing single phase solvers are used and a provision is given to the user to add an other velocity field and define explicit the interfacial interaction physics. This strategy does not account for the feed back of the strong interfacial interactions on the mathematical solution methods - see the discussion in *Miettinen* and *Schmidt* (2002). Multi-phase flow simulations require specific solution methods accounting for this specific physics - see for instance the discussion by *Antal* et al. (2000).

There are groups of methods that are solving single phase conservation equations with surface tracking, see the state of the art part of *Tryggavson* et al. (2001) work. This is in fact a direct numerical simulation that is outside of the scope of this chapter. To mention few of them: In Japan a powerful family of cubic-interpolation methods (CIP) is developed based on the pseudo-characteristic method of lines *Takewaki*, *Nishiguchi* and *Yabe* (1985), *Takewaki* and *Yabe* (1987), *Nakamura*, *Tanaka*, *Yabe* and *Takizawa* (2001), *Yabe*, *Xiao* and *Utsumi* (2001), *Yabe*, *Tanaka*, *Nakamura* and *Xiao* (2001), *Yabe*, *Xiao* and *Utsumi* (2001), *Yabe* and *Takei* (1988), *Xiao* and *Yabe* (2001), *Xiao*, *Yabe*, *Peng* and *Kobayashi* (2002), *Xiao* (2003), *Xiao* and *Ikebata* (2003), *Yabe* and *Wang* (1991), *Yabe* and *Aoki* (1991), *Yabe* et al. (1991). In USA particle tracking and level-set surface tracking methods are very popular; see for instance *Sussman*, *Smereka* and *Oslier* (1994), *Osher* and *Fredkiw* (2003), *Swthian* (1996), *Tryggavson* at al. (2001). The third group of DNS method with surface tracking is the lattice-*Boltzman* family, see *Hou* et al. (1995), *Nourgaliev* et al. (2002) and the references given there. To the family of emerging methods the so called diffuse interface methods based on high order thermodynamics can be mentioned, see *Verschueren* (1999), *Jamet* et al. (2001). Let as emphasize once again, that unlike those methods, our work is concentrated on methods solving the local volume and time averaged multiphase flow equations which are much different then the single phase equations.

In Europe two developments for solving two-fluid conservation equations in unstructured grids are known to me. *Staedke* et al. (1998) developed a solution method based on the method of characteristics using unstructured grid in a single domain. The authors added artificial terms to enforce hyperbolicy in the initially incomplete system of partial differential equations that contain derivatives which do not have any physical meaning. *Toumi* et al. (2000) started again from the incomplete system for two-fluid two phase flows without interaction terms and included them later for a specific class of processes; see *Kumbaro* et al. (2002). These authors extended the approximate *Riemann* solver originally developed for single phase flows by *Roe* to two-fluid flows. One application example of the method is demonstrated in a single space domain in *Toumi* et al. (2000), *Kumbaro* et al. (2002). No industrial applications of these two methods have been reported so far. One should note that it is well know that if proper local volume averaging is applied the originating interfacial interaction terms provide naturally hyperbolicy of the system of PDS and there is no need for artificial terms without any physical meaning. An example for the resolution of this problem is given by *van Wijngaarden* in 1976 among many others.

In USA *Lahey* and *Drew* demonstrated clearly in 1999 haw by careful elaboration of the constitutive relationships starting from first principles variety of steady state processes including *frequency dependent acoustics* can be successfully simulated. Actually, the idea by *Lahey* and *Drew* (1999) is a further development of the proposal made by *Harlow* and *Amsden* in 1975 where liquid (1) in vapor (2) and vapor (3) in liquid (4) are grouped in two velocity fields 1 + 2 and 3 + 4. The treatment of *Lahey* and *Drew* (1999) is based on four velocity fields. *Antal* et al. (2000) started developing the NPHASE multi-domain multi-phase flows code based on the single phase *Rhie* and *Chow* numerical method extended to multiphase flows. Application example is given for T-pipe bubble flows with 10 groups of bubble diameters. Two works that can be considered as a subset of this approach are reported in *Tomiyama* et al. (2000) *Gregor*, *Petelin* and *Tiselj* (2000). Another direction of development in USA that can be observed is the use of the volume of fluid method with computing the surface tension force as a volumetric force *Hirt* (1993), *Kothe* et al. (1996), *Brackbill* et al. (1992), *Rider* and *Kothe* (1998).

## 13.2 Nodes, grids, meshes, topology - some basic definitions

**Database concept:** Let as consider the data base concept. The data volume is made up of points, or *nodes*, which themselves define in their neighborhood a volume element. We use hexahedrons (Fig. 4 in Appendix 1). A hexahedron is a 3D volume element with six sides and eight vertices. The vertices are connected in an order that mimics the way nodes are numbered in the data volume. The nodes in the data volume are numbered by beginning with 1 at the data volume's origin. Node numbering increases, with $x$ changing fastest. This means node numbering increases along the $x$ axis first, the $y$ axis second, and the $z$ axis last, until all nodes are numbered. The numbering of the vertices of the volume elements follows the same rule. It starts with the vertex being closest to the data volume's origin, moves along $x$, then $y$, and then $z$.

**Grid:** A *grid* is a set of locations in a 3D data volume defined with $x$, $y$, and $z$ coordinates. The locations are called *nodes*, which are connected in a specific order to create the topology of the grid. A grid can be regular or irregular depending on how its nodes are represented as points.

A *regular grid*'s nodes are evenly spaced in $x$, $y$, and $z$ directions, respectively. A *regular grid*'s nodes are specified with $x$, $y$, and $z$ offsets from the data volume's origin. A regular grid may have equidistant or non-equidistant spacing. If equidistant spacing is used all areas of the data volumes have the same resolution. This suits data with regular sample intervals.

An *irregular grid*'s nodes need not be evenly spaced or in a rectangular configuration. This suits data with a specific area of interest that require finer sampling. Because nodes may not be evenly spaced, each node's $xyz$ coordinates must be explicitly listed.

**Topology:** A *topology* defines an array of elements by specifying the connectivity of the element's vertices or nodes. It builds a volume from separate elements by specifying how they are connected together. The elements can be

3D volume elements or 2D surface elements. A topology is either regular or irregular, depending upon what types of elements it defines and how they are structured.

A *regular topology* defines a data volume's node connectivity. We assume a hexahedron volume element type. A regular topology can be used for regular or irregular grids.

An *irregular topology* defines the node connectivity of either a data volume or geometric surface elements. An irregular topology data volume can be composed of either hexahedron or tetrahedron volume elements. Geometry objects are composed of points, lines, or polygons. An element list has to explicitly specify how the nodes connect to form these elements.

**Volume elements:** The volume elements are the smallest building blocks of a data volume topology.

**Mesh:** A *mesh* is a grid combined with specific topology for the volume of data. We distinguish the following mesh types: regular meshes, irregular or structured meshes, unstructured meshes, and geometry meshes.

A *regular mesh* consists of grid having regular spacing and regular topology that consists of simple, rectangular array of volume elements.

An *irregular mesh* explicitly specifies the *xyz* coordinates of each node in a node list. As in the regular mesh, the topology is regular, although individual elements are formed by explicit *xyz* node locations. The grid may be irregular or rectilinear.

An unstructured mesh explicitly defines the topology. Each topology element is explicitly defined by its node connectivity in an element list. The grid may be regular or irregular.

In this sense we are dealing in this Chapter with *multi-blocks* each of them consisting of

- irregular grid's nodes, irregular meshes,
- regular topology with hexahedron volume element type.

The integration space is built by a specified number of interconnected blocks.

## 13.3 Formulation of the mathematical problem

Consider the following mathematical problem: A multi-phase flow is described by the following vector of dependent variables

$$\mathbf{U}^T = (\alpha_m, T_1, s_2, s_3, C_{il}, n_l, p, u_l, v_l, w_l),$$

where

$$l = 1,\ 2,\ 3,\ i1 = 1...n1,\ i2 = 1...n2,\ i3 = 1...n3$$

which is a function of the three space coordinates $(x, y, z)$, and of the time $\tau$,

$$\mathbf{U} = \mathbf{U}(x, y, z, \tau).$$

The relationship $\mathbf{U} = \mathbf{U}(x, y, z, \tau)$ is defined by the volume-averaged and successively time-averaged mass, momentum and energy conservation equations derived in Chapters 1, 2, 5 *Kolev* (1994a, b, 1995, 1997, 1998) as well as by initial conditions, boundary conditions, and geometry. The conservation equations are transformed in a curvilinear coordinate system $\xi, \eta, \zeta$ as shown in Chapter 11, *Kolev* (2001). The flux form of these equations is given in Chapter 11. As shown in Chapter 11, *Kolev* (2001), the conservation principles lead to a system of 19+*n1*+*n2*+*n3* non-linear, non-homogeneous partial differential equations with variable coefficients. This system is defined in the three-dimensional domain **R**. The initial conditions of $\mathbf{U}(\tau = 0) = \mathbf{U}_a$ in **R** and the boundary conditions acting at the interface separating the integration space from its environment are given. The solution required is for conditions after the time interval $\Delta\tau$ has elapsed. The previous time variables are assigned the index *a*. The time variables not denoted with *a* are either in the new time plane, or are the best available guesses for the new time plane.

In order to enable modeling of flows with arbitrary obstacles and inclusions in the integration space as is usually expected for technical applications, surface permeabilities are defined

$$(\gamma_\xi, \gamma_\eta, \gamma_\zeta) = \text{functions of } (\xi, \eta, \zeta, \tau),$$

at the virtual surfaces that separate each computational cell from its environment. By definition, the surface permeabilities have values between one and zero,

$$0 \le \text{each of all } (\gamma_\xi, \gamma_\eta, \gamma_\zeta)\text{'s} \le 1.$$

A volumetric porosity

$$\gamma_v = \gamma_v(\xi, \eta, \zeta, \tau)$$

is assigned to each computational cell, with

$$0 < \gamma_v \le 1.$$

The surface permeabilities and the volume porosities are not expected to be smooth functions of the space coordinates in the region **R** and of time. For this reason, one constructs a frame of geometrical flow obstacles which are functions of space and time. This permits a large number of extremely interesting technical applications of this type of approach.

In order to construct useful numerical solutions it is essential that an appropriate set of constitutive relations be available: state equations, thermodynamic derivatives, equations for estimation of the transport properties, correlations modeling the heat, mass and momentum transport across the surfaces dividing the separate velocity fields, etc. These relationships together are called closure equations. This very complex problem will not be discussed in Volume II. Only the numerics will be addressed here.

# 13.4 Discretization of the mass conservation equations

## 13.4.1 Integration over a finite time step and finite control volume

We start with the conservation equation (10.56) for the species $i$ inside the velocity field $l$ in the curvilinear coordinate system

$$\frac{\partial}{\partial\tau}\left(\alpha_l\rho_l C_{il}\sqrt{g}\,\gamma_v\right)+\frac{\partial}{\partial\xi}\left(\gamma_\xi\sqrt{g}\,\mathbf{a}^1\cdot\mathbf{G}_{il}\right)+\frac{\partial}{\partial\eta}\left(\gamma_\eta\sqrt{g}\,\mathbf{a}^2\cdot\mathbf{G}_{il}\right)$$
$$+\frac{\partial}{\partial\zeta}\left(\gamma_\zeta\sqrt{g}\,\mathbf{a}^3\cdot\mathbf{G}_{il}\right)=\gamma_v\sqrt{g}\,\mu_{il}, \tag{13.1}$$

where the species mass flow rate vector is defined as follows

$$\mathbf{G}_{il}=\alpha_l\rho_l\left[C_{il}\left(\mathbf{V}_l-\mathbf{V}_{cs}\right)-D_{il}^*\left(\mathbf{a}^1\frac{\partial C_{il}}{\partial\xi}+\mathbf{a}^2\frac{\partial C_{il}}{\partial\eta}+\mathbf{a}^3\frac{\partial C_{il}}{\partial\zeta}\right)\right]. \tag{13.2}$$

Note that for $C_{il}=1$ we have the mass flow vector of the velocity field

$$\mathbf{G}_l=\alpha_l\rho_l\left(\mathbf{V}_l-\mathbf{V}_{cs}\right). \tag{13.3}$$

Next we will use the following basic relationships from Appendix 2 between the surface vectors and the contravariant vectors, and between the *Jacobian* determinant and the infinitesimal spatial and volume increments

$$\sqrt{g}\mathbf{a}^1=\frac{\mathbf{S}^1}{\partial\eta\partial\zeta},\ \sqrt{g}\mathbf{a}^2=\frac{\mathbf{S}^2}{\partial\xi\partial\zeta},\ \sqrt{g}\mathbf{a}^3=\frac{\mathbf{S}^3}{\partial\xi\partial\eta},\ \sqrt{g}=\frac{dV}{d\xi d\eta d\zeta}. \tag{13.4-7}$$

We will integrate both sides of the equation over the time, and spatial intervals $\partial\tau$, $\partial\xi$, $\partial\eta$, and $\partial\zeta$ respectively. We start with the first term

$$\iiint\limits_{\Delta V}\left[\int_0^{\Delta\tau}\frac{\partial}{\partial\tau}\left(\alpha_l\rho_l C_{il}\sqrt{g}\,\gamma_v\right)\partial\tau\right]\partial\xi\partial\eta\partial\zeta=\left[\int_0^{\Delta\tau}\frac{\partial}{\partial\tau}\left(\alpha_l\rho_l C_{il}\gamma_v\right)\partial\tau\right]\iiint\limits_{\Delta V}dV$$
$$=\left[\left(\alpha_l\rho_l C_{il}\gamma_v\right)-\left(\alpha_l\rho_l C_{il}\gamma_v\right)_a\right]\Delta V\,. \tag{13.8}$$

This result is obtained under the assumption that there is no spatial variation of the properties $\left(\alpha_l\rho_l C_{il}\gamma_v\right)$ inside the cell. The integration of the other terms gives the following results:

$$\int_0^{\Delta\tau}\iiint\limits_{\Delta V}\frac{\partial}{\partial\xi}\left(\gamma_\xi\sqrt{g}\,\mathbf{a}^1\cdot\mathbf{G}_{il}\right)\partial\xi\partial\eta\partial\zeta\partial\tau=\Delta\tau\int_0^{\Delta\xi}\frac{\partial}{\partial\xi}\left(\gamma_\xi\mathbf{S}^1\cdot\mathbf{G}_{il}\right)\partial\xi$$
$$=\Delta\tau\left[\left(\gamma_\xi\mathbf{S}^1\cdot\mathbf{G}_{il}\right)-\left(\gamma_\xi\mathbf{S}^1\cdot\mathbf{G}_{il}\right)_{i-1}\right]$$

$$= \Delta\tau\Delta V\left[\gamma_\xi \frac{S_1}{\Delta V}\left(\mathbf{e}^1 \cdot \mathbf{G}_{il}\right) - \gamma_{\xi,i-1}\frac{S_2}{\Delta V}\left(\mathbf{e}^1 \cdot \mathbf{G}_{il}\right)_{i-1}\right], \qquad (13.9)$$

$$\int_0^{\Delta\tau}\iiint\limits_{\Delta V}\frac{\partial}{\partial\eta}\left(\gamma_\eta\sqrt{g}\,\mathbf{a}^2\cdot\mathbf{G}_{il}\right)\partial\xi\partial\eta\partial\zeta\partial\tau = \Delta\tau\int_0^{\Delta\eta}\frac{\partial}{\partial\eta}\left(\gamma_\eta\mathbf{S}^2\cdot\mathbf{G}_{il}\right)\partial\eta$$

$$= \Delta\tau\left[\left(\gamma_\eta\mathbf{S}^2\cdot\mathbf{G}_{il}\right) - \left(\gamma_\eta\mathbf{S}^2\cdot\mathbf{G}_{il}\right)_{j-1}\right]$$

$$= \Delta\tau\Delta V\left[\gamma_\eta \frac{S_3}{\Delta V}\left(\mathbf{e}^2 \cdot \mathbf{G}_{il}\right) - \gamma_{\eta,j-1}\frac{S_4}{\Delta V}\left(\mathbf{e}^2 \cdot \mathbf{G}_{il}\right)_{j-1}\right], \qquad (13.10)$$

$$\int_0^{\Delta\tau}\iiint\limits_{\Delta V}\frac{\partial}{\partial\zeta}\left(\gamma_\zeta\sqrt{g}\,\mathbf{a}^3\cdot\mathbf{G}_{il}\right)\partial\xi\partial\eta\partial\zeta\partial\tau = \Delta\tau\int_0^{\Delta\zeta}\frac{\partial}{\partial\zeta}\left(\gamma_\zeta\mathbf{S}^3\cdot\mathbf{G}_{il}\right)\partial\zeta$$

$$= \Delta\tau\left[\left(\gamma_\zeta\mathbf{S}^3\cdot\mathbf{G}_{il}\right) - \left(\gamma_\zeta\mathbf{S}^3\cdot\mathbf{G}_{il}\right)_{k-1}\right]$$

$$= \Delta\tau\Delta V\left[\gamma_\zeta \frac{S_5}{\Delta V}\left(\mathbf{e}^3 \cdot \mathbf{G}_{il}\right) - \gamma_{\zeta,k-1}\frac{S_6}{\Delta V}\left(\mathbf{e}^3 \cdot \mathbf{G}_{il}\right)_{k-1}\right], \qquad (13.11)$$

$$\int_0^{\Delta\tau}\iiint\limits_{\Delta V}\gamma_v\sqrt{g}\,\mu_{il}\partial\xi\partial\eta\partial\zeta\partial\tau = \Delta\tau\iiint\limits_{\Delta V}\gamma_v\mu_{il}dV = \Delta\tau\gamma_v\mu_{il}\Delta V\,. \qquad (13.12)$$

It is convenient to introduce the numbering at the surfaces of the control volumes 1 to 6 corresponding to high-$i$, low-$i$, high-$j$, low-$j$, high-$k$ and low-$k$, respectively. We first define the unit surface vector $(\mathbf{e})^m$ at each surface $m$ as outwards directed:

$$(\mathbf{e})^1 = \mathbf{e}^1,\ (\mathbf{e})^2 = -\mathbf{e}^1_{i-1},\ (\mathbf{e})^3 = \mathbf{e}^2,\ (\mathbf{e})^4 = -\mathbf{e}^2_{j-1},\ (\mathbf{e})^5 = \mathbf{e}^3,\ (\mathbf{e})^6 = -\mathbf{e}^3_{k-1}. \qquad (13.13\text{-}18)$$

With this we have a short notation of the corresponding discretized concentration conservation equation

$$\alpha_l\rho_l C_{il}\gamma_v - \alpha_{la}\rho_{la}C_{ila}\gamma_{va} + \Delta\tau\sum_{m=1}^{6}\beta_m(\mathbf{e})^m\cdot\mathbf{G}_{il,m} = \Delta\tau\gamma_v\mu_{il}\,. \qquad (13.19)$$

We immediately recognize that it is effective to compute once the geometry coefficients

$$\beta_1 = \gamma_\xi\frac{S_1}{\Delta V},\ \beta_2 = \gamma_{\xi,i-1}\frac{S_2}{\Delta V},\ \beta_3 = \gamma_\eta\frac{S_3}{\Delta V},\ \beta_4 = \gamma_{\eta,j-1}\frac{S_4}{\Delta V},$$

$$\beta_5 = \gamma_\zeta\frac{S_5}{\Delta V},\ \beta_6 = \gamma_{\zeta,k-1}\frac{S_6}{\Delta V}, \qquad (13.20\text{-}25)$$

before the process simulation, to store them, and to update only those that change during the computation. Secondly, we see that these coefficients contain exact physical geometry information. Note that for cylindrical coordinate systems we have

$$\beta_1 = \frac{r_h^\kappa \gamma_r}{r^\kappa \Delta r}, \ \beta_2 = \frac{(r_h^\kappa \gamma_r)_{i-1}}{r^\kappa \Delta r}, \ \beta_3 = \frac{\gamma_\theta}{r^\kappa \Delta \theta}, \ \beta_4 = \frac{\gamma_{\theta,j-1}}{r^\kappa \Delta \theta},$$

$$\beta_5 = \frac{\gamma_z}{\Delta z}, \ \beta_6 = \frac{\gamma_{z,k-1}}{\Delta z}, \tag{13.26-31}$$

and for Cartesian setting $\kappa = 0$ and $r = x$, $\theta = y$,

$$\beta_1 = \frac{\gamma_x}{\Delta x}, \ \beta_2 = \frac{\gamma_{x,i-1}}{\Delta x}, \ \beta_3 = \frac{\gamma_y}{\Delta y}, \ \beta_4 = \frac{\gamma_{y,j-1}}{\Delta y}, \ \beta_5 = \frac{\gamma_z}{\Delta z}, \ \beta_6 = \frac{\gamma_{z,k-1}}{\Delta z}, \tag{13.32-39}$$

compare with Section 11.4. Setting $C_{il} = 1$ in Eq. (13.19) we obtain the discretized mass conservation equation of each velocity field

$$\alpha_l \rho_l \gamma_v - \alpha_{la} \rho_{la} \gamma_{va} + \Delta\tau \sum_{m=1}^{6} \beta_m (\mathbf{e})^m \cdot \mathbf{G}_{l,m} = \Delta\tau \gamma_v \mu_l . \tag{13.40}$$

Next we derive the useful non-conservative form of the concentration equations. We multiply Eq. (13.40) by the concentration at the new time plane and subtract the resulting equation from Eq. (13.19). Then the field mass source term is split in two non-negative parts $\mu_l = \mu_l^+ + \mu_l^-$. The result is

$$\alpha_{la} \rho_{la} \left( C_{il} - C_{ila} \right) \gamma_{va} + \Delta\tau \sum_{m=1}^{6} \beta_m (\mathbf{e})^m \cdot \left( \mathbf{G}_{il,m} - C_{il} \mathbf{G}_{l,m} \right) + \Delta\tau \gamma_v \mu_l^+ C_{il} = \Delta\tau \gamma_v DC_{il} . \tag{13.41}$$

where $DC_{il} = \mu_{il} + \mu_l^- C_{il}$. Note that

$$\mathbf{G}_{il,m} - C_{il} \mathbf{G}_{l,m}$$
$$= \left[ \alpha_l \rho_l \left( \mathbf{V}_l - \mathbf{V}_{cs} \right) \right]_m \left( C_{il,m} - C_{il} \right) - \left[ \alpha_l \rho_l D_{il}^* \left( \mathbf{a}^1 \frac{\partial C_{il}}{\partial \xi} + \mathbf{a}^2 \frac{\partial C_{il}}{\partial \eta} + \mathbf{a}^3 \frac{\partial C_{il}}{\partial \zeta} \right) \right]_m . \tag{13.42}$$

Up to this point of the derivation we did not made any assumption about the computation of the properties at the surfaces of the control volume.

### 13.4.2 The donor-cell concept

The concept of the so called *donor-cell* for the convective terms is now introduced. Flow of given scalars takes the values of the scalars at the cell where the flow is coming from. Mathematically it is expressed as follows. First we define velocity normal to the cell surfaces and outwards directed

$$V_{l,m}^n = (\mathbf{e})^m \cdot \left( \mathbf{V}_l - \mathbf{V}_{cs} \right)_m , \tag{13.43}$$

then the switch functions (to store them use *signet integers* in computer codes, it saves memory)

$$\xi_{lm+} = \frac{1}{2}\left[1 + sign\left(V_{lm}^{n}\right)\right], \tag{13.44}$$

$$\xi_{lm-} = 1 - \xi_{lm+}, \tag{13.45}$$

and then the $b$ coefficients as follows

$$b_{lm+} = \beta_m \xi_{lm+} V_{lm}^{n} \geq 0, \tag{13.46}$$

$$b_{lm-} = -\beta_m \xi_{lm-} V_{lm}^{n} \geq 0. \tag{13.47}$$

If the normal outwards directed velocity is positive the $+b$ coefficients are unity and the $-b$ coefficients are zero and vice versa. In this case the normal mass flow rate at the surfaces is

$$(\mathbf{e})^{m} \cdot \mathbf{G}_{l,m} = \left[\alpha_l \rho_l \mathbf{e} \cdot \left(\mathbf{V}_l - \mathbf{V}_{cs}\right)\right]_m = \left(\xi_{lm+}\alpha_l \rho_l + \xi_{lm-}\alpha_{l,m}\rho_{l,m}\right) V_{lm}^{n}. \tag{13.48}$$

Using the above result the mass conservation equations for each field result is

$$\alpha_l \rho_l \gamma_v - \alpha_{la}\rho_{la}\gamma_{va} + \Delta\tau \sum_{m=1}^{6}\left(b_{lm+}\alpha_l \rho_l - B_{lm-}\right) - \Delta\tau \gamma_v \mu_l = 0. \tag{13.49}$$

In the donor-cell concept the term

$$B_{lm-} = b_{lm-}\alpha_{l,m}\rho_{l,m} \tag{13.50}$$

plays an important role. $B_{lm-}$ is in fact the mass flow entering the cell from the face $m$ divided by the volume of the cell. Once computed for the mass conservation equation it is stored and used subsequently in all other conservation equations.

At this point the method used for computation of the field volumetric fractions by iteration using the point *Gauss-Seidel* method for known velocity vectors and thermal properties will be described.

Consider the field variables $\alpha_l \rho_l$ in the convective terms associated with the output flow in the new time plane, and $\alpha_{lm}\rho_{lm}$ in the neighboring cells $m$ as the best available guesses for the new time plane. Solving Eq. (13.49) with respect to $\alpha_l \rho_l$ gives

$$\overline{\alpha}_l \overline{\rho}_l = \left[\gamma_{va}\left(\mu_l + \frac{\alpha_{la}\rho_{la}}{\Delta\tau}\right) + \sum_{m=1}^{6} B_{lm-}\right] \Bigg/ \left(\frac{\gamma_v}{\Delta\tau} + \sum_{m=1}^{6} b_{lm+}\right). \tag{13.51}$$

Here

$$\frac{\gamma_v}{\Delta\tau} + \sum_{m=1}^{6} b_{lm+} > 0 \tag{13.52}$$

is ensured because $\gamma_v$ is not allowed to be zero. For a field that is just originating we have

$$\overline{\alpha}_l = \frac{\Delta\tau}{\overline{\rho}_l} \frac{\gamma_{va}\mu_l + \sum_{m=1}^{6} B_{lm-}}{\gamma_v + \Delta\tau \sum_{m=1}^{6} b_{lm+}}. \qquad (13.53)$$

Obviously the field can originate due to convection, $\sum_{m=1}^{6} B_{lm-} > 0$, or due to an in-cell mass source, $\mu_l > 0$, or due to the simultaneous appearance of both phenomena. In case of origination caused by in-cell mass source terms it is important to define the initial density, $\overline{\rho}_l$, in order to compute $\overline{\alpha}_l = \Delta\tau\mu_l / \overline{\rho}_l$.

The best mass conservation in such procedures is ensured if the following sequence is used for computation of the volume fractions:

$$\alpha_2 = \overline{\alpha}_2\overline{\rho}_2 / \rho_2, \; \alpha_3 = \overline{\alpha}_3\overline{\rho}_3 / \rho_3, \; \alpha_1 = 1 - \alpha_2 - \alpha_3. \qquad (13.54\text{-}56)$$

For designing the pressure-velocity coupling the form of the discretized mass conservation is required that explicitly contains the normal velocities,

$$(\alpha_l\rho_l\gamma_v - \alpha_{la}\rho_{la}\gamma_{va}) / \Delta\tau + \sum_{m=1}^{6} \beta_m \left(\xi_{lm+}\alpha_l\rho_l + \xi_{lm-}\alpha_{lm}\rho_{lm}\right)V_{lm}^n - \gamma_v\mu_l = 0. \qquad (13.57)$$

The mass flow rate of the species *i* inside the field *l* at the cell surface *m* is then

$$(\mathbf{e})^m \cdot \mathbf{G}_{il,m} = \left[\alpha_l\rho_l C_{il}\mathbf{e}\cdot\left(\mathbf{V}_l - \mathbf{V}_{cs}\right)\right]_m - \left[\alpha_l\rho_l D_{il}^*\mathbf{e}\cdot\left(\mathbf{a}^1\frac{\partial C_{il}}{\partial\xi} + \mathbf{a}^2\frac{\partial C_{il}}{\partial\eta} + \mathbf{a}^3\frac{\partial C_{il}}{\partial\zeta}\right)\right]_m$$

$$= \left(\xi_{lm+}\alpha_l\rho_l C_{il} + \xi_{lm-}\alpha_{l,m}\rho_{l,m}C_{il,m}\right)V_{lm}^n - \left[\alpha_l\rho_l D_{il}^*\mathbf{e}\cdot\left(\mathbf{a}^1\frac{\partial C_{il}}{\partial\xi} + \mathbf{a}^2\frac{\partial C_{il}}{\partial\eta} + \mathbf{a}^3\frac{\partial C_{il}}{\partial\zeta}\right)\right]_m, \qquad (13.58)$$

and consequently

$$(\mathbf{e})^m \cdot \left(\mathbf{G}_{il,m} - C_{il}\mathbf{G}_{l,m}\right)$$

$$= \xi_{lm-}\alpha_{l,m}\rho_{l,m}V_{lm}^n\left(C_{il,m} - C_{il}\right) - \left[\alpha_l\rho_l D_{il}^*\mathbf{e}\cdot\left(\mathbf{a}^1\frac{\partial C_{il}}{\partial\xi} + \mathbf{a}^2\frac{\partial C_{il}}{\partial\eta} + \mathbf{a}^3\frac{\partial C_{il}}{\partial\zeta}\right)\right]_m. \qquad (13.59)$$

Thus Eq. (13.41) takes the intermediate form

$$\alpha_{la}\rho_{la}\left(C_{il}-C_{ila}\right)\gamma_{va}-\Delta\tau\sum_{m=1}^{6}\left\{\begin{array}{l}B_{lm-}\left(C_{il,m}-C_{il}\right)\\ +\beta_m\left[\alpha_l\rho_l D_{il}^{*}\mathbf{e}\cdot\left(\mathbf{a}^1\dfrac{\partial C_{il}}{\partial\xi}+\mathbf{a}^2\dfrac{\partial C_{il}}{\partial\eta}+\mathbf{a}^3\dfrac{\partial C_{il}}{\partial\zeta}\right)\right]_m\end{array}\right\}$$

$$=\Delta\tau\gamma_v\left(\mu_{il}-C_{il}\mu_l\right). \tag{13.60}$$

### 13.4.3 Two methods for computing the finite difference approximations of the contravariant vectors at the cell center

The contravariant vectors for each particular surface can be expressed by

$$\mathbf{a}^1=\frac{\mathbf{S}^1}{dV}\partial\xi,\ \mathbf{a}^2=\frac{\mathbf{S}^2}{dV}\partial\eta,\ \mathbf{a}^3=\frac{\mathbf{S}^3}{dV}\partial\zeta. \tag{13.61-63}$$

Note that the contravariant vectors normal to each control volume surface are conveniently computed for **equidistant discretization in the computational space** as follows

$$\left(\mathbf{a}^1\right)_1=\frac{\mathbf{S}^1}{\overline{\Delta V_1}}=\frac{\left(\mathbf{S}\right)_1}{\overline{\Delta V_1}}=\frac{S_1}{\overline{\Delta V_1}}\left(\mathbf{e}\right)^1,\quad \left(\mathbf{a}^1\right)_2=\frac{\mathbf{S}^1}{\overline{\Delta V_2}}=-\frac{\left(\mathbf{S}\right)_2}{\overline{\Delta V_2}}=-\frac{S_2}{\overline{\Delta V_2}}\left(\mathbf{e}\right)^2, \tag{13.64-65}$$

$$\left(\mathbf{a}^2\right)_3=\frac{\mathbf{S}^2}{\overline{\Delta V_3}}=\frac{\left(\mathbf{S}\right)_3}{\overline{\Delta V_3}}=\frac{S_3}{\overline{\Delta V_3}}\left(\mathbf{e}\right)^3,\quad \left(\mathbf{a}^2\right)_4=\frac{\mathbf{S}^2}{\overline{\Delta V_4}}=-\frac{\left(\mathbf{S}\right)_4}{\overline{\Delta V_4}}=-\frac{S_4}{\overline{\Delta V_4}}\left(\mathbf{e}\right)^4, \tag{13.66-67}$$

$$\left(\mathbf{a}^3\right)_5=\frac{\mathbf{S}^3}{\overline{\Delta V_5}}=\frac{\left(\mathbf{S}\right)_5}{\overline{\Delta V_5}}=\frac{S_5}{\overline{\Delta V_5}}\left(\mathbf{e}\right)^5,\quad \left(\mathbf{a}^3\right)_6=\frac{\mathbf{S}^3}{\overline{\Delta V_6}}=-\frac{\left(\mathbf{S}\right)_6}{\overline{\Delta V_6}}=-\frac{S_6}{\overline{\Delta V_6}}\left(\mathbf{e}\right)^6, \tag{13.68-69}$$

where the volume associated with these vectors is

$$\overline{\Delta V_m}=\frac{1}{2}\left(\Delta V+\Delta V_m\right). \tag{13.70}$$

*The finite volume method*: There are two practicable methods for approximation of the contravariant vectors at the cell center. The first one makes use of the already computed normal interface vectors in the following way:

$$\mathbf{a}_c^1=\frac{1}{2}\left[\left(\mathbf{a}^1\right)_1+\left(\mathbf{a}^1\right)_2\right],\ \mathbf{a}_c^2=\frac{1}{2}\left[\left(\mathbf{a}^2\right)_3+\left(\mathbf{a}^2\right)_4\right],\ \mathbf{a}_c^3=\frac{1}{2}\left[\left(\mathbf{a}^3\right)_5+\left(\mathbf{a}^3\right)_6\right] \tag{13.71-73}$$

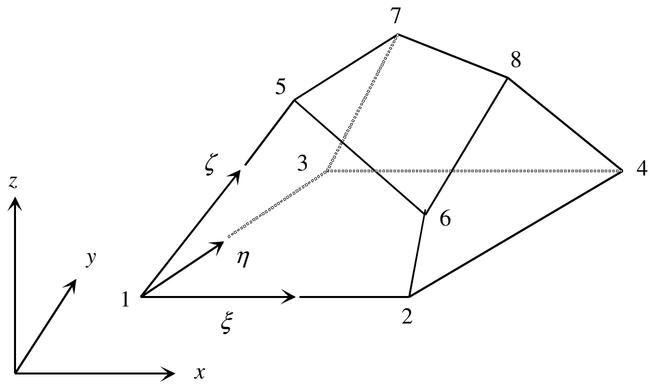


**Fig. 13.1** Numbering of the vertices

*The finite difference method*: The second method uses the coordinates of the vertices of the control volume directly, Fig. 13.1. First we define the position at the cell surfaces that will be used to compute the transformation metrics as follows:

$$\mathbf{r}_{S1} = \frac{1}{4}\left(\mathbf{r}_2 + \mathbf{r}_4 + \mathbf{r}_8 + \mathbf{r}_6\right), \qquad \mathbf{r}_{S2} = \frac{1}{4}\left(\mathbf{r}_1 + \mathbf{r}_3 + \mathbf{r}_7 + \mathbf{r}_5\right), \tag{13.74-75}$$

$$\mathbf{r}_{S3} = \frac{1}{4}\left(\mathbf{r}_3 + \mathbf{r}_4 + \mathbf{r}_8 + \mathbf{r}_7\right), \qquad \mathbf{r}_{S4} = \frac{1}{4}\left(\mathbf{r}_1 + \mathbf{r}_2 + \mathbf{r}_6 + \mathbf{r}_5\right), \tag{13.76-77}$$

$$\mathbf{r}_{S5} = \frac{1}{4}\left(\mathbf{r}_5 + \mathbf{r}_6 + \mathbf{r}_8 + \mathbf{r}_7\right), \qquad \mathbf{r}_{S6} = \frac{1}{4}\left(\mathbf{r}_1 + \mathbf{r}_2 + \mathbf{r}_4 + \mathbf{r}_3\right). \tag{13.78-79}$$

Then we compute the *inverse metrics* of the coordinate transformation for **equidistant discretization in the transformed space**

$$\begin{pmatrix} \dfrac{\partial x}{\partial \xi} & \dfrac{\partial x}{\partial \eta} & \dfrac{\partial x}{\partial \zeta} \\ \dfrac{\partial y}{\partial \xi} & \dfrac{\partial y}{\partial \eta} & \dfrac{\partial y}{\partial \zeta} \\ \dfrac{\partial z}{\partial \xi} & \dfrac{\partial z}{\partial \eta} & \dfrac{\partial z}{\partial \zeta} \end{pmatrix} = \begin{pmatrix} x_{s1} - x_{s2} & x_{s3} - x_{s4} & x_{s5} - x_{s6} \\ y_{s1} - y_{s2} & y_{s3} - y_{s4} & y_{s5} - y_{s6} \\ z_{s1} - z_{s2} & z_{s3} - z_{s4} & z_{s5} - z_{s6} \end{pmatrix}. \tag{13.80}$$

Then we compute the *Jacobian determinant* and the *metrics* of the coordinate transformation for equidistant discretization in the transformed space.

As already mentioned all this information belongs to the center of the cell. However, the off-diagonal geometry information is required at the cell surfaces. For both cases we use the two corresponding neighbor vectors to compute the contravariant vectors at the cell surfaces as follows

$$\left(\mathbf{a}^2\right)_1 = \frac{1}{2}\left(\mathbf{a}_c^2 + \mathbf{a}_{c,i+1}^2\right),\ \left(\mathbf{a}^3\right)_1 = \frac{1}{2}\left(\mathbf{a}_c^3 + \mathbf{a}_{c,i+1}^3\right),$$

$$\left(\mathbf{a}^2\right)_2 = \frac{1}{2}\left(\mathbf{a}_c^2 + \mathbf{a}_{c,i-1}^2\right),\ \left(\mathbf{a}^3\right)_2 = \frac{1}{2}\left(\mathbf{a}_c^3 + \mathbf{a}_{c,i-1}^3\right),$$

$$\left(\mathbf{a}^1\right)_3 = \frac{1}{2}\left(\mathbf{a}_c^1 + \mathbf{a}_{c,j+1}^1\right),\ \left(\mathbf{a}^3\right)_3 = \frac{1}{2}\left(\mathbf{a}_c^3 + \mathbf{a}_{c,j+1}^3\right),$$

$$\left(\mathbf{a}^1\right)_4 = \frac{1}{2}\left(\mathbf{a}_c^1 + \mathbf{a}_{c,j-1}^1\right),\ \left(\mathbf{a}^3\right)_4 = \frac{1}{2}\left(\mathbf{a}_c^3 + \mathbf{a}_{c,j-1}^3\right),$$

$$\left(\mathbf{a}^1\right)_5 = \frac{1}{2}\left(\mathbf{a}_c^1 + \mathbf{a}_{c,k+1}^1\right),\ \left(\mathbf{a}^2\right)_5 = \frac{1}{2}\left(\mathbf{a}_c^2 + \mathbf{a}_{c,k+1}^2\right),$$

$$\left(\mathbf{a}^1\right)_6 = \frac{1}{2}\left(\mathbf{a}_c^1 + \mathbf{a}_{c,k-1}^1\right),\ \left(\mathbf{a}^2\right)_6 = \frac{1}{2}\left(\mathbf{a}_c^2 + \mathbf{a}_{c,k-1}^2\right). \quad (13.81\text{-}94)$$

### 13.4.4 Discretization of the diffusion terms

#### *13.4.4.1 General*

Our next task is to find appropriate finite difference approximation for the six diffusion terms

$$\left[\alpha_l \rho_l D_{il}^* \mathbf{e} \cdot \left(\mathbf{a}^1 \frac{\partial C_{il}}{\partial \xi} + \mathbf{a}^2 \frac{\partial C_{il}}{\partial \eta} + \mathbf{a}^3 \frac{\partial C_{il}}{\partial \zeta}\right)\right]_m,$$

The geometric properties computed by using the control volume approach in the previous section are used to transform the diagonal diffusion terms as direct finite differences

$$\sum_{m=1}^{6} \beta_m \left[\alpha_l \rho_l D_{il}^* \mathbf{e} \cdot \left(\mathbf{a}^1 \frac{\partial C_{il}}{\partial \xi} + \mathbf{a}^2 \frac{\partial C_{il}}{\partial \eta} + \mathbf{a}^3 \frac{\partial C_{il}}{\partial \zeta}\right)\right]_m$$

$$= \beta_1 \left(\frac{\alpha_l \rho_l D_{il}^*}{\overline{\Delta V}}\right)_1 S_1 \left[C_{il,i+1} - C_{il} + \frac{\overline{\Delta V}_1}{S_1}\left(\mathbf{e}\cdot\mathbf{a}^2 \frac{\partial C_{il}}{\partial \eta} + \mathbf{e}\cdot\mathbf{a}^3 \frac{\partial C_{il}}{\partial \zeta}\right)_1\right]$$

$$+ \beta_2 \left(\frac{\alpha_l \rho_l D_{il}^*}{\overline{\Delta V}}\right)_2 S_2 \left[C_{il,i-1} - C_{il} + \frac{\overline{\Delta V}_2}{S_2}\left(\mathbf{e}\cdot\mathbf{a}^2 \frac{\partial C_{il}}{\partial \eta} + \mathbf{e}\cdot\mathbf{a}^3 \frac{\partial C_{il}}{\partial \zeta}\right)_2\right]$$

$$+ \beta_3 \left(\frac{\alpha_l \rho_l D_{il}^*}{\overline{\Delta V}}\right)_3 S_3 \left[C_{il,j+1} - C_{il} + \frac{\overline{\Delta V}_3}{S_3}\left(\mathbf{e}\cdot\mathbf{a}^1 \frac{\partial C_{il}}{\partial \xi} + \mathbf{e}\cdot\mathbf{a}^3 \frac{\partial C_{il}}{\partial \zeta}\right)_3\right]$$

$$+ \beta_4 \left(\frac{\alpha_l \rho_l D_{il}^*}{\overline{\Delta V}}\right)_4 S_4 \left[C_{il,j-1} - C_{il} + \frac{\overline{\Delta V}_4}{S_4}\left(\mathbf{e}\cdot\mathbf{a}^1 \frac{\partial C_{il}}{\partial \xi} + \mathbf{e}\cdot\mathbf{a}^3 \frac{\partial C_{il}}{\partial \zeta}\right)_4\right]$$

$$+\beta_5\left(\frac{\alpha_l\rho_l D_{il}^*}{\overline{\Delta V}}\right)_5 S_5\left[C_{il,k+1}-C_{il}+\frac{\overline{\Delta V}_5}{S_5}\left(\mathbf{e}\cdot\mathbf{a}^1\frac{\partial C_{il}}{\partial\xi}+\mathbf{e}\cdot\mathbf{a}^2\frac{\partial C_{il}}{\partial\eta}\right)_5\right]$$

$$+\beta_6\left(\frac{\alpha_l\rho_l D_{il}^*}{\overline{\Delta V}}\right)_6 S_6\left[C_{il,k-1}-C_{il}+\frac{\overline{\Delta V}_6}{S_6}\left(\mathbf{e}\cdot\mathbf{a}^1\frac{\partial C_{il}}{\partial\xi}+\mathbf{e}\cdot\mathbf{a}^2\frac{\partial C_{il}}{\partial\eta}\right)_6\right]. \tag{13.95}$$

A natural averaging of the diffusion coefficients is then the harmonic averaging as given in Appendix 12.1

$$\frac{D_{il,m}^C}{\Delta L_{h,m}}=\left(\frac{\alpha_l\rho_l D_{il}^*}{\overline{\Delta V}}\right)_m S_m=S_m\frac{2\left(\alpha_l\rho_l D_{il}^*\right)\left(\alpha_l\rho_l D_{il}^*\right)_m}{\Delta V_m\left(\alpha_l\rho_l D_{il}^*\right)+\Delta V\left(\alpha_l\rho_l D_{il}^*\right)_m}, \tag{13.96}$$

where in the right hand side $m$ = 1, 2, 3, 4, 5, 6 is equivalent to $i$ + 1, $i$ - 1, $j$ + 1, $j$ - 1, $k$ + 1, $k$ - 1, respectively regarding the properties inside a control volumes. It guaranties that if the field in one of the neighboring cells is missing the diffusion coefficient is zero.

#### 13.4.4.2 Orthogonal coordinate systems

In the case of orthogonal coordinate systems we see that:

- the off-diagonal diffusion terms are equal to zero,
- the finite volume approximations of the diagonal terms are obtained without the need to know anything about the contravariant vectors.

This illustrates the advantage of using orthogonal coordinate systems. This is valid for any diffusion terms in the conservation equations, e.g. the thermal heat diffusion terms in the energy conservation equations, the viscous diffusion terms in the momentum equations etc.

#### 13.4.4.3 Off-diagonal diffusion terms in the general case

The geometric coefficients of the off-diagonal diffusion terms can then be computed as follows

$$d_{12}=(\mathbf{e})^1\cdot\left(\mathbf{a}^2\right)_1=(e)^{11}\left(a^{21}\right)_1+(e)^{12}\left(a^{22}\right)_1+(e)^{13}\left(a^{23}\right)_1, \tag{13.97}$$

$$d_{13}=(\mathbf{e})^1\cdot\left(\mathbf{a}^3\right)_1=(e)^{11}\left(a^{31}\right)_1+(e)^{12}\left(a^{32}\right)_1+(e)^{13}\left(a^{33}\right)_1, \tag{13.98}$$

$$d_{22}=(\mathbf{e})^2\cdot\left(\mathbf{a}^2\right)_2=(e)^{21}\left(a^{21}\right)_2+(e)^{22}\left(a^{22}\right)_2+(e)^{23}\left(a^{23}\right)_2=-\left(d_{12}\right)_{i-1}, \tag{13.99}$$

$$d_{23}=(\mathbf{e})^2\cdot\left(\mathbf{a}^3\right)_2=(e)^{21}\left(a^{31}\right)_2+(e)^{22}\left(a^{32}\right)_2+(e)^{23}\left(a^{33}\right)_2=-\left(d_{13}\right)_{i-1}, \tag{13.100}$$

$$d_{31}=(\mathbf{e})^3\cdot\left(\mathbf{a}^1\right)_3=(e)^{31}\left(a^{11}\right)_3+(e)^{32}\left(a^{12}\right)_3+(e)^{33}\left(a^{13}\right)_3, \tag{13.101}$$

$$d_{33} = (\mathbf{e})^3 \cdot (\mathbf{a}^3)_3 = (e)^{31}(a^{31})_3 + (e)^{32}(a^{32})_3 + (e)^{33}(a^{33})_3, \tag{13.102}$$

$$d_{41} = (\mathbf{e})^4 \cdot (\mathbf{a}^1)_4 = (e)^{41}(a^{11})_4 + (e)^{42}(a^{12})_4 + (e)^{43}(a^{13})_4 = -(d_{31})_{j-1}, \tag{13.103}$$

$$d_{43} = (\mathbf{e})^4 \cdot (\mathbf{a}^3)_4 = (e)^{41}(a^{31})_4 + (e)^{42}(a^{32})_4 + (e)^{43}(a^{33})_4 = -(d_{33})_{j-1}, \tag{13.104}$$

$$d_{51} = (\mathbf{e})^5 \cdot (\mathbf{a}^1)_5 = (e)^{51}(a^{11})_5 + (e)^{52}(a^{12})_5 + (e)^{53}(a^{13})_5, \tag{13.105}$$

$$d_{52} = (\mathbf{e})^5 \cdot (\mathbf{a}^2)_5 = (e)^{51}(a^{21})_5 + (e)^{52}(a^{22})_5 + (e)^{53}(a^{23})_5, \tag{13.106}$$

$$d_{61} = (\mathbf{e})^6 \cdot (\mathbf{a}^1)_6 = (e)^{61}(a^{11})_6 + (e)^{62}(a^{12})_6 + (e)^{63}(a^{13})_6 = -(d_{51})_{k-1}, \tag{13.107}$$

$$d_{62} = (\mathbf{e})^6 \cdot (\mathbf{a}^2)_6 = (e)^{61}(a^{21})_6 + (e)^{62}(a^{22})_6 + (e)^{63}(a^{23})_6 = -(d_{52})_{k-1}. \tag{13.108}$$

With this notation the diffusion term takes the form

$$\sum_{m=1}^{6} \beta_m \left[ \alpha_l \rho_l D_{il}^* \mathbf{e} \cdot \left( \mathbf{a}^1 \frac{\partial C_{il}}{\partial \xi} + \mathbf{a}^2 \frac{\partial C_{il}}{\partial \eta} + \mathbf{a}^3 \frac{\partial C_{il}}{\partial \zeta} \right) \right]_m$$
$$= \sum_{m=1}^{6} \beta_m \frac{D_{il,m}^C}{\Delta L_{h,m}} \left( C_{il,m} - C_{il} + \frac{\overline{\Delta V}_m}{S_m} DI\_C_{il,m} \right) \tag{13.109}$$

where

$$DI\_C_{il,1} = d_{12} \left. \frac{\partial C_{il}}{\partial \eta} \right|_1 + d_{13} \left. \frac{\partial C_{il}}{\partial \zeta} \right|_1, \qquad DI\_C_{il,2} = d_{22} \left. \frac{\partial C_{il}}{\partial \eta} \right|_2 + d_{23} \left. \frac{\partial C_{il}}{\partial \zeta} \right|_2, \tag{13.110-111}$$

$$DI\_C_{il,3} = d_{31} \left. \frac{\partial C_{il}}{\partial \xi} \right|_3 + d_{33} \left. \frac{\partial C_{il}}{\partial \zeta} \right|_3, \qquad DI\_C_{il,4} = d_{41} \left. \frac{\partial C_{il}}{\partial \xi} \right|_4 + d_{43} \left. \frac{\partial C_{il}}{\partial \zeta} \right|_4, \tag{13.112-113}$$

$$DI\_C_{il,5} = d_{51} \left. \frac{\partial C_{il}}{\partial \xi} \right|_5 + d_{52} \left. \frac{\partial C_{il}}{\partial \eta} \right|_5, \qquad DI\_C_{il,6} = d_{61} \left. \frac{\partial C_{il}}{\partial \xi} \right|_6 + d_{62} \left. \frac{\partial C_{il}}{\partial \eta} \right|_6. \tag{13.114-115}$$

The twelve concentration derivatives are computed as follows

$$\left. \frac{\partial C_{il}}{\partial \eta} \right|_1 = \frac{1}{4} \left( C_{il,j+1} + C_{il,i+1,j+1} - C_{il,j-1} - C_{il,i+1,j-1} \right), \tag{13.116}$$

$$\left. \frac{\partial C_{il}}{\partial \zeta} \right|_1 = \frac{1}{4} \left( C_{il,k+1} + C_{il,i+1,k+1} - C_{il,k-1} - C_{il,i+1,k-1} \right), \tag{13.117}$$

$$\left.\frac{\partial C_{il}}{\partial \eta}\right|_2 = \frac{1}{4}\left(C_{il,i-1\,j+1} + C_{il,j+1} - C_{il,i-1\,j-1} - C_{il,j-1}\right), \tag{13.118}$$

$$\left.\frac{\partial C_{il}}{\partial \zeta}\right|_2 = \frac{1}{4}\left(C_{il,k+1} + C_{il,i-1,k+1} - C_{il,k-1} - C_{il,i-1,k-1}\right), \tag{13.119}$$

$$\left.\frac{\partial C_{il}}{\partial \xi}\right|_3 = \frac{1}{4}\left(C_{il,i+1} + C_{il,i+1,j+1} - C_{il,i-1} - C_{il,i-1,j+1}\right), \tag{13.120}$$

$$\left.\frac{\partial C_{il}}{\partial \zeta}\right|_3 = \frac{1}{4}\left(C_{il,k+1} + C_{il,j+1,k+1} - C_{il,k-1} - C_{il,j+1,k-1}\right), \tag{13.121}$$

$$\left.\frac{\partial C_{il}}{\partial \xi}\right|_4 = \frac{1}{4}\left(C_{il,i+1} + C_{il,i+1,j-1} - C_{il,i-1} - C_{il,i-1,j-1}\right), \tag{13.122}$$

$$\left.\frac{\partial C_{il}}{\partial \zeta}\right|_4 = \frac{1}{4}\left(C_{il,k+1} + C_{il,j-1,k+1} - C_{il,k-1} - C_{il,j-1,k-1}\right), \tag{13.123}$$

$$\left.\frac{\partial C_{il}}{\partial \xi}\right|_5 = \frac{1}{4}\left(C_{il,i+1,k+1} + C_{il,i+1} - C_{il,i-1,k+1} - C_{il,i-1}\right), \tag{13.124}$$

$$\left.\frac{\partial C_{il}}{\partial \eta}\right|_5 = \frac{1}{4}\left(C_{il,j+1} + C_{il,j+1,k+1} - C_{il,j-1} - C_{il,j-1,k+1}\right), \tag{13.125}$$

$$\left.\frac{\partial C_{il}}{\partial \xi}\right|_6 = \frac{1}{4}\left(C_{il,i+1} + C_{il,i+1,k-1} - C_{il,i-1} - C_{il,i-1,k-1}\right), \tag{13.126}$$

$$\left.\frac{\partial C_{il}}{\partial \eta}\right|_6 = \frac{1}{4}\left(C_{il,j+1} + C_{il,j+1,k-1} - C_{il,j-1} - C_{il,j-1,k-1}\right). \tag{13.127}$$

#### *13.4.4.4 Final form of the finite volume concentration equation*

Thus the final form of the discretized concentration equation (13.1) is

$$\alpha_{la}\rho_{la}\left(C_{il} - C_{ila}\right)\gamma_{va} - \Delta\tau\sum_{m=1}^{6}\left(B_{lm-} + \beta_m \frac{D_{il,m}^{C}}{\Delta L_{h,m}}\right)\left(C_{il,m} - C_{il}\right) + \Delta\tau\gamma_v\mu_l^{+}C_{il}$$

$$= \Delta\tau\gamma_v DC_{il} + \Delta\tau\sum_{m=1}^{6}\beta_m \frac{D_{il,m}^{C}}{\Delta L_{h,m}}\frac{\overline{\Delta V}_m}{S_m} DI\_C_{il,m}\ , \tag{13.128}$$

Solving with respect to the unknown concentration we obtain

$$C_{il} = \frac{\alpha_{la}\rho_{la}\gamma_{va}C_{ila} + \Delta\tau\left\{\gamma_v DC_{il} + \sum_{m=1}^{6}\left[\begin{array}{l} B_{lm-}C_{il,m} \\ +\beta_m \dfrac{D_{il,m}^C}{\Delta L_{h,m}}\left(C_{il,m} + \dfrac{\overline{\Delta V}_m}{S_m} DI\_C_{il,m}\right)\end{array}\right]\right\}}{\alpha_{la}\gamma_{va}\rho_{la} + \Delta\tau\left[\gamma_v\mu_l^+ + \sum_{m=1}^{6}\left(B_{lm-} + \beta_m \dfrac{D_{il,m}^C}{\Delta L_{h,m}}\right)\right]}. \quad (13.129)$$

For the case of a just originating velocity field, $\alpha_{la} = 0$ and

$$\gamma_v\mu_l^+ + \sum_{m=1}^{6}\left(b_{lm-}\alpha_{l,m}\rho_{l,m} + \beta_m \frac{D_{il,m}^C}{\Delta L_{h,m}}\right) > 0, \quad (13.130)$$

we have

$$C_{il} = \frac{\gamma_v DC_{il} + \sum_{m=1}^{6}\gamma_v DC_{il} + \sum_{m=1}^{6}\left[B_{lm-}C_{il,m} + \beta_m \dfrac{D_{il,m}^C}{\Delta L_{h,m}}\left(C_{il,m} + \dfrac{\overline{\Delta V}_m}{S_m} DI\_C_{il,m}\right)\right]}{\gamma_v\mu_l^+ + \sum_{m=1}^{6}\left(B_{lm-} + \beta_m \dfrac{D_{il,m}^C}{\Delta L_{h,m}}\right)}. \quad (13.131)$$

## 13.5 Discretization of the entropy equation

The entropy equation (10.62) is discretized following the procedure already described in the previous section. The result is

$$\alpha_{la}\rho_{la}\left(s_l - s_{la}\right)\gamma_{va} - \Delta\tau\sum_{m=1}^{6} B_{lm-}\left(s_{l,m} - s_l\right) + \Delta\tau\gamma_v\mu_l^+ s_l = \Delta\tau\gamma_v Ds_l^*, \quad (13.132)$$

where

$$Ds_l^* = Ds_l + \frac{1}{\gamma_v}\sum_{m=1}^{6}\beta_m\left[\begin{array}{l}\dfrac{1}{T_l}\dfrac{D_{l,m}^T}{\Delta L_{h,m}}\left(T_{l,m} - T_l + \dfrac{\overline{\Delta V}_m}{S_m} DI\_T_{l,m}\right) \\ + \dfrac{D_{l,m}^{sC}}{\Delta L_{h,m}}\sum_{i=2}^{i_{\max}}\left(C_{il,m} - C_{il} + \dfrac{\overline{\Delta V}_m}{S_m} DI\_C_{il}\right)\end{array}\right]. \quad (13.133)$$

The term $DI\_T_{l,m}$ is computed by replacing the concentrations in Eqs. (11.110-127) with the corresponding temperatures. The computation of the harmonic averaged thermal conductivity coefficients is given in Appendix 12.1. Solving with respect to the unknown specific entropy we obtain

$$s_l = \frac{\alpha_{la}\rho_{la}\gamma_{va}s_{la} + \Delta\tau\left(\gamma_v Ds_l^* + \sum_{m=1}^{6} B_{lm-}s_{lm}\right)}{\alpha_{la}\rho_{la}\gamma_{va} + \Delta\tau\left(\sum_{m=1}^{6} B_{lm-} + \gamma_v\mu_l^+\right)}. \tag{13.134}$$

For the case of a just originating velocity field, $\alpha_{la} = 0$ and $\sum_{m=1}^{6} B_{lm-} + \gamma_v\mu_l^+ > 0$, we have

$$s_l = \frac{\gamma_v Ds_l^* + \sum_{m=1}^{6} B_{lm-}s_{lm}}{\sum_{m=1}^{6} B_{lm-} + \gamma_v\mu_l^+}. \tag{13.135}$$

## 13.6 Discretization of the temperature equation

The temperature equation (10.65) is discretized following the procedure already described in the previous section. The result is

$$\alpha_{la}\rho_{la}c_{pla}\left(T_l - T_{la}\right)\gamma_{va} - \Delta\tau\sum_{m=1}^{6}\left(B_{lm-}c_{pl,m} + \beta_m\frac{D_{l,m}^T}{\Delta L_{h,m}}\right)\left(T_{l,m} - T_l\right)$$

$$\left[1 - \rho_l\left(\frac{\partial h_l}{\partial p}\right)_{T_l,all\_C's}\right]\left[\alpha_{la}\left(p - p_a\right)\gamma_{va} - \Delta\tau\sum_{m=1}^{6}\frac{B_{lm-}}{\rho_{lm}}\left(p_m - p\right)\right]$$

$$= \Delta\tau\gamma_v\left[DT_l^N - T_l\sum_{i=2}^{i_{\max}}\Delta s_{il}^{np}\left(\mu_{il} - C_{il}\mu_l\right)\right]$$

$$-\Delta\tau\sum_{m=1}^{6}\beta_m\left[\frac{D_{l,m}^C}{\Delta L_{h,m}}T_l\sum_{i=2}^{i_{\max}}\Delta s_{il}^{np}\left(C_{il,m} - C_{il} + \frac{\overline{\Delta V}_m}{S_m}DI\_C_{il}\right) - \frac{D_{l,m}^T}{\Delta L_{h,m}}\frac{\overline{\Delta V}_m}{S_m}DI\_T_l\right]. \tag{13.136}$$

## 13.7 Discretization of the particle number density equation

The particle number density equation (10.66) is discretized following the procedure already described in the previous section. The result is

$$n_l\gamma_v - n_{la}\gamma_{va} + \Delta\tau\sum_{m=1}^{6}\beta_m\left[(\mathbf{e})^m\cdot\left(\mathbf{V}_{l,m}-\mathbf{V}_{cs}\right)n_{l,m} - \frac{D^n_{l,m}}{\Delta L_{h,m}}\left(n_{l,m}-n_l\right)\right]$$

$$= \Delta\tau\gamma_v\left(\dot{n}_{l,kin} - \dot{n}_{l,coal} + \dot{n}_{l,sp}\right) + \Delta\tau\sum_{m=1}^{6}\beta_m\frac{D^n_{l,m}}{\Delta L_{h,m}}\frac{\overline{\Delta V}_m}{S_m}DI\_n_{l,m} \ . \qquad (13.137)$$

The turbulent diffusion coefficient is again a result of harmonic volume averaging – Appendix 12.1.

$$\frac{D^n_{l,m}}{\Delta L_{h,m}} = \left(\frac{\dfrac{\nu_l^t}{Sc^t}}{\Delta V}\right)_m S_m = S_m\frac{2\left(\dfrac{\nu_l^t}{Sc^t}\right)\left(\dfrac{\nu_l^t}{Sc^t}\right)_m}{\Delta V_m\left(\dfrac{\nu_l^t}{Sc^t}\right) + \Delta V\left(\dfrac{\nu_l^t}{Sc^t}\right)_m} \ . \qquad (13.138)$$

## 13.8 Discretization of the *x* momentum equation

The $x$ momentum equation (10.68) is discretized as already discussed in the previous Section. The result is

$$\alpha_{la}\rho_{la}\left(u_l - u_{la}\right)\gamma_{va} - \Delta\tau\sum_{m=1}^{6}\left\{B_{lm-} + \beta_m\frac{D^\nu_{l,m}}{\Delta L_{h,m}}\left[1+\frac{1}{3}(e)^{m1}(e)^{m1}\right]\right\}\left(u_{l,m}-u_l\right)$$

$$+\Delta\tau\alpha_l\left(a^{11}\gamma_\xi\frac{\partial p}{\partial\xi} + a^{21}\gamma_\eta\frac{\partial p}{\partial\eta} + a^{31}\gamma_\zeta\frac{\partial p}{\partial\zeta}\right)$$

$$-\Delta\tau\gamma_v\left[\sum_{\substack{m=1\\m\neq l}}^{3}\bar{c}^d_{ml}\left|\Delta\mathbf{V}_{ml}\right|\left(u_m-u_l\right) + \bar{c}^d_{wl}\left|\Delta\mathbf{V}_{wl}\right|\left(u_{cs}-u_l\right)\right]$$

$$-\Delta\tau\gamma_v\sum_{\substack{m=1\\m\neq l}}^{l_{\max}}\bar{c}^L_{ml}\left[\left(v_l-v_m\right)b_{m,3} - \left(w_l-w_m\right)b_{m,2}\right]$$

$$-\Delta\tau\gamma_v\bar{c}^L_{wl}\left[\left(v_l-v_{cs}\right)b_{w,3} - \left(w_l-w_{cs}\right)b_{w,2}\right]$$

$$-\Delta\tau\gamma_v\sum_{\substack{m=1\\m\neq l}}^{3}\bar{c}^{vm}_{ml}\left(\frac{\partial\Delta u_{ml}}{\partial\tau} + V^1\frac{\partial\Delta u_{ml}}{\partial\xi} + V^2\frac{\partial\Delta u_{ml}}{\partial\eta} + V^3\frac{\partial\Delta u_{ml}}{\partial\zeta}\right)$$

$$-\gamma_v \Delta \tau \overline{c}_{wl}^{vm} \left( \frac{\partial \Delta u_{csl}}{\partial \tau} + \overline{V}^1 \frac{\partial \Delta u_{csl}}{\partial \xi} + \overline{V}^2 \frac{\partial \Delta u_{csl}}{\partial \eta} + \overline{V}^3 \frac{\partial \Delta u_{csl}}{\partial \zeta} \right)$$

$$= \Delta \tau \gamma_v \left[ -\alpha_l \rho_l g_x + \sum_{m=1}^{3,w} \left[ \mu_{ml} \left( u_m - u_l \right) \right] + \mu_{lw} \left( u_{lw} - u_l \right) \right]$$

$$+\Delta \tau \sum_{m=1}^{6} \beta_m \frac{D_{l,m}^{v}}{\Delta L_{h,m}} \left( \begin{array}{l} DI\_u_{l,m} - \frac{2}{3} (e)^{m1} DI\_u_{l,m}^{b} + DI\_vis_{lm}^{uT} \\ \\ + \frac{1}{3} (e)^{m1} \left[ (e)^{m2} \left( v_{l,m} - v_l \right) + (e)^{m3} \left( w_{l,m} - w_l \right) \right] \end{array} \right). \quad (13.139)$$

A natural averaging of the diffusion coefficients is the harmonic averaging – Appendix 12.1

$$\frac{D_{il,m}^{v}}{\Delta L_{h,m}} = \left( \frac{\alpha_l^e \rho_l \nu_l^*}{\Delta V} \right)_m S_m = S_m \frac{2 \left( \alpha_l^e \rho_l \nu_l^* \right) \left( \alpha_l^e \rho_l \nu_l^* \right)_m}{\Delta V_m \left( \alpha_l^e \rho_l \nu_l^* \right) + \Delta V \left( \alpha_l^e \rho_l \nu_l^* \right)_m} . \quad (13.140)$$

It is valid for all momentum equations. Note how we arrive to the integral form of the pressure term:

$$\frac{1}{\Delta V} \int_0^{\Delta \tau} \iiint_{\Delta V} \sqrt{g} \alpha_l \left( a^{11} \gamma_\xi \frac{\partial p}{\partial \xi} + a^{21} \gamma_\eta \frac{\partial p}{\partial \eta} + a^{31} \gamma_\zeta \frac{\partial p}{\partial \zeta} \right) \partial \xi \partial \eta \partial \zeta \partial \tau$$

$$= \Delta \tau \alpha_l \left( a^{11} \gamma_\xi \frac{\partial p}{\partial \xi} + a^{21} \gamma_\eta \frac{\partial p}{\partial \eta} + a^{31} \gamma_\zeta \frac{\partial p}{\partial \zeta} \right). \quad (13.141)$$

The $b$ coefficients of in the lift force expressions result from the Cartesian component decomposition:

$$b_{m,1} = a^{12} \frac{\partial w_m}{\partial \xi} - a^{13} \frac{\partial v_m}{\partial \xi} + a^{22} \frac{\partial w_m}{\partial \eta} - a^{23} \frac{\partial v_m}{\partial \eta} + a^{32} \frac{\partial w_m}{\partial \zeta} - a^{33} \frac{\partial v_m}{\partial \zeta}, \quad (13.142)$$

$$b_{m,2} = a^{13} \frac{\partial u_m}{\partial \xi} - a^{11} \frac{\partial w_m}{\partial \xi} + a^{23} \frac{\partial u_m}{\partial \eta} - a^{21} \frac{\partial w_m}{\partial \eta} + a^{33} \frac{\partial u_m}{\partial \zeta} - a^{31} \frac{\partial w_m}{\partial \zeta}, \quad (13.143)$$

$$b_{m,3} = a^{11} \frac{\partial v_m}{\partial \xi} - a^{12} \frac{\partial u_m}{\partial \xi} + a^{21} \frac{\partial v_m}{\partial \eta} - a^{22} \frac{\partial u_m}{\partial \eta} + a^{31} \frac{\partial v_m}{\partial \zeta} - a^{32} \frac{\partial u_m}{\partial \zeta}, \quad (13.144)$$

and

$$b_{w,1} = a^{12} \frac{\partial w_{cs}}{\partial \xi} - a^{13} \frac{\partial v_{cs}}{\partial \xi} + a^{22} \frac{\partial w_{cs}}{\partial \eta} - a^{23} \frac{\partial v_{cs}}{\partial \eta} + a^{32} \frac{\partial w_{cs}}{\partial \zeta} - a^{33} \frac{\partial v_{cs}}{\partial \zeta}, \quad (13.145)$$

$$b_{w,2} = a^{13} \frac{\partial u_{cs}}{\partial \xi} - a^{11} \frac{\partial w_{cs}}{\partial \xi} + a^{23} \frac{\partial u_{cs}}{\partial \eta} - a^{21} \frac{\partial w_{cs}}{\partial \eta} + a^{33} \frac{\partial u_{cs}}{\partial \zeta} - a^{31} \frac{\partial w_{cs}}{\partial \zeta}, \quad (13.146)$$

$$b_{w,3} = a^{11}\frac{\partial v_{cs}}{\partial \xi} - a^{12}\frac{\partial u_{cs}}{\partial \xi} + a^{21}\frac{\partial v_{cs}}{\partial \eta} - a^{22}\frac{\partial u_{cs}}{\partial \eta} + a^{31}\frac{\partial v_{cs}}{\partial \zeta} - a^{32}\frac{\partial u_{cs}}{\partial \zeta}. \qquad (13.147)$$

We proceed in a similar way for the other momentum equations.

## 13.9 Discretization of the *y* momentum equation

The result of the discretization of the *y* momentum equation (10.73) is

$$\alpha_{la}\rho_{la}\left(v_l - v_{la}\right)\gamma_{va} - \Delta\tau\sum_{m=1}^{6}\left\{B_{lm-} + \beta_m \frac{D^v_{l,m}}{\Delta L_{h,m}}\left[1 + \frac{1}{3}(e)^{m2}(e)^{m2}\right]\right\}\left(v_{l,m} - v_l\right)$$

$$+\Delta\tau\alpha_l\left(a^{12}\gamma_\xi\frac{\partial p}{\partial \xi} + a^{22}\gamma_\eta\frac{\partial p}{\partial \eta} + a^{32}\gamma_\zeta\frac{\partial p}{\partial \zeta}\right)$$

$$-\Delta\tau\gamma_v\left[\sum_{\substack{m=1\\m\neq l}}^{3}\bar{c}^d_{ml}\left|\Delta\mathbf{V}_{ml}\right|\left(v_m - v_l\right) + \bar{c}^d_{wl}\left|\Delta\mathbf{V}_{wl}\right|\left(v_{cs} - v_l\right)\right]$$

$$-\Delta\tau\gamma_v\sum_{\substack{m=1\\m\neq l}}^{l_{\max}}\bar{c}^L_{ml}\left[\left(w_l - w_m\right)b_{m,1} - \left(u_l - u_m\right)b_{m,3}\right]$$

$$-\Delta\tau\gamma_v\bar{c}^L_{wl}\left[\left(w_l - w_{cs}\right)b_{w,1} - \Delta u_{lw}\left(u_l - u_{cs}\right)b_{w,3}\right]$$

$$-\Delta\tau\gamma_v\sum_{\substack{m=1\\m\neq l}}^{3}\bar{c}^{vm}_{ml}\left(\frac{\partial \Delta v_{ml}}{\partial \tau} + \bar{V}^1\frac{\partial \Delta v_{ml}}{\partial \xi} + \bar{V}^2\frac{\partial \Delta v_{ml}}{\partial \eta} + \bar{V}^3\frac{\partial \Delta v_{ml}}{\partial \zeta}\right)$$

$$-\gamma_v\Delta\tau\bar{c}^{vm}_{wl}\left(\frac{\partial \Delta v_{csl}}{\partial \tau} + \bar{V}^1\frac{\partial \Delta v_{csl}}{\partial \xi} + \bar{V}^2\frac{\partial \Delta v_{csl}}{\partial \eta} + \bar{V}^3\frac{\partial \Delta v_{csl}}{\partial \zeta}\right)$$

$$= \Delta\tau\gamma_v\left[-\alpha_l\rho_l g_y + \sum_{m=1}^{3,w}\left[\mu_{ml}\left(v_m - v_l\right)\right] + \mu_{lw}\left(v_{lw} - v_l\right)\right]$$

$$+\Delta\tau\sum_{m=1}^{6}\beta_m\frac{D^v_{l,m}}{\Delta L_{h,m}}\left(\begin{array}{l} DI\_v_{l,m} - \frac{2}{3}(e)^{m2}DI\_u^b_{l,m} + DI\_vis^{vT}_{lm} \\ \\ +\frac{1}{3}(e)^{m2}\left[(e)^{m1}\left(u_{l,m} - u_l\right) + (e)^{m3}\left(w_{l,m} - w_l\right)\right] \end{array}\right). \qquad (13.148)$$

## 13.10 Discretization of the *z* momentum equation

The result of the discretization of the $z$ momentum equation (10.77) is

$$
\begin{aligned}
&\alpha_{la}\rho_{la}\left(w_l - w_{la}\right)\gamma_{va} - \Delta\tau\sum_{m=1}^{6}\left\{B_{lm-} + \beta_m \frac{D_{l,m}^{v}}{\Delta L_{h,m}}\left[1+\frac{1}{3}(e)^{m3}(e)^{m3}\right]\right\}\left(w_{l,m} - w_l\right)\\
&+\Delta\tau\alpha_l\left(a^{13}\gamma_\xi \frac{\partial p}{\partial \xi} + a^{23}\gamma_\eta \frac{\partial p}{\partial \eta} + a^{33}\gamma_\zeta \frac{\partial p}{\partial \zeta}\right)\\
&-\Delta\tau\gamma_v\left[\sum_{\substack{m=1\\ m\neq l}}^{3}\bar{c}_{ml}^{d}\left|\Delta\mathbf{V}_{ml}\right|\left(w_m - w_l\right) + \bar{c}_{wl}^{d}\left|\Delta\mathbf{V}_{wl}\right|\left(w_{cs} - w_l\right)\right]\\
&-\Delta\tau\gamma_v\sum_{\substack{m=1\\ m\neq l}}^{l_{\max}}\bar{c}_{ml}^{L}\left[\left(u_l - u_m\right)b_{m,2} - \left(v_l - v_m\right)b_{m,1}\right]\\
&-\Delta\tau\gamma_v\bar{c}_{wl}^{L}\left[\left(u_l - u_{cs}\right)b_{w,2} - \left(v_l - v_{cs}\right)b_{w,1}\right]\\
&-\Delta\tau\gamma_v\sum_{\substack{m=1\\ m\neq l}}^{3}\bar{c}_{ml}^{vm}\left(\frac{\partial\Delta w_{ml}}{\partial\tau} + \bar{V}^1\frac{\partial\Delta w_{ml}}{\partial\xi} + \bar{V}^2\frac{\partial\Delta w_{ml}}{\partial\eta} + \bar{V}^3\frac{\partial\Delta w_{ml}}{\partial\zeta}\right)\\
&-\gamma_v\Delta\tau\bar{c}_{wl}^{vm}\left(\frac{\partial\Delta w_{csl}}{\partial\tau} + \bar{V}^1\frac{\partial\Delta w_{csl}}{\partial\xi} + \bar{V}^2\frac{\partial\Delta w_{csl}}{\partial\eta} + \bar{V}^3\frac{\partial\Delta w_{csl}}{\partial\zeta}\right)\\
&=\Delta\tau\gamma_v\left[-\alpha_l\rho_l g_z + \sum_{m=1}^{3,w}\left[\mu_{ml}\left(w_m - w_l\right)\right] + \mu_{lw}\left(w_{lw} - w_l\right)\right]\\
&+\Delta\tau\sum_{m=1}^{6}\beta_m\frac{D_{l,m}^{v}}{\Delta L_{h,m}}\left(\begin{array}{l} DI\_w_{l,m} - \frac{2}{3}(e)^{m3}DI\_u_{l,m}^{b} + DI\_vis_{lm}^{wT}\\[2ex] +\frac{1}{3}(e)^{m3}\left[(e)^{m1}\left(u_{l,m} - u_l\right) + (e)^{m2}\left(v_{l,m} - v_l\right)\right]\end{array}\right).
\end{aligned}
\tag{13.149}
$$

## 13.11 Pressure-velocity coupling

*The IVA3 method:* An important target of the numerical methods is to guarantee a strict mass conservation in the sense of the overall mass balance as for the single cell as well for the sum of the cells inside the physical domain of interest. We use the discretized mass conservation equations of each field in a special way to construct the so called pressure-velocity coupling keeping in mind the above requirement. First we note that the difference resulting from the time derivative divided by the new time level density can be rearranged as follows

$$\frac{1}{\rho_l}\left(\alpha_l\rho_l\gamma_v - \alpha_{la}\rho_{la}\gamma_{va}\right) = \left(\alpha_l - \alpha_{la}\right)\gamma_v + \alpha_{la}\left(\gamma_v - \gamma_{va}\right) + \frac{\alpha_{la}}{\rho_l}\left(\rho_l - \rho_{la}\right)\gamma_{va} . \tag{13.150}$$

Then, we divide each of the discretized field mass conservation equations by the corresponding new time level density. Having in mind Eq. (13.150) we obtain

$$\left(\alpha_l - \alpha_{la}\right)\gamma_v + \frac{\alpha_{la}}{\rho_l}\left(\rho_l - \rho_{la}\right)\gamma_{va} + \Delta\tau\frac{1}{\rho_l}\sum_{m=1}^{6}\beta_m\left(\xi_{lm+}\alpha_l\rho_l + \xi_{lm-}\alpha_{lm}\rho_{lm}\right)V_{lm}^n$$
$$= \frac{1}{\rho_l}\Delta\tau\gamma_v\mu_l - \alpha_{la}\left(\gamma_v - \gamma_{va}\right). \tag{13.151}$$

We sum all of the $l_{max}$ mass conservation equations. The first term disappears because the sum of all volume fractions is equal to unity. In the resulting equation the temporal density difference is replaced by the linearized form of the equation of state, Eq. (3.173),

$$\rho_l - \rho_{la} = \frac{1}{a_{la}^2}\left(p - p_a\right) + \left(\frac{\partial\rho_l}{\partial s_l}\right)_a\left(s_l - s_{la}\right) + \sum_{i=2}^{i_{\max}}\left(\frac{\partial\rho_l}{\partial C_{i,l}}\right)_a\left(C_{i,l} - C_{i,la}\right). \tag{13.152}$$

The result is

$$\left(p - p_a\right)\gamma_{va}\sum_{l=1}^{l_{\max}}\frac{\alpha_{la}}{\rho_l a_{la}^2} + \Delta\tau\sum_{l=1}^{l_{\max}}\frac{1}{\rho_l}\sum_{m=1}^{6}\beta_m\left(\xi_{lm+}\alpha_l\rho_l + \xi_{lm-}\alpha_{lm}\rho_{lm}\right)V_{lm}^n = \Delta\tau\sum_{l=1}^{l_{\max}}D\alpha_l , \tag{13.153}$$

where

$$\Delta\tau D\alpha_l = \frac{1}{\rho_l}\Delta\tau\gamma_v\mu_l - \alpha_{la}\left(\gamma_v - \gamma_{va}\right)$$
$$-\gamma_{va}\frac{\alpha_{la}}{\rho_l}\left[\left(\frac{\partial\rho_l}{\partial s_l}\right)_a\left(s_l - s_{la}\right) + \sum_{i=2}^{i_{\max}}\left(\frac{\partial\rho_l}{\partial C_{i,l}}\right)_a\left(C_{i,l} - C_{i,la}\right)\right]. \tag{13.154}$$

This equation is equivalent exactly to the sum of the discretized mass conservation equations divided by the corresponding densities. It takes into account the influence of the variation of the density with the time on the pressure change. The spatial variation of the density in the second term is still not resolved. With the next step we will derive a approximated approach to change also the influence of the spatial variation of the density on the pressure change.

Writing the discretized momentum equation in the linearized form

$$V_{lm}^n = dV_{lm}^n - \left(\mathbf{e}\right)^m \cdot \mathbf{V}_{cs,m} - RVel_{lm}\left(p_m - p\right), \tag{13.155}$$

and replacing we finally obtain the so called pressure equation

$$p\gamma_{va}\sum_{l=1}^{l_{\max}}\frac{\alpha_{la}}{\rho_l a_{la}^2}-\Delta\tau\sum_{m=1}^{6}\beta_m\left[\sum_{l=1}^{l_{\max}}\left(\xi_{lm+}\alpha_l+\xi_{lm-}\alpha_{lm}\frac{\rho_{lm}}{\rho_l}\right)RVel_{lm}\right](p_m-p)$$

$$=p_a\gamma_{va}\sum_{l=1}^{l_{\max}}\frac{\alpha_{la}}{\rho_l a_{la}^2}-\Delta\tau\sum_{l=1}^{l_{\max}}\frac{1}{\rho_l}\sum_{m=1}^{6}\beta_m\left(\xi_{lm+}\alpha_l\rho_l+\xi_{lm-}\alpha_{lm}\rho_{lm}\right)\left[dV_{lm}^n-(\mathbf{e})^m\cdot\mathbf{V}_{cs,m}\right]$$

$$+\Delta\tau\sum_{l=1}^{l_{\max}}D\alpha_l\ . \tag{13.156}$$

Defining the coefficients

$$c_m=-\Delta\tau\beta_m\sum_{l=1}^{l_{\max}}\left(\xi_{lm+}\alpha_l+\xi_{lm-}\alpha_{lm}\frac{\rho_{lm}}{\rho_l}\right)RVel_{lm}\ , \tag{13.157}$$

$$c=p\gamma_{va}\sum_{l=1}^{l_{\max}}\frac{\alpha_{la}}{\rho_l a_{la}^2}-\sum_{m=1}^{6}c_m\ , \tag{13.158}$$

$$d=p_a\gamma_{va}\sum_{l=1}^{l_{\max}}\frac{\alpha_{la}}{\rho_l a_{la}^2}+\Delta\tau\sum_{l=1}^{l_{\max}}D\alpha_l$$

$$-\Delta\tau\sum_{m=1}^{6}\beta_m\sum_{l=1}^{l_{\max}}\left(\xi_{lm+}\alpha_l+\xi_{lm-}\alpha_{lm}\frac{\rho_{lm}}{\rho_l}\right)\left[dV_{lm}^n-(\mathbf{e})^m\cdot\mathbf{V}_{cs,m}\right], \tag{13.159}$$

we obtain the pressure equation

$$cp+\sum_{m=1}^{6}c_m p_m=d\ , \tag{13.160}$$

connecting each cell pressure with the pressure of the surrounding cells. We see that the system of algebraic equations *has positive diagonal elements*, is *symmetric* and *strictly diagonally dominant* because

$$|c|>\sum_{m=1}^{6}|c_m|\ . \tag{13.161}$$

These are very important properties.

*The IVA2 method*: The spatial deviation of the density of the surrounding cells from the density of the cell considered can be introduced into Eq. (13.153) as follows

$$\beta_m\left(\xi_{lm+}\alpha_l\rho_l+\xi_{lm-}\alpha_{lm}\rho_{lm}\right)=\beta_m\left(\xi_{lm+}\alpha_l+\xi_{lm-}\alpha_{lm}\right)\rho_l+\beta_m\xi_{lm-}\alpha_{lm}\left(\rho_{lm}-\rho_l\right). \tag{13.161}$$

The result is

$$\left(p-p_a\right)\gamma_{va}\sum_{l=1}^{l_{\max}}\frac{\alpha_{la}}{\rho_l a_{la}^2}+\Delta\tau\sum_{l=1}^{l_{\max}}\sum_{m=1}^{6}\beta_m\left(\xi_{lm+}\alpha_l+\xi_{lm-}\alpha_{lm}\right)V_{lm}^n$$

$$+\Delta\tau\sum_{l=1}^{l_{\max}}\frac{1}{\rho_l}\sum_{m=1}^{6}\beta_m\xi_{lm-}\alpha_{lm}\left(\rho_{lm}-\rho_l\right)V_{lm}^n$$

$$=\sum_{l=1}^{l_{\max}}\left[\begin{array}{l}\frac{1}{\rho_l}\Delta\tau\gamma_v\mu_l-\alpha_{la}\left(\gamma_v-\gamma_{va}\right)\\ -\gamma_{va}\frac{\alpha_{la}}{\rho_l}\left[\left(\frac{\partial\rho_l}{\partial s_l}\right)_a\left(s_l-s_{la}\right)+\sum_{i=2}^{i_{\max}}\left(\frac{\partial\rho_l}{\partial C_{i,l}}\right)_a\left(C_{i,l}-C_{i,la}\right)\right]\end{array}\right]. \qquad (13.163)$$

The spatial density variation can again be expressed as follows, Eq. (3.173),

$$\rho_{lm}-\rho_l=\frac{1}{a_{la}^2}\left(p_m-p\right)+\left(\frac{\partial\rho_l}{\partial s_l}\right)_a\left(s_{lm}-s_l\right)+\sum_{i=2}^{i_{\max}}\left(\frac{\partial\rho_l}{\partial C_{i,l}}\right)_a\left(C_{i,lm}-C_{i,l}\right). \qquad (13.164)$$

With this we obtain

$$\left(p-p_a\right)\gamma_{va}\sum_{l=1}^{l_{\max}}\frac{\alpha_{la}}{\rho_l a_{la}^2}+\Delta\tau\sum_{l=1}^{l_{\max}}\sum_{m=1}^{6}\beta_m\left[\xi_{lm+}\alpha_l+\xi_{lm-}\alpha_{lm}\left(1+\frac{p_m-p}{\rho_l a_{la}^2}\right)\right]V_{lm}^n$$

$$=\Delta\tau\sum_{l=1}^{l_{\max}}D\alpha_l\ , \qquad (13.165)$$

where

$$\rho_l\Delta\tau D\alpha_l=\Delta\tau\gamma_v\mu_l-\alpha_{la}\rho_l\left(\gamma_v-\gamma_{va}\right)-\left(\frac{\partial\rho_l}{\partial s_l}\right)_a\left[\begin{array}{l}\gamma_{va}\alpha_{la}\left(s_l-s_{la}\right)\\ -\Delta\tau\sum_{m=1}^{6}b_{lm-}\alpha_{lm}\left(s_{lm}-s_l\right)\end{array}\right]$$

$$-\sum_{i=2}^{i_{\max}}\left(\frac{\partial\rho_l}{\partial C_{i,l}}\right)_a\left[\gamma_{va}\alpha_{la}\left(C_{i,l}-C_{i,la}\right)-\Delta\tau\sum_{m=1}^{6}b_{lm-}\alpha_{lm}\left(C_{i,lm}-C_{i,l}\right)\right], \qquad (13.166)$$

Equation (13.165) is equivalent exactly to the sum of the discretized mass conservation equations. The discretized concentration equation divided by the old time level density is

$$\gamma_{va}\alpha_{la}\left(C_{il}-C_{ila}\right)-\Delta\tau\sum_{m=1}^{6}b_{lm-}\alpha_{l,m}\frac{\rho_{l,m}}{\rho_{la}}\left(C_{il,m}-C_{il}\right)=\frac{\Delta\tau}{\rho_{la}}DC_{il}^{N}, \quad (13.167)$$

where

$$DC_{il}^{N}=\gamma_{v}\left(DC_{il}-\mu_{l}^{+}C_{il}\right)+\sum_{m=1}^{6}\beta_{m}\frac{D_{il,m}^{*}}{\Delta L_{h,m}}\left(C_{il,m}-C_{il}+DI\_C_{il,m}\right), \quad (13.168)$$

does not contain time derivatives and convection terms. Even these terms are the most strongly varying in transient processes during a single time step. In the case of negligible diffusion $DC_{il}^{N}$ contains only source terms.

We realize that the expression on the right hand side is very similar to the left hand side of the concentration equation divided by the old time level density. A very useful approximation is then

$$\gamma_{va}\alpha_{la}\left(C_{i,l}-C_{i,la}\right)-\Delta\tau\sum_{m=1}^{6}b_{lm-}\alpha_{lm}\left(C_{i,lm}-C_{i,l}\right)$$
$$\approx\alpha_{la}\left(C_{il}-C_{ila}\right)\gamma_{va}-\Delta\tau\sum_{m=1}^{6}b_{lm-}\alpha_{l,m}\frac{\rho_{l,m}}{\rho_{la}}\left(C_{il,m}-C_{il}\right)=\frac{\Delta\tau}{\rho_{la}}DC_{il}^{N} \quad (13.169)$$

and

$$\gamma_{va}\alpha_{la}\left(s_{l}-s_{la}\right)-\Delta\tau\sum_{m=1}^{6}b_{lm-}\alpha_{lm}\left(s_{lm}-s_{l}\right)$$
$$\approx\alpha_{la}\left(s_{l}-s_{la}\right)\gamma_{va}-\Delta\tau\sum_{m=1}^{6}b_{lm-}\alpha_{l,m}\frac{\rho_{l,m}}{\rho_{la}}\left(s_{l,m}-s_{l}\right)=\frac{\Delta\tau}{\rho_{la}}Ds_{l}^{N}, \quad (13.170)$$

Thus $D\alpha_{l}$ can be approximated as follows

$$D\alpha_{l}=\gamma_{v}\frac{\mu_{l}}{\rho_{l}}-\alpha_{la}\left(\frac{\gamma_{v}-\gamma_{va}}{\Delta\tau}\right)-\frac{1}{\rho_{l}\rho_{la}}\left\{\left(\frac{\partial\rho_{l}}{\partial s_{l}}\right)_{a}Ds_{l}^{N}+\sum_{i=2}^{i_{\max}}\left(\frac{\partial\rho_{l}}{\partial C_{i,l}}\right)_{a}DC_{il}^{N}\right\}. \quad (13.171)$$

Replacing with the normal velocities computed from the discretized momentum equation in linearized form we finally obtain the so called pressure equation

$$p\gamma_{va}\sum_{l=1}^{l_{\max}}\frac{\alpha_{la}}{\rho_{l}a_{la}^{2}}-\Delta\tau\sum_{m=1}^{6}\beta_{m}\sum_{l=1}^{l_{\max}}\left[\xi_{lm+}\alpha_{l}+\xi_{lm-}\alpha_{lm}\left(1+\frac{p_{m}-p}{\rho_{l}a_{la}^{2}}\right)\right]RVel_{lm}(p_{m}-p)$$
$$=p_{a}\gamma_{va}\sum_{l=1}^{l_{\max}}\frac{\alpha_{la}}{\rho_{l}a_{la}^{2}}+\Delta\tau\sum_{l=1}^{l_{\max}}D\alpha_{l}$$
$$-\Delta\tau\sum_{m=1}^{6}\beta_{m}\sum_{l=1}^{l_{\max}}\left[\xi_{lm+}\alpha_{l}+\xi_{lm-}\alpha_{lm}\left(1+\frac{p_{m}-p}{\rho_{l}a_{la}^{2}}\right)\right]\left[dV_{lm}^{n}-(\mathbf{e})^{m}\cdot\mathbf{V}_{cs,m}\right] \quad (13.172)$$

or

$$cp + \sum_{m=1}^{6} c_m p_m = d \ , \tag{13.173}$$

where

$$c_m = -\Delta\tau\beta_m \sum_{l=1}^{l_{\max}} \left[ \xi_{lm+}\alpha_l + \xi_{lm-}\alpha_{lm} \left( 1 + \frac{p_m - p}{\rho_l a_{la}^2} \right) \right] RVel_{lm} \ , \tag{13.174}$$

$$c = p\gamma_{va} \sum_{l=1}^{l_{\max}} \frac{\alpha_{la}}{\rho_l a_{la}^2} - \sum_{m=1}^{6} c_m \ , \tag{13.175}$$

$$d = p_a \gamma_{va} \sum_{l=1}^{l_{\max}} \frac{\alpha_{la}}{\rho_l a_{la}^2} + \Delta\tau \sum_{l=1}^{l_{\max}} D\alpha_l$$
$$- \Delta\tau \sum_{m=1}^{6} \beta_m \sum_{l=1}^{l_{\max}} \left[ \xi_{lm+}\alpha_l + \xi_{lm-}\alpha_{lm} \left( 1 + \frac{p_m - p}{\rho_l a_{la}^2} \right) \right] \left[ dV_{lm}^n - \left(\mathbf{e}\right)^m \cdot \mathbf{V}_{cs,m} \right] . \tag{13.176}$$

The advantage of Eq. (13.172) for the very first outer iteration step is that it takes the influence of all sources on the pressure change which is not the case in Eq. (13.156). The advantage of Eq. (13.156) for all subsequent outer iterations is that it reduces the residuals to very low value which is not the case with Eq. (13.172) because of the approximations (13.169) and (13.170). An additional source of numerical error is that the new density is usually computed within the outer iteration by using Eq. (13.159) and not Eq. (13.164). Combined, both equations result in a useful algorithm. As a predictor step use Eq. (13.172) and for all other iterations use Eq. (13.156).

## 13.12 Staggered *x* momentum equation

Two families of methods are known in the literature for solving partial differential equations with low order methods, the so called co-located and staggered grid methods. In the co-located methods all dependent variables are defined at the center of the mass control volume. In these methods unless the staggered grid method is used, discretization of order higher then the first order is required to create a stable numerical method. In the staggered grid method all dependent variables are defined in the center of the mass control volume except the velocities which are defined at the faces of the volume. In both cases the velocities are required for the center as well for the faces, so that the one group of velocities is usually computed by interpolation from the known other group. The control volume for the staggered grid methods consists of the half of the volumes belonging to each face. Strictly speaking the required geometrical information that has to be stored for these methods is four times those for the co-located methods. A compromise between low order methods using low storage and stability is to derive the discretized form of the momentum equation in the staggered cell from already discretized momentum equations in the two neighboring cells. This is possible for the following reason. Momentum equations are force balances per unit mixture volume and therefore they can be volumetrically averaged over the staggered grids. In this section we will use this idea. As already mentioned the staggered computational cell in the $\xi$ direction consists of the half of the mass control volumes belonging to the both sites of the $\xi$ face. We will discretize the three components of the momentum equation in this staggered cell. Then we will use the dot product of the so discretized vector momentum equation with the unit face vector to obtain the normal velocity at the cell face. In doing this, we will try to keep the computational effort small by finding common coefficients for all three equations. This approach leads to a pressure gradient component normal to the face instead of a pressure gradient to each of the Cartesian directions, which is simply numerically treated. This is the key for designing implicit or semi-implicit methods.

**Time derivatives:** We start with the term $\alpha_{la}\rho_{la}\left(u_l - u_{la}\right)\gamma_{va}$, perform volume averaging

$$\overline{\alpha_{la}\rho_{la}\left(u_l - u_{la}\right)\gamma_{va}}$$
$$= \alpha_{la}\rho_{la}\left(u_l - u_{la}\right)\frac{\gamma_{va}\Delta V}{\Delta V + \Delta V_{i+1}} + \alpha_{la,i+1}\rho_{la,i+1}\left(u_{l,i+1} - u_{la,i+1}\right)\frac{\gamma_{va,i+1}\Delta V_{i+1}}{\Delta V + \Delta V_{i+1}} \quad (13.177)$$

and approximate the average with

$$\overline{\alpha_{la}\rho_{la}\left(u_l - u_{la}\right)\gamma_{va}} \approx \left(\alpha_{la}\rho_{la}\gamma_{va}\right)_u \left(u_l^u - u_{la}^u\right), \quad (13.178)$$

where

$$\left(\alpha_{la}\rho_{la}\gamma_{va}\right)_u = \alpha_{la}\rho_{la}\frac{\gamma_{va}\Delta V}{\Delta V + \Delta V_{i+1}} + \alpha_{la,i+1}\rho_{la,i+1}\frac{\gamma_{va,i+1}\Delta V_{i+1}}{\Delta V + \Delta V_{i+1}}. \quad (13.179)$$

Note that this procedure of averaging does not give

$$u_l^u = \frac{1}{2}\left(u_l + u_{l,i+1}\right) \quad (13.180)$$

in the general case. Similarly we have for the other directions momentum equations

$$\overline{\alpha_{la}\rho_{la}\left(v_l - v_{la}\right)\gamma_{va}} \approx \left(\alpha_{la}\rho_{la}\gamma_{va}\right)_u \left(v_l^u - v_{la}^u\right), \quad (13.181)$$

$$\overline{\alpha_{la}\rho_{la}\left(w_l - w_{la}\right)\gamma_{va}} \approx \left(\alpha_{la}\rho_{la}\gamma_{va}\right)_u \left(w_l^u - w_{la}^u\right). \quad (13.182)$$

We realize that in this way of approximation the component velocity differences for all three Cartesian directions possess a common coefficient.

**Convective terms:** The following approximation for the convective terms is proposed

$$\overline{\sum_{m=1}^{6} b_{lm-}\alpha_{l,m}\rho_{l,m}\left(u_{l,m}-u_{l}\right)}$$
$$=\frac{1}{\Delta V+\Delta V_{i+1}}\left\{\Delta V\sum_{m=1}^{6} B_{lm-}\left(u_{l,m}-u_{l}\right)+\Delta V_{i+1}\sum_{m=1}^{6}\left[B_{lm-}\left(u_{l,m}-u_{l}\right)\right]_{i+1}\right\}$$
$$\approx\sum_{m=1}^{6} b_{lm-}^{u}\alpha_{l,m}^{u}\rho_{l,m}^{u}\left(u_{l,m}^{u}-u_{l}^{u}\right), \tag{13.183}$$

where

$$b_{lm-}^{u}\alpha_{l,m}^{u}\rho_{l,m}^{u}=C^{*}B_{lm-}+\left(1-C^{*}\right)\left(B_{lm-}\right)_{i+1}, \tag{13.184}$$

is the $m$-th face mass flow into the staggered cell divided by its volume and

$$C^{*}=\frac{\Delta V}{\Delta V+\Delta V_{i+1}}. \tag{13.185}$$

As in the case of the time derivatives we realize that in this way of approximation the component velocity differences for all three Cartesian directions possess a common coefficient.

**Diagonal diffusion terms**: We apply a similar procedure to the diagonal diffusion terms

$$\overline{\sum_{m=1}^{6}\beta_{m}\frac{D_{l,m}^{\nu}}{\Delta L_{h,m}}\left[1+\frac{1}{3}(e)^{m1}(e)^{m1}\right]\left(u_{l,m}-u_{l}\right)}=$$
$$=C^{*}\sum_{m=1}^{6}\beta_{m}\frac{D_{l,m}^{\nu}}{\Delta L_{h,m}}\left[1+\frac{1}{3}(e)^{m1}(e)^{m1}\right]\left(u_{l,m}-u_{l}\right)$$
$$+\left(1-C^{*}\right)\sum_{m=1}^{6}\left\{\beta_{m}\frac{D_{l,m}^{\nu}}{\Delta L_{h,m}}\left[1+\frac{1}{3}(e)^{m1}(e)^{m1}\right]\left(u_{l,m}-u_{l}\right)\right\}_{i+1}$$
$$\approx\sum_{m=1}^{6}\begin{pmatrix} C^{*}\beta_{m}\frac{D_{l,m}^{\nu}}{\Delta L_{h,m}}\left[1+\frac{1}{3}(e)^{m1}(e)^{m1}\right] \\ \\ +\left\{\left(1-C^{*}\right)\beta_{m}\frac{D_{l,m}^{\nu}}{\Delta L_{h,m}}\left[1+\frac{1}{3}(e)^{m1}(e)^{m1}\right]\right\}_{i+1}\end{pmatrix}\left(u_{l,m}^{u}-u_{l}^{u}\right). \tag{13.186}$$

Thus the combined convection-diffusion terms are finally approximated as follows

$$\overline{-\sum_{m=1}^{6}\left\{B_{lm-}+\beta_m \frac{D_{l,m}^{\nu}}{\Delta L_{h,m}}\left[1+\frac{1}{3}(e)^{m1}(e)^{m1}\right]\right\}\left(u_{l,m}-u_l\right)}$$

$$\approx \sum_{m=1}^{6} a_{lm,cd}\left(u_{l,m}^{u}-u_l^{u}\right)+\sum_{m=1}^{6} a_{lm,u\_dif}\left(u_{l,m}^{u}-u_l^{u}\right), \qquad (13.187)$$

where

$$a_{lm,cd}=-C^*\left(B_{lm-}+\beta_m \frac{D_{l,m}^{\nu}}{\Delta L_{h,m}}\right)-\left(1-C^*\right)\left(B_{lm-}+\beta_m \frac{D_{l,m}^{\nu}}{\Delta L_{h,m}}\right)_{i+1}, \qquad (13.188)$$

$$a_{lm,u\_dif}=-\frac{1}{3}\left\{C^*\beta_m \frac{D_{l,m}^{\nu}}{\Delta L_{h,m}}(e)^{m1}(e)^{m1}+\left(1-C^*\right)\left[\beta_m \frac{D_{l,m}^{\nu}}{\Delta L_{h,m}}(e)^{m1}(e)^{m1}\right]_{i+1}\right\}. \qquad (13.189)$$

Similarly we have

$$\overline{-\sum_{m=1}^{6}\left\{B_{lm-}+\beta_m \frac{D_{l,m}^{\nu}}{\Delta L_{h,m}}\left[1+\frac{1}{3}(e)^{m2}(e)^{m2}\right]\right\}\left(v_{l,m}-v_l\right)}$$

$$\approx \sum_{m=1}^{6} a_{lm,cd}\left(v_{l,m}^{u}-v_l^{u}\right)+\sum_{m=1}^{6} a_{lm,v\_dif}\left(v_{l,m}^{u}-v_l^{u}\right), \qquad (13.190)$$

$$a_{lm,v\_dif}=-\frac{1}{3}\left\{C^*\beta_m \frac{D_{l,m}^{\nu}}{\Delta L_{h,m}}(e)^{m2}(e)^{m2}+\left(1-C^*\right)\left[\beta_m \frac{D_{l,m}^{\nu}}{\Delta L_{h,m}}(e)^{m2}(e)^{m2}\right]_{i+1}\right\}. \qquad (13.191)$$

$$\overline{-\sum_{m=1}^{6}\left\{B_{lm-}+\beta_m \frac{D_{l,m}^{\nu}}{\Delta L_{h,m}}\left[1+\frac{1}{3}(e)^{m3}(e)^{m3}\right]\right\}\left(w_{l,m}-w_l\right)}$$

$$\approx \sum_{m=1}^{6} a_{lm,cd}\left(w_{l,m}^{u}-w_l^{u}\right)+\sum_{m=1}^{6} a_{lm,w\_dif}\left(w_{l,m}^{u}-w_l^{u}\right), \qquad (13.192)$$

$$a_{lm,w\_dif}=-\frac{1}{3}\left\{C^*\beta_m \frac{D_{l,m}^{\nu}}{\Delta L_{h,m}}(e)^{m3}(e)^{m3}+\left(1-C^*\right)\left[\beta_m \frac{D_{l,m}^{\nu}}{\Delta L_{h,m}}(e)^{m3}(e)^{m3}\right]_{i+1}\right\}. \qquad (13.193)$$

We realize again that the coefficients $a_{lm,cd}$ are common for all the momentum equations in the staggered cell.

**Drag force terms:** The following approximation contains in fact computation of the volume averages of the linearized drag coefficients.

$$\overline{\gamma_v \left[ \sum_{\substack{m=1 \\ m \ne l}}^{3} \overline{c}_{ml}^{d} \left| \Delta \mathbf{V}_{ml} \right| \left( u_m - u_l \right) + \overline{c}_{wl}^{d} \left| \Delta \mathbf{V}_{wl} \right| \left( u_{cs} - u_l \right) \right]}$$
$$\approx \sum_{\substack{m=1 \\ m \ne l}}^{3} \left( \gamma_v c_{ml}^{d} \right)_u \left( u_m^u - u_l^u \right) + \left( \gamma_v c_{wl}^{d} \right)_u \left( u_{cs}^u - u_l^u \right), \tag{13.194}$$

where

$$\left( \gamma_v c_{ml}^{d} \right)_u = \frac{1}{\Delta V + \Delta V_{i+1}} \left( \gamma_v \Delta V \overline{c}_{ml}^{d} \left| \Delta \mathbf{V}_{ml} \right| + \gamma_{v,i+1} \Delta V_{i+1} \overline{c}_{ml,i+1}^{d} \left| \Delta \mathbf{V}_{ml} \right|_{i+1} \right), \tag{13.195}$$

$$\left( \gamma_v c_{wl}^{d} \right)_u = \frac{1}{\Delta V + \Delta V_{i+1}} \left( \gamma_v \Delta V \overline{c}_{wl}^{d} \left| \Delta \mathbf{V}_{csl} \right| + \gamma_{v,i+1} \Delta V_{i+1} \overline{c}_{wl,i+1}^{d} \left| \Delta \mathbf{V}_{csl} \right|_{i+1} \right). \tag{13.196}$$

Similarly we have

$$\overline{\gamma_v \left[ \sum_{\substack{m=1 \\ m \ne l}}^{3} \overline{c}_{ml}^{d} \left| \Delta \mathbf{V}_{ml} \right| \left( v_m - v_l \right) + \overline{c}_{wl}^{d} \left| \Delta \mathbf{V}_{wl} \right| \left( v_{cs} - v_l \right) \right]}$$
$$\approx \sum_{\substack{m=1 \\ m \ne l}}^{3} \left( \gamma_v c_{ml}^{d} \right)_u \left( v_m^u - v_l^u \right) + \left( \gamma_v c_{wl}^{d} \right)_u \left( v_{cs}^u - v_l^u \right), \tag{13.197}$$

$$\overline{\gamma_v \left[ \sum_{\substack{m=1 \\ m \ne l}}^{3} \overline{c}_{ml}^{d} \left| \Delta \mathbf{V}_{ml} \right| \left( w_m - w_l \right) + \overline{c}_{wl}^{d} \left| \Delta \mathbf{V}_{wl} \right| \left( w_{cs} - w_l \right) \right]}$$
$$\approx \sum_{\substack{m=1 \\ m \ne l}}^{3} \left( \gamma_v c_{ml}^{d} \right)_u \left( w_m^u - w_l^u \right) + \left( \gamma_v c_{wl}^{d} \right)_u \left( w_{cs}^u - w_l^u \right). \tag{13.198}$$

Again the drag term coefficients for the momentum equations in the staggered cell are common.

**Gravitational force:** The volume averaging for the gravitational force gives

$$\overline{\alpha_l \rho_l g_x \gamma_v} = g_x \left( \alpha_{la} \rho_{la} \gamma_{va} \right)_u, \tag{13.199}$$

$$\overline{\alpha_l \rho_l g_y \gamma_v} = g_y \left( \alpha_{la} \rho_{la} \gamma_{va} \right)_u, \tag{13.200}$$

$$\overline{\alpha_l \rho_l g_z \gamma_v} = g_z \left( \alpha_{la} \rho_{la} \gamma_{va} \right)_u. \tag{13.201}$$

**Interfacial momentum transfer due to mass transfer:** The interfacial momentum transfer is again approximated by first volume averaging the volume mass source terms due to interfacial mass transfer. The source terms due to external injection or suction are computed exactly because it is easy to prescribe the velocities corresponding to the sources at the mass cell center.

$$-\overline{\left[\sum_{m=1}^{3,w}\left[\mu_{ml}\gamma_v\left(u_m-u_l\right)\right]+\mu_{lw}\gamma_v\left(u_{lw}-u_l\right)\right]}$$

$$\approx\sum_{m=1}^{3}\left(\gamma_v\mu_{ml}\right)_u\left(u_m^u-u_l^u\right)+\left(\gamma_v\mu_{wl}\right)_u\left(u_{wl}^u-u_l^u\right)-\left(\gamma_v\mu_{lw}\right)_u\left(u_{lw}^u-u_l^u\right) \quad (13.202)$$

$$\left(\gamma_v\mu_{ml}\right)_u=\frac{1}{\Delta V+\Delta V_{i+1}}\left(\gamma_v\Delta V\mu_{ml}+\gamma_{v,i+1}\Delta V_{i+1}\mu_{ml,i+1}\right), \quad (13.203)$$

$$\left(\gamma_v\mu_{wl}\right)_u=\frac{1}{\Delta V+\Delta V_{i+1}}\left(\gamma_v\Delta V\mu_{wl}+\gamma_{v,i+1}\Delta V_{i+1}\mu_{wl,i+1}\right), \quad (13.204)$$

$$\left(\gamma_v\mu_{lw}\right)_u=\frac{1}{\Delta V+\Delta V_{i+1}}\left(\gamma_v\Delta V\mu_{lw}+\gamma_{v,i+1}\Delta V_{i+1}\mu_{lw,i+1}\right), \quad (13.205)$$

$$\left(\gamma_v\mu_{wl}\right)_u u_{wl}=\frac{1}{\Delta V+\Delta V_{i+1}}\left(\gamma_v\Delta V\mu_{wl}u_{wl}+\gamma_{v,i+1}\Delta V_{i+1}\mu_{wl,i+1}u_{wl,i+1}\right), \quad (13.206)$$

$$\left(\gamma_v\mu_{lw}\right)_u u_{lw}=\frac{1}{\Delta V+\Delta V_{i+1}}\left(\gamma_v\Delta V\mu_{lw}u_{lw}+\gamma_{v,i+1}\Delta V_{i+1}\mu_{lw,i+1}u_{lw,i+1}\right), \quad (13.207)$$

Similarly we have

$$-\overline{\left[\sum_{m=1}^{3,w}\left[\mu_{ml}\gamma_v\left(v_m-v_l\right)\right]+\mu_{lw}\gamma_v\left(v_{lw}-v_l\right)\right]}$$

$$\approx\sum_{m=1}^{3}\left(\gamma_v\mu_{ml}\right)_u\left(v_m^u-v_l^u\right)+\left(\gamma_v\mu_{wl}\right)_u\left(v_{wl}^u-v_l^u\right)-\left(\gamma_v\mu_{lw}\right)_u\left(v_{lw}^u-v_l^u\right), \quad (13.208)$$

$$-\overline{\left[\sum_{m=1}^{3,w}\left[\mu_{ml}\gamma_v\left(w_m-w_l\right)\right]+\mu_{lw}\gamma_v\left(w_{lw}-w_l\right)\right]}$$

$$\approx\sum_{m=1}^{3}\left(\gamma_v\mu_{ml}\right)_u\left(w_m^u-w_l^u\right)+\left(\gamma_v\mu_{wl}\right)_u\left(w_{wl}^u-w_l^u\right)-\left(\gamma_v\mu_{lw}\right)_u\left(w_{lw}^u-w_l^u\right). \quad (13.209)$$

**Lift force, off-diagonal viscous forces:** The lift force and the off-diagonal viscous forces are explicitly computed by strict volume averaging.

Pressure gradient:

$$\overline{\alpha_l \gamma_\xi (\nabla p)\cdot \mathbf{i}} = \alpha_{lu}\gamma_\xi (\nabla p)\cdot \mathbf{i} \,, \tag{13.210}$$

where

$$\alpha_{lu} = \frac{\gamma_v \Delta V \alpha_l + \gamma_{v,i+1}\Delta V_{i+1}\alpha_{l,i+1}}{\gamma_v \Delta V + \gamma_{v,i+1}\Delta V_{i+1}} \,. \tag{13.211}$$

Similarly we have

$$\overline{\alpha_l \gamma_\xi (\nabla p)\cdot \mathbf{j}} = \alpha_{lu}\gamma_\xi (\nabla p)\cdot \mathbf{j} \,, \tag{13.212}$$

$$\overline{\alpha_l \gamma_\xi (\nabla p)\cdot \mathbf{k}} = \alpha_{lu}\gamma_\xi (\nabla p)\cdot \mathbf{k} \,. \tag{13.213}$$

Virtual mass force:

$$\gamma_v \sum_{\substack{m=1\\ m\neq l}}^{3,cs} \overline{c}_{ml}^{vm} \left( \frac{\partial \Delta u_{ml}}{\partial \tau} + \overline{V}^1 \frac{\partial \Delta u_{ml}}{\partial \xi} + \overline{V}^2 \frac{\partial \Delta u_{ml}}{\partial \eta} + \overline{V}^3 \frac{\partial \Delta u_{ml}}{\partial \zeta} \right)$$

$$= \sum_{\substack{m=1\\ m\neq l}}^{3,cs} \left(\gamma_v \overline{c}_{ml}^{vm}\right)_u \left( \begin{array}{l} \dfrac{u_m^u - u_l^u}{\Delta \tau} - \dfrac{u_{ma}^u - u_{la}^u}{\Delta \tau} + \left(\overline{V}^1\right)_1 \left(u_{m,i+1} - u_{l,i+1} - u_m + u_l\right) \\ + \left(\overline{V}^2\right)_1 \left( \left.\dfrac{\partial u_m}{\partial \eta}\right|_1 - \left.\dfrac{\partial u_l}{\partial \eta}\right|_1 \right) + \left(\overline{V}^3\right)_1 \left( \left.\dfrac{\partial u_m}{\partial \zeta}\right|_1 - \left.\dfrac{\partial u_l}{\partial \zeta}\right|_1 \right) \end{array} \right). \tag{13.214}$$

Similarly we have

$$\gamma_v \sum_{\substack{m=1\\ m\neq l}}^{3,cs} \overline{c}_{ml}^{vm} \left( \frac{\partial \Delta v_{ml}}{\partial \tau} + \overline{V}^1 \frac{\partial \Delta v_{ml}}{\partial \xi} + \overline{V}^2 \frac{\partial \Delta v_{ml}}{\partial \eta} + \overline{V}^3 \frac{\partial \Delta v_{ml}}{\partial \zeta} \right)$$

$$= \sum_{\substack{m=1\\ m\neq l}}^{3,cs} \left(\gamma_v \overline{c}_{ml}^{vm}\right)_u \left( \begin{array}{l} \dfrac{v_m^u - v_l^u}{\Delta \tau} - \dfrac{v_{ma}^u - v_{la}^u}{\Delta \tau} + \left(\overline{V}^1\right)_1 \left(v_{m,i+1} - v_{l,i+1} - v_m + v_l\right) \\ + \left(\overline{V}^2\right)_1 \left( \left.\dfrac{\partial v_m}{\partial \eta}\right|_1 - \left.\dfrac{\partial v_l}{\partial \eta}\right|_1 \right) + \left(\overline{V}^3\right)_1 \left( \left.\dfrac{\partial v_m}{\partial \zeta}\right|_1 - \left.\dfrac{\partial v_l}{\partial \zeta}\right|_1 \right) \end{array} \right), \tag{13.215}$$

$$\gamma_v \sum_{\substack{m=1\\ m\neq l}}^{3,cs} \overline{c}_{ml}^{vm} \left( \frac{\partial \Delta w_{ml}}{\partial \tau} + \overline{V}^1 \frac{\partial \Delta w_{ml}}{\partial \xi} + \overline{V}^2 \frac{\partial \Delta w_{ml}}{\partial \eta} + \overline{V}^3 \frac{\partial \Delta w_{ml}}{\partial \zeta} \right)$$

$$= \sum_{\substack{m=1 \\ m \neq l}}^{3,cs} \left( \gamma_v \overline{c}_{ml}^{vm} \right)_u \left( \begin{array}{l} \dfrac{w_m^u - w_l^u}{\Delta \tau} - \dfrac{w_{ma}^u - w_{la}^u}{\Delta \tau} + \left( \overline{V}^1 \right)_1 \left( w_{m,i+1} - w_{l,i+1} - w_m + w_l \right) \\ + \left( \overline{V}^2 \right)_1 \left( \left. \dfrac{\partial w_m}{\partial \eta} \right|_1 - \left. \dfrac{\partial w_l}{\partial \eta} \right|_1 \right) + \left( \overline{V}^3 \right)_1 \left( \left. \dfrac{\partial w_m}{\partial \zeta} \right|_1 - \left. \dfrac{\partial w_l}{\partial \zeta} \right|_1 \right) \end{array} \right). \quad (13.216)$$

Implicit treatment of the interfacial interaction:

$$\left( \alpha_{la} \rho_{la} \gamma_{va} \right)_u \frac{u_l^u - u_{la}^u}{\Delta \tau} + \sum_{m=1}^{6} a_{lm,cd} \left( u_{l,m}^u - u_l^u \right) + \alpha_{l,u} \gamma_\xi \left( \nabla p \right) \cdot \mathbf{i}$$

$$- \sum_{\substack{m=1 \\ m \neq l}}^{3,cs} \left( \gamma_v \overline{c}_{ml}^{vm} \right)_u \left( \begin{array}{l} \dfrac{u_m^u - u_l^u}{\Delta \tau} - \dfrac{u_{ma}^u - u_{la}^u}{\Delta \tau} + \left( \overline{V}^1 \right)_1 \left( u_{m,i+1} - u_{l,i+1} - u_m + u_l \right) \\ + \left( \overline{V}^2 \right)_1 \left( \left. \dfrac{\partial u_m}{\partial \eta} \right|_1 - \left. \dfrac{\partial u_l}{\partial \eta} \right|_1 \right) + \left( \overline{V}^3 \right)_1 \left( \left. \dfrac{\partial u_m}{\partial \zeta} \right|_1 - \left. \dfrac{\partial u_l}{\partial \zeta} \right|_1 \right) \end{array} \right) - \left( \gamma_v f_l^L \right)_u$$

$$= - \sum_{m=1}^{6} a_{lm,u\_dif} \left( u_{l,m}^u - u_l^u \right) - g_x \left( \alpha_{la} \rho_{la} \gamma_{va} \right)_u$$

$$+ \sum_{m=1}^{3} \left( \gamma_v \mu_{ml} \right)_u \left( u_m^u - u_l^u \right) + \left( \gamma_v \mu_{wl} \right)_u \left( u_{wl}^u - u_l^u \right) - \left( \gamma_v \mu_{lw} \right)_u \left( u_{lw}^u - u_l^u \right)$$

$$+ \sum_{\substack{m=1 \\ m \neq l}}^{3} \left( \gamma_v c_{ml}^d \right)_u \left( u_m^u - u_l^u \right) + \left( \gamma_v c_{wl}^d \right)_u \left( u_{cs}^u - u_l^u \right) + Vis_l^u \,. \quad (13.217)$$

For all three velocity fields we have a system of algebraic equations with respect to the corresponding field velocity components in the $x$ direction

$$\left[ \left( \alpha_{la} \rho_{la} \gamma_{va} \right)_u \frac{1}{\Delta \tau} - \sum_{\substack{m=1 \\ m \neq l}}^{3} a_{lm} + a_{l,cd} + \left( \gamma_v \overline{c}_{wl}^{vm} \right)_u \frac{1}{\Delta \tau} + \left( \gamma_v c_{wl}^d \right)_u + \left( \gamma_v \mu_{wl} \right)_u - \left( \gamma_v \mu_{lw} \right)_u \right] u_l^u$$

$$+ \sum_{\substack{m=1 \\ m \neq l}}^{3} a_{lm} u_m^u = b_l - \alpha_{l,u} \gamma_\xi \left( \nabla p \right) \cdot \mathbf{i} \quad (13.218)$$

or

$$\mathbf{A}^u \mathbf{u}^u = \mathbf{b} \mathbf{u}^u - \mathbf{a}^u \gamma_\xi \left( \nabla p \right) \cdot \mathbf{i} \,. \quad (13.219)$$

The non-diagonal and the diagonal elements of the $\mathbf{A}^u$ matrix are

$$a_{ml} = -\left[\left(\gamma_v \overline{c}_{ml}^{vm}\right)_u \frac{1}{\Delta\tau} + \left(\gamma_v \mu_{ml}\right)_u + \left(\gamma_v c_{ml}^{d}\right)_u\right], \tag{13.220}$$

and

$$a_{ll} = \left(\alpha_{la}\rho_{la}\gamma_{va}\right)_u \frac{1}{\Delta\tau} - \sum_{\substack{m=1 \\ m\neq l}}^{3} a_{lm} + a_{l,cd} + \left(\gamma_v \overline{c}_{wl}^{vm}\right)_u \frac{1}{\Delta\tau} + \left(\gamma_v c_{wl}^{d}\right)_u + \left(\gamma_v \mu_{wl}\right)_u - \left(\gamma_v \mu_{lw}\right)_u, \tag{13.221}$$

respectively, where

$$a_{l,cd} = -\sum_{m=1}^{6} a_{lm,cd} \ . \tag{13.222}$$

The elements of the algebraic vector $\mathbf{bu}^u$ are

$$bu_l = bu_{l,conv} + Vis_l^u + \left(\alpha_{la}\rho_{la}\gamma_{va}\right)_u \left(\frac{u_{la}^u}{\Delta\tau} - g_x\right) - \sum_{\substack{m=1 \\ m\neq l}}^{3,cs} bu_{lm} + \left(\gamma_v f_l^L\right)_u$$

$$+\left[\left(\gamma_v \overline{c}_{csl}^{vm}\right)_u \frac{1}{\Delta\tau} + \left(\gamma_v c_{wl}^{d}\right)_u\right] u_{cs}^u + \left[\left(\gamma_v \mu_{wl}\right)_u - \left(\gamma_v \mu_{lw}\right)_u\right] u_{lw}^u \tag{13.223}$$

where

$$bu_{ml} = -bu_{lm} = \left(\gamma_v \overline{c}_{ml}^{vm}\right)_u \left[\begin{array}{l} -\dfrac{u_{ma}^u - u_{la}^u}{\Delta\tau} + \left(\overline{V}^1\right)_1 \left(u_{m,i+1} - u_{l,i+1} - u_m + u_l\right) \\ \\ +\left(\overline{V}^2\right)_1 \left(\left.\dfrac{\partial u_m}{\partial \eta}\right|_{1} - \left.\dfrac{\partial u_l}{\partial \eta}\right|_{1}\right) + \left(\overline{V}^3\right)_1 \left(\left.\dfrac{\partial u_m}{\partial \zeta}\right|_{1} - \left.\dfrac{\partial u_l}{\partial \zeta}\right|_{1}\right) \end{array}\right] \tag{13.224}$$

and

$$bu_{l,conv} = -\sum_{m=1}^{6}\left[\left(a_{lm,cd} + a_{lm,u\_dif}\right) u_{l,m}^u - a_{lm,u\_dif} u_l^u\right]. \tag{13.225}$$

The elements of the algebraic vector $\mathbf{a}^u$ are $\alpha_{l,u}$, where $l$ = 1,2,3. Note that by definition, if one velocity field does not exist, $\alpha_l = 0$, the coefficients describing its coupling with the other fields are then equal to zero. Similarly we can discretize the momentum equations in the same staggered control volume for the other Cartesian components. The result in component form is then

$$\mathbf{A}^u\mathbf{u}^u = \mathbf{b}\mathbf{u}^u - \mathbf{a}^u\gamma_\xi\left(\nabla p\right)\cdot\mathbf{i}\,, \qquad (13.226)$$

$$\mathbf{A}^u\mathbf{v}^u = \mathbf{b}\mathbf{v}^u - \mathbf{a}^u\gamma_\xi\left(\nabla p\right)\cdot\mathbf{j}\,, \qquad (13.227)$$

$$\mathbf{A}^u\mathbf{w}^u = \mathbf{b}\mathbf{w}^u - \mathbf{a}^u\gamma_\xi\left(\nabla p\right)\cdot\mathbf{k}\,. \qquad (13.228)$$

It is remarkable that the **A** matrix and the coefficients of the pressure gradient are common for all the three systems of equations. If we take the dot product of each *u*-*v*-*w* equation with the unit normal vector at the control volume face we then obtain

$$\mathbf{A}^u\left[\left(e^{11}\right)_1\mathbf{u}^u + \left(e^{12}\right)_1\mathbf{v}^u + \left(e^{13}\right)_1\mathbf{w}^u\right]$$
$$= \left(e^{11}\right)_1\mathbf{b}\mathbf{u}^u + \left(e^{12}\right)_1\mathbf{b}\mathbf{v}^u + \left(e^{13}\right)_1\mathbf{b}\mathbf{w}^u - \mathbf{a}^u\gamma_\xi\left[\left(\mathbf{e}^1\right)_1\cdot\left(\nabla p\right)\right]. \qquad (13.229)$$

Having in mind that the outwards pointing normal face velocity is

$$\overline{\mathbf{V}}^n = \left(\mathbf{e}\right)^1\cdot\mathbf{V}^u\,, \qquad (13.230)$$

and

$$\frac{\partial p}{\partial \xi} = \left(\mathbf{e}\right)^1\cdot\left(\nabla p\right), \qquad (13.231)$$

we obtain finally

$$\mathbf{A}^u\overline{\mathbf{V}}^n = \mathbf{b}^u - \mathbf{a}^u\gamma_\xi\frac{\partial p}{\partial \xi}\,, \qquad (13.232)$$

where

$$\mathbf{b}^u = \left(e^{11}\right)_1\mathbf{b}\mathbf{u}^u + \left(e^{12}\right)_1\mathbf{b}\mathbf{v}^u + \left(e^{13}\right)_1\mathbf{b}\mathbf{w}^u\,. \qquad (13.233)$$

This algebraic system can be solved with respect to each field velocity provided that

$$\det\mathbf{A}^u = a_{11}a_{22}a_{33} + a_{12}a_{23}a_{31} + a_{21}a_{32}a_{13} - a_{31}a_{22}a_{13} - a_{32}a_{23}a_{11} - a_{12}a_{21}a_{33} \neq 0\,. \qquad (13.234)$$

The result is

$$\overline{\mathbf{V}}^n = \mathbf{d}\mathbf{V}_\xi - \mathbf{R}\mathbf{V}_\xi\gamma_\xi\left(p_{i+1} - p\right), \qquad (13.235)$$

where

$$\mathbf{dV}_\xi = \left(\mathbf{A}^u\right)^{-1} \mathbf{b}^u \tag{13.236}$$

with components

$$d\overline{V}_{\xi,l} = \left( \sum_{m=1}^{3} b_m \overline{a}_{lm} \right) / \det \mathbf{A}^u , \tag{13.237}$$

and

$$\mathbf{RV}_\xi = \left(\mathbf{A}^u\right)^{-1} \mathbf{a}_u , \tag{13.238}$$

with components

$$RU_l = \left( \sum_{m=1}^{3} \alpha_{ma,u} \overline{a}_{lm} \right) / \det \mathbf{A}_u , \tag{13.239}$$

and the $\overline{a}$ values are

$$\overline{a}_{11} = a_{22}a_{33} - a_{32}a_{23} , \quad \overline{a}_{12} = a_{32}a_{13} - a_{12}a_{33} , \quad \overline{a}_{13} = a_{12}a_{23} - a_{22}a_{13} ,$$

$$\overline{a}_{21} = a_{23}a_{31} - a_{21}a_{33} , \quad \overline{a}_{22} = a_{11}a_{33} - a_{31}a_{13} , \quad \overline{a}_{23} = a_{21}a_{13} - a_{23}a_{11} ,$$

$$\overline{a}_{31} = a_{21}a_{32} - a_{31}a_{22} , \quad \overline{a}_{32} = a_{12}a_{31} - a_{32}a_{11} , \quad \overline{a}_{33} = a_{11}a_{22} - a_{21}a_{12} . \tag{13.240-248}$$

Actually, not the absolute but the relative normal face velocity is required to construct the pressure equation which is readily obtained

$$\mathbf{V}^n = \overline{\mathbf{V}}^n - \left(\mathbf{e}\right)^1 \cdot \mathbf{V}_{cs} . \tag{13.249}$$

## Appendix 13.1 Harmonic averaged diffusion coefficients

A natural averaging of the coefficients describing diffusion across the face $m$, having surface cross section $S_m$ is then the harmonic averaging

$$\frac{D_{l,m}^{\Phi}}{\Delta L_{h,m}} = \left( \frac{\Phi_l}{\Delta V} \right)_m S_m = S_m \frac{2\left(\Phi_l\right)\left(\Phi_l\right)_m}{\Delta V_m \left(\Phi_l\right) + \Delta V \left(\Phi_l\right)_m}$$

where on the right hand side $m$ = 1, 2, 3, 4, 5, 6 is equivalent to $i$ + 1, $i$ - 1, $j$ + 1, $j$ - 1, $k$ + 1, $k$ - 1, respectively regarding the properties inside a control volumes. $\Delta V$ is the non-staggered cell volume, and $\Delta V_m$ is the volume of the cell at the other side of face $m$. It guaranties that if the field in one of the neighboring cells is missing the diffusion coefficient is zero. This property is derived from the solution of the steady state one-dimensional diffusion equations.

For computation of

$$\frac{D_{il,m}^*}{\Delta L_{h,m}} = \left(\frac{\alpha_l \rho_l D_{il}^*}{\Delta V}\right)_m S_m = S_m \frac{2\left(\alpha_l \rho_l D_{il}^*\right)\left(\alpha_l \rho_l D_{il}^*\right)_m}{\Delta V_m \left(\alpha_l \rho_l D_{il}^*\right) + \Delta V \left(\alpha_l \rho_l D_{il}^*\right)_m}$$

we simply set $\Phi_l = \alpha_l \rho_l D_{il}^*$.

For computation of $\frac{D_{l,m}^T}{\Delta L_{h,m}}$ we simply set $\Phi_l = \alpha_l \lambda_l$.

For computation of $\frac{D_{il,m}^{sC}}{\Delta L_{h,m}}$ we simply set $\Phi_l = \alpha_l \rho_l D_{il}^* \left(s_{il} - s_{1l}\right)$. Note that

$$\frac{D_{il,m}^C}{\Delta L_{h,m}} = 0$$

for $s_{il} = s_{1l}$ or $s_{il,m} = s_{1l,m}$.

For computation of the turbulent particle diffusion coefficient $\frac{D_{l,m}^n}{\Delta L_{h,m}}$ we simply set $\Phi_l = \frac{\nu_l^t}{Sc^t}$.

For computation of $\frac{D_{l,m}^\nu}{\Delta L_{h,m}}$ we simply set $\Phi_l = \alpha_l \rho_l \nu_l^*$.

In the case of cylindrical or Cartesian coordinate systems we have zero off-diagonal diffusion terms and

$$\frac{D_{l1}^\Phi}{\Delta r_h} = \frac{2\left(\Phi_l\right)\left(\Phi_l\right)_{i+1}}{\Delta r \left(\Phi_l\right)_{i+1} + \Delta r_{i+1} \Phi_l},$$

$$\frac{D_{l2}^\Phi}{\Delta r_{h,i-1}} = \frac{2\left(\Phi_l\right)\left(\Phi_l\right)_{i-1}}{\Delta r \left(\Phi_l\right)_{i-1} + \Delta r_{i-1} \Phi_l},$$

$$\frac{D_{l3}^\Phi}{r^\kappa \Delta \theta_h} = \frac{2\left(\Phi_l\right)\left(\Phi_l\right)_{j+1}}{r^\kappa \left[\Delta \theta \left(\Phi_l\right)_{j+1} + \Delta \theta_{j+1} \Phi_l\right]},$$

$$\frac{D_{l4}^\Phi}{r^\kappa \Delta \theta_{h,j-1}} = \frac{2\left(\Phi_l\right)\left(\Phi_l\right)_{j-1}}{r^\kappa \left[\Delta \theta \left(\Phi_l\right)_{j-1} + \Delta \theta_{j-1} \Phi_l\right]},$$

$$\frac{D_{l5}^\Phi}{\Delta z_h} = \frac{2\left(\Phi_l\right)\left(\Phi_l\right)_{k+1}}{\Delta z \left(\Phi_l\right)_{k+1} + \Delta z_{k+1} \Phi_l},$$

$$\frac{D^{\Phi}_{l6}}{\Delta z_{h,k-1}} = \frac{2\left(\Phi_l\right)\left(\Phi_l\right)_{k-1}}{\Delta z\left(\Phi_l\right)_{k-1} + \Delta z_{k-1}\Phi_l} .$$

## Appendix 13.2 Off-diagonal viscous diffusion terms of the *x* momentum equation

The off-diagonal viscous diffusion terms in the $x$ momentum equation are

$$\sum_{m=1}^{6} \beta_m \frac{D^{\nu}_{l,m}}{\Delta L_{h,m}} \left( DI\_u_{l,m} - \frac{2}{3}\left(e\right)^{m1} DI\_u^{b}_{l,m} + DI\_vis^{uT}_{lm} \right)$$

$$= \beta_1^* \left\{ q_{x1,12} \left.\frac{\partial u_l}{\partial \eta}\right|_1 + q_{x1,13} \left.\frac{\partial u_l}{\partial \zeta}\right|_1 + q_{x1,22} \left.\frac{\partial v_l}{\partial \eta}\right|_1 + q_{x1,23} \left.\frac{\partial v_l}{\partial \zeta}\right|_1 + q_{x1,32} \left.\frac{\partial w_l}{\partial \eta}\right|_1 + q_{x1,33} \left.\frac{\partial w_l}{\partial \zeta}\right|_1 \right\}$$

$$+ \beta_2^* \left\{ q_{x2,12} \left.\frac{\partial u_l}{\partial \eta}\right|_2 + q_{x2,13} \left.\frac{u_l}{\partial \zeta}\right|_2 q_{x2,22} \left.\frac{\partial v_l}{\partial \eta}\right|_2 + q_{x2,23} \left.\frac{\partial v_l}{\partial \zeta}\right|_2 + q_{x2,32} \left.\frac{\partial w_l}{\partial \eta}\right|_2 + q_{x2,33} \left.\frac{\partial w_l}{\partial \zeta}\right|_2 \right\}$$

$$+ \beta_3^* \left\{ q_{x3,11} \left.\frac{\partial u_l}{\partial \xi}\right|_3 + q_{x3,13} \left.\frac{\partial u_l}{\partial \zeta}\right|_3 + q_{x3,21} \left.\frac{\partial v_l}{\partial \xi}\right|_3 + q_{x3,23} \left.\frac{\partial v_l}{\partial \zeta}\right|_3 + q_{x3,31} \left.\frac{\partial w_l}{\partial \xi}\right|_3 + q_{x3,33} \left.\frac{\partial w_l}{\partial \zeta}\right|_3 \right\}$$

$$+ \beta_4^* \left\{ q_{x4,11} \left.\frac{\partial u_l}{\partial \xi}\right|_4 + q_{x4,13} \left.\frac{\partial u_l}{\partial \zeta}\right|_4 + q_{x4,21} \left.\frac{\partial v_l}{\partial \xi}\right|_4 + q_{x4,23} \left.\frac{\partial v_l}{\partial \zeta}\right|_4 + q_{x4,31} \left.\frac{\partial w_l}{\partial \xi}\right|_4 + q_{x4,33} \left.\frac{\partial w_l}{\partial \zeta}\right|_4 \right\}$$

$$+ \beta_5^* \left\{ q_{x5,11} \left.\frac{\partial u_l}{\partial \xi}\right|_5 + q_{x5,12} \left.\frac{\partial u_l}{\partial \eta}\right|_5 + q_{x5,21} \left.\frac{\partial v_l}{\partial \xi}\right|_5 + q_{x5,22} \left.\frac{\partial v_l}{\partial \eta}\right|_5 + q_{x5,31} \left.\frac{\partial w_l}{\partial \xi}\right|_5 + q_{x5,32} \left.\frac{\partial w_l}{\partial \eta}\right|_5 \right\}$$

$$+ \beta_6^* \left\{ q_{x6,11} \left.\frac{\partial u_l}{\partial \xi}\right|_6 + q_{x6,12} \left.\frac{\partial u_l}{\partial \eta}\right|_6 + q_{x6,21} \left.\frac{\partial v_l}{\partial \xi}\right|_6 + q_{x6,22} \left.\frac{\partial v_l}{\partial \eta}\right|_6 + q_{x6,31} \left.\frac{\partial w_l}{\partial \xi}\right|_6 + q_{x6,32} \left.\frac{\partial w_l}{\partial \eta}\right|_6 \right\} .$$

Here the coefficients

$$\beta_m^* = \beta_m = \frac{D^{\nu}_{l,m}}{\Delta L_{h,m}} \frac{\overline{\Delta V}_m}{S_m}$$

are used also in the other momentum equations. The following 36 coefficients are functions of the geometry only.

$$q_{x1,12} = \frac{4}{3}\left(e\right)^{11}\left(a^{21}\right)_1 + \left(e\right)^{12}\left(a^{22}\right)_1 + \left(e\right)^{13}\left(a^{23}\right)_1 = d_{12} + \frac{1}{3}\left(e\right)^{11}\left(a^{21}\right)_1 ,$$

$$q_{x1,13} = \frac{4}{3}\left(e\right)^{11}\left(a^{31}\right)_1 + \left(e\right)^{12}\left(a^{32}\right)_1 + \left(e\right)^{13}\left(a^{33}\right)_1 = d_{13} + \frac{1}{3}\left(e\right)^{11}\left(a^{31}\right)_1 ,$$

$$q_{x1,22} = (e)^{12} \left(a^{21}\right)_1 - \frac{2}{3}(e)^{11} \left(a^{22}\right)_1 ,$$

$$q_{x1,23} = (e)^{12} \left(a^{31}\right)_1 - \frac{2}{3}(e)^{11} \left(a^{32}\right)_1 ,$$

$$q_{x1,32} = (e)^{13} \left(a^{21}\right)_1 - \frac{2}{3}(e)^{11} \left(a^{23}\right)_1 ,$$

$$q_{x1,33} = (e)^{13} \left(a^{31}\right)_1 - \frac{2}{3}(e)^{11} \left(a^{33}\right)_1 ,$$

$$q_{x2,12} = \frac{4}{3}(e)^{21} \left(a^{21}\right)_2 + (e)^{22} \left(a^{22}\right)_2 + (e)^{23} \left(a^{23}\right)_2 = d_{22} + \frac{1}{3}(e)^{21} \left(a^{21}\right)_2$$

$$= -\left(q_{x1,12}\right)_{i-1} ,$$

$$q_{x2,13} = \frac{4}{3}(e)^{21} \left(a^{31}\right)_2 + (e)^{22} \left(a^{32}\right)_2 + (e)^{23} \left(a^{33}\right)_2 = d_{23} + \frac{1}{3}(e)^{21} \left(a^{31}\right)_2$$

$$= -\left(q_{x1,13}\right)_{i-1} ,$$

$$q_{x2,22} = (e)^{22} \left(a^{21}\right)_2 - \frac{2}{3}(e)^{21} \left(a^{22}\right)_2 = -\left(q_{x1,22}\right)_{i-1} ,$$

$$q_{x2,23} = (e)^{22} \left(a^{31}\right)_2 - \frac{2}{3}(e)^{21} \left(a^{32}\right)_2 = -\left(q_{x1,23}\right)_{i-1} ,$$

$$q_{x2,32} = (e)^{23} \left(a^{21}\right)_2 - \frac{2}{3}(e)^{21} \left(a^{23}\right)_2 = -\left(q_{x1,32}\right)_{i-1} ,$$

$$q_{x2,33} = (e)^{23} \left(a^{31}\right)_2 - \frac{2}{3}(e)^{21} \left(a^{33}\right)_2 = -\left(q_{x1,33}\right)_{i-1} ,$$

$$q_{x3,11} = \frac{4}{3}(e)^{31} \left(a^{11}\right)_3 + (e)^{32} \left(a^{12}\right)_3 + (e)^{33} \left(a^{13}\right)_3 = d_{31} + \frac{1}{3}(e)^{31} \left(a^{11}\right)_3 ,$$

$$q_{x3,13} = \frac{4}{3}(e)^{31} \left(a^{31}\right)_3 + (e)^{32} \left(a^{32}\right)_3 + (e)^{33} \left(a^{33}\right)_3 = d_{33} + \frac{1}{3}(e)^{31} \left(a^{31}\right)_3 ,$$

$$q_{x3,21} = (e)^{32} \left(a^{11}\right)_3 - \frac{2}{3}(e)^{31} \left(a^{12}\right)_3 ,$$

$$q_{x3,23} = (e)^{32} \left(a^{31}\right)_3 - \frac{2}{3}(e)^{31} \left(a^{32}\right)_3 ,$$

$$q_{x3,31} = (e)^{33} \left(a^{11}\right)_3 - \frac{2}{3}(e)^{31} \left(a^{13}\right)_3 ,$$

$$q_{x3,33} = (e)^{33} \left(a^{31}\right)_3 - \frac{2}{3}(e)^{31} \left(a^{33}\right)_3 ,$$

$$q_{x4,11} = \frac{4}{3}(e)^{41} \left(a^{11}\right)_4 + (e)^{42} \left(a^{12}\right)_4 + (e)^{43} \left(a^{13}\right)_4 = d_{41} + \frac{1}{3}(e)^{41} \left(a^{11}\right)_4$$

$$= -\left(q_{x3,11}\right)_{j-1} ,$$

$$q_{x4,13} = \frac{4}{3}(e)^{41} \left(a^{31}\right)_4 + (e)^{42} \left(a^{32}\right)_4 + (e)^{43} \left(a^{33}\right)_4 = d_{43} + \frac{1}{3}(e)^{41} \left(a^{31}\right)_4$$

$$= -\left(q_{x3,13}\right)_{j-1} ,$$

$$q_{x4,21} = (e)^{42} \left(a^{11}\right)_4 - \frac{2}{3}(e)^{41} \left(a^{12}\right)_4 = -\left(q_{x3,21}\right)_{j-1} ,$$

$$q_{x4,23} = (e)^{42} \left(a^{31}\right)_4 - \frac{2}{3}(e)^{41} \left(a^{32}\right)_4 = -\left(q_{x3,23}\right)_{j-1} ,$$

$$q_{x4,31} = (e)^{43} \left(a^{11}\right)_4 - \frac{2}{3}(e)^{41} \left(a^{13}\right)_4 = -\left(q_{x3,31}\right)_{j-1} ,$$

$$q_{x4,33} = (e)^{43} \left(a^{31}\right)_4 - \frac{2}{3}(e)^{41} \left(a^{33}\right)_4 = -\left(q_{x3,33}\right)_{j-1} ,$$

$$q_{x5,11} = \frac{4}{3}(e)^{51} \left(a^{11}\right)_5 + (e)^{52} \left(a^{12}\right)_5 + (e)^{53} \left(a^{13}\right)_5 = d_{51} + \frac{1}{3}(e)^{51} \left(a^{11}\right)_5 ,$$

$$q_{x5,12} = \frac{4}{3}(e)^{51} \left(a^{21}\right)_5 + (e)^{52} \left(a^{22}\right)_5 + (e)^{53} \left(a^{23}\right)_5 = d_{52} + \frac{1}{3}(e)^{51} \left(a^{21}\right)_5 ,$$

$$q_{x5,21} = (e)^{52} \left(a^{11}\right)_5 - \frac{2}{3}(e)^{51} \left(a^{12}\right)_5 ,$$

$$q_{x5,22} = (e)^{52} \left(a^{21}\right)_5 - \frac{2}{3}(e)^{51} \left(a^{22}\right)_5 ,$$

$$q_{x5,31} = (e)^{53} \left(a^{11}\right)_5 - \frac{2}{3}(e)^{51} \left(a^{13}\right)_5 ,$$

$$q_{x5,32} = (e)^{53} \left(a^{21}\right)_5 - \frac{2}{3}(e)^{51} \left(a^{23}\right)_5 ,$$

$$q_{x6,11} = \frac{4}{3}(e)^{61} \left(a^{11}\right)_6 + (e)^{62} \left(a^{12}\right)_6 + (e)^{63} \left(a^{13}\right)_6 = d_{61} + \frac{1}{3}(e)^{61} \left(a^{11}\right)_6$$

$$= -\left(q_{x5,11}\right)_{k-1} ,$$

$$q_{x6,12} = \frac{4}{3}(e)^{61}\left(a^{21}\right)_6 + (e)^{62}\left(a^{22}\right)_6 + (e)^{63}\left(a^{23}\right)_6 = d_{62} + \frac{1}{3}(e)^{61}\left(a^{21}\right)_6$$

$$= -\left(q_{x5,12}\right)_{k-1},$$

$$q_{x6,21} = (e)^{62}\left(a^{11}\right)_6 - \frac{2}{3}(e)^{61}\left(a^{12}\right)_6 = -\left(q_{x5,21}\right)_{k-1},$$

$$q_{x6,22} = (e)^{62}\left(a^{21}\right)_6 - \frac{2}{3}(e)^{61}\left(a^{22}\right)_6 = -\left(q_{x5,22}\right)_{k-1},$$

$$q_{x6,31} = (e)^{63}\left(a^{11}\right)_6 - \frac{2}{3}(e)^{61}\left(a^{13}\right)_6 = -\left(q_{x5,31}\right)_{k-1},$$

$$q_{x6,32} = (e)^{63}\left(a^{21}\right)_6 - \frac{2}{3}(e)^{61}\left(a^{23}\right)_6 = -\left(q_{x5,32}\right)_{k-1}.$$

## Appendix 13.3 Off-diagonal viscous diffusion terms of the *y* momentum equation

The off-diagonal viscous diffusion terms in the $y$ momentum equation

$$\sum_{m=1}^{6} \beta_m \frac{D_{l,m}^{\nu}}{\Delta L_{h,m}} \left( DI\_v_{l,m} - \frac{2}{3}(e)^{m2} DI\_u_{l,m}^{b} + DI\_vis_{lm}^{vT} \right)$$

are computed using the same procedure as those for $x$ equation replacing simply the subscript $x$ with $y$ and using the following geometry coefficients.

$$q_{y1,12} = (e)^{11}\left(a^{22}\right)_1 - \frac{2}{3}(e)^{12}\left(a^{21}\right)_1,$$

$$q_{y1,13} = (e)^{11}\left(a^{32}\right)_1 - \frac{2}{3}(e)^{12}\left(a^{31}\right)_1,$$

$$q_{y1,22} = (e)^{11}\left(a^{21}\right)_1 + \frac{4}{3}(e)^{12}\left(a^{22}\right)_1 + (e)^{13}\left(a^{23}\right)_1,$$

$$q_{y1,23} = (e)^{11}\left(a^{31}\right)_1 + \frac{4}{3}(e)^{12}\left(a^{32}\right)_1 + (e)^{13}\left(a^{33}\right)_1,$$

$$q_{y1,32} = (e)^{13}\left(a^{22}\right)_1 - \frac{2}{3}(e)^{12}\left(a^{23}\right)_1,$$

$$q_{y1,33} = (e)^{13}\left(a^{32}\right)_1 - \frac{2}{3}(e)^{12}\left(a^{33}\right)_1,$$

$$q_{y2,12} = (e)^{21}\left(a^{22}\right)_2 - \frac{2}{3}(e)^{22}\left(a^{21}\right)_2 = -\left(q_{y1,12}\right)_{i-1},$$

$$q_{y2,13} = (e)^{21}\left(a^{32}\right)_2 - \frac{2}{3}(e)^{22}\left(a^{31}\right)_2 = -\left(q_{y1,13}\right)_{i-1},$$

$$q_{y2,22} = (e)^{21}\left(a^{21}\right)_2 + \frac{4}{3}(e)^{22}\left(a^{22}\right)_2 + (e)^{23}\left(a^{23}\right)_2 = -\left(q_{y1,22}\right)_{i-1},$$

$$q_{y2,23} = (e)^{21}\left(a^{31}\right)_2 + \frac{4}{3}(e)^{22}\left(a^{32}\right)_2 + (e)^{23}\left(a^{33}\right)_2 = -\left(q_{y1,23}\right)_{i-1},$$

$$q_{y2,32} = (e)^{23}\left(a^{22}\right)_2 - \frac{2}{3}(e)^{22}\left(a^{23}\right)_2 = -\left(q_{y1,32}\right)_{i-1},$$

$$q_{y2,33} = (e)^{23}\left(a^{32}\right)_2 - \frac{2}{3}(e)^{22}\left(a^{33}\right)_2 = -\left(q_{y1,33}\right)_{i-1},$$

$$q_{y3,11} = (e)^{31}\left(a^{12}\right)_3 - \frac{2}{3}(e)^{32}\left(a^{11}\right)_3,$$

$$q_{y3,13} = (e)^{31}\left(a^{32}\right)_3 - \frac{2}{3}(e)^{32}\left(a^{31}\right)_3,$$

$$q_{y3,21} = (e)^{31}\left(a^{11}\right)_3 + \frac{4}{3}(e)^{32}\left(a^{12}\right)_3 + (e)^{33}\left(a^{13}\right)_3,$$

$$q_{y3,23} = (e)^{31}\left(a^{31}\right)_3 + \frac{4}{3}(e)^{32}\left(a^{32}\right)_3 + (e)^{33}\left(a^{33}\right)_3,$$

$$q_{y3,31} = (e)^{33}\left(a^{12}\right)_3 - \frac{2}{3}(e)^{32}\left(a^{13}\right)_3,$$

$$q_{y3,33} = (e)^{33}\left(a^{32}\right)_3 - \frac{2}{3}(e)^{32}\left(a^{33}\right)_3,$$

$$q_{y4,11} = (e)^{41}\left(a^{12}\right)_4 - \frac{2}{3}(e)^{42}\left(a^{11}\right)_4 = -\left(q_{y3,11}\right)_{j-1},$$

$$q_{y4,13} = (e)^{41}\left(a^{32}\right)_4 - \frac{2}{3}(e)^{42}\left(a^{31}\right)_4 = -\left(q_{y3,13}\right)_{j-1},$$

$$q_{y4,21} = (e)^{41}\left(a^{11}\right)_4 + \frac{4}{3}(e)^{42}\left(a^{12}\right)_4 + (e)^{43}\left(a^{13}\right)_4 = -\left(q_{y3,21}\right)_{j-1},$$

$$q_{y4,23} = (e)^{41}\left(a^{31}\right)_4 + \frac{4}{3}(e)^{42}\left(a^{32}\right)_4 + (e)^{43}\left(a^{33}\right)_4 = -\left(q_{y3,23}\right)_{j-1},$$

$$q_{y4,31} = (e)^{43}\left(a^{12}\right)_4 - \frac{2}{3}(e)^{42}\left(a^{13}\right)_4 = -\left(q_{y3,31}\right)_{j-1},$$

$$q_{y4,33} = (e)^{43}\left(a^{32}\right)_4 - \frac{2}{3}(e)^{42}\left(a^{33}\right)_4 = -\left(q_{y3,33}\right)_{j-1},$$

$$q_{y5,11} = (e)^{51}\left(a^{12}\right)_5 - \frac{2}{3}(e)^{52}\left(a^{11}\right)_5,$$

$$q_{y5,12} = (e)^{51}\left(a^{22}\right)_5 - \frac{2}{3}(e)^{52}\left(a^{21}\right)_5,$$

$$q_{y5,21} = (e)^{51}\left(a^{11}\right)_5 + \frac{4}{3}(e)^{52}\left(a^{12}\right)_5 + (e)^{53}\left(a^{13}\right)_5,$$

$$q_{y5,22} = (e)^{51}\left(a^{21}\right)_5 + \frac{4}{3}(e)^{52}\left(a^{22}\right)_5 + (e)^{53}\left(a^{23}\right)_5,$$

$$q_{y5,31} = (e)^{53}\left(a^{12}\right)_5 - \frac{2}{3}(e)^{52}\left(a^{13}\right)_5,$$

$$q_{y5,32} = (e)^{53}\left(a^{22}\right)_5 - \frac{2}{3}(e)^{52}\left(a^{23}\right)_5,$$

$$q_{y6,11} = (e)^{61}\left(a^{12}\right)_6 - \frac{2}{3}(e)^{62}\left(a^{11}\right)_6 = -\left(q_{y5,11}\right)_{k-1},$$

$$q_{y6,12} = (e)^{61}\left(a^{22}\right)_6 - \frac{2}{3}(e)^{62}\left(a^{21}\right)_6 = -\left(q_{y5,12}\right)_{k-1},$$

$$q_{y6,21} = (e)^{61}\left(a^{11}\right)_6 + \frac{4}{3}(e)^{62}\left(a^{12}\right)_6 + (e)^{63}\left(a^{13}\right)_6 = -\left(q_{y5,21}\right)_{k-1},$$

$$q_{y6,22} = (e)^{61}\left(a^{21}\right)_6 + \frac{4}{3}(e)^{62}\left(a^{22}\right)_6 + (e)^{63}\left(a^{23}\right)_6 = -\left(q_{y5,22}\right)_{k-1},$$

$$q_{y6,31} = (e)^{63}\left(a^{12}\right)_6 - \frac{2}{3}(e)^{62}\left(a^{13}\right)_6 = -\left(q_{y5,31}\right)_{k-1},$$

$$q_{y6,32} = (e)^{63}\left(a^{22}\right)_6 - \frac{2}{3}(e)^{62}\left(a^{23}\right)_6 = -\left(q_{y5,32}\right)_{k-1}.$$

## Appendix 13.4 Off-diagonal viscous diffusion terms of the *z* momentum equation

The off-diagonal viscous diffusion terms in the $z$ momentum equation

$$\sum_{m=1}^{6} \beta_m \frac{D^{\nu}_{l,m}}{\Delta L_{h,m}} \left( DI\_w_{l,m} - \frac{2}{3} (e)^{m3} DI\_u^{b}_{l,m} + DI\_vis^{wT}_{lm} \right)$$

are computed using the same procedure as those for $x$ equation replacing simply the subscript $x$ with $z$ and using the following geometry coefficients.

$$q_{z1,12} = (e)^{11} \left(a^{23}\right)_1 - \frac{2}{3}(e)^{13} \left(a^{21}\right)_1 ,$$

$$q_{z1,13} = (e)^{11} \left(a^{33}\right)_1 - \frac{2}{3}(e)^{13} \left(a^{31}\right)_1 ,$$

$$q_{z1,22} = (e)^{12} \left(a^{23}\right)_1 - \frac{2}{3}(e)^{13} \left(a^{22}\right)_1 ,$$

$$q_{z1,23} = (e)^{12} \left(a^{33}\right)_1 - \frac{2}{3}(e)^{13} \left(a^{32}\right)_1 ,$$

$$q_{z1,32} = (e)^{11} \left(a^{21}\right)_1 + (e)^{12} \left(a^{22}\right)_1 + \frac{4}{3}(e)^{13} \left(a^{23}\right)_1 ,$$

$$q_{z1,33} = (e)^{11} \left(a^{31}\right)_1 + (e)^{12} \left(a^{32}\right)_1 + \frac{4}{3}(e)^{13} \left(a^{33}\right)_1 ,$$

$$q_{z2,12} = (e)^{21} \left(a^{23}\right)_2 - \frac{2}{3}(e)^{23} \left(a^{21}\right)_2 = -\left(q_{z1,12}\right)_{i-1} ,$$

$$q_{z2,13} = (e)^{21} \left(a^{33}\right)_2 - \frac{2}{3}(e)^{23} \left(a^{31}\right)_2 = -\left(q_{z1,13}\right)_{i-1} ,$$

$$q_{z2,22} = (e)^{22} \left(a^{23}\right)_2 - \frac{2}{3}(e)^{23} \left(a^{22}\right)_2 = -\left(q_{z1,22}\right)_{i-1} ,$$

$$q_{z2,23} = (e)^{22} \left(a^{33}\right)_2 - \frac{2}{3}(e)^{23} \left(a^{32}\right)_2 = -\left(q_{z1,23}\right)_{i-1} ,$$

$$q_{z2,32} = (e)^{21} \left(a^{21}\right)_2 + (e)^{22} \left(a^{22}\right)_2 + \frac{4}{3}(e)^{23} \left(a^{23}\right)_2 = -\left(q_{z1,32}\right)_{i-1} ,$$

$$q_{z2,33} = (e)^{21} \left(a^{31}\right)_2 + (e)^{22} \left(a^{32}\right)_2 + \frac{4}{3}(e)^{23} \left(a^{33}\right)_2 = -\left(q_{z1,33}\right)_{i-1} ,$$

$$q_{z3,11} = (e)^{31} \left(a^{13}\right)_3 - \frac{2}{3}(e)^{33} \left(a^{11}\right)_3 ,$$

$$q_{z3,13} = (e)^{31} \left(a^{33}\right)_3 - \frac{2}{3}(e)^{33} \left(a^{31}\right)_3 ,$$

$$q_{z3,21} = (e)^{32}(a^{13})_3 - \frac{2}{3}(e)^{33}(a^{12})_3,$$

$$q_{z3,23} = (e)^{32}(a^{33})_3 - \frac{2}{3}(e)^{33}(a^{32})_3,$$

$$q_{z3,31} = (e)^{31}(a^{11})_3 + (e)^{32}(a^{12})_3 + \frac{4}{3}(e)^{33}(a^{13})_3,$$

$$q_{z3,33} = (e)^{31}(a^{31})_3 + (e)^{32}(a^{32})_3 + \frac{4}{3}(e)^{33}(a^{33})_3,$$

$$q_{z4,11} = (e)^{41}(a^{13})_4 - \frac{2}{3}(e)^{43}(a^{11})_4 = -(q_{z3,11})_{j-1},$$

$$q_{z4,13} = (e)^{41}(a^{33})_4 - \frac{2}{3}(e)^{43}(a^{31})_4 = -(q_{z3,13})_{j-1},$$

$$q_{z4,21} = (e)^{42}(a^{13})_4 - \frac{2}{3}(e)^{43}(a^{12})_4 = -(q_{z3,21})_{j-1},$$

$$q_{z4,23} = (e)^{42}(a^{33})_4 - \frac{2}{3}(e)^{43}(a^{32})_4 = -(q_{z3,23})_{j-1},$$

$$q_{z4,31} = (e)^{41}(a^{11})_4 + (e)^{42}(a^{12})_4 + \frac{4}{3}(e)^{43}(a^{13})_4 = -(q_{z3,31})_{j-1},$$

$$q_{z4,33} = (e)^{41}(a^{31})_4 + (e)^{42}(a^{32})_4 + \frac{4}{3}(e)^{43}(a^{33})_4 = -(q_{z3,33})_{j-1},$$

$$q_{z5,11} = (e)^{51}(a^{13})_5 - \frac{2}{3}(e)^{53}(a^{11})_5,$$

$$q_{z5,12} = (e)^{51}(a^{23})_5 - \frac{2}{3}(e)^{53}(a^{21})_5,$$

$$q_{z5,21} = (e)^{52}(a^{13})_5 - \frac{2}{3}(e)^{53}(a^{12})_5,$$

$$q_{z5,22} = (e)^{52}(a^{23})_5 - \frac{2}{3}(e)^{53}(a^{22})_5,$$

$$q_{z5,31} = (e)^{51}(a^{11})_5 + (e)^{52}(a^{12})_5 + \frac{4}{3}(e)^{53}(a^{13})_5,$$

$$q_{z5,32} = (e)^{51}(a^{21})_5 + (e)^{52}(a^{22})_5 + \frac{4}{3}(e)^{53}(a^{23})_5,$$

$$q_{z6,11} = (e)^{61}\left(a^{13}\right)_6 - \frac{2}{3}(e)^{63}\left(a^{11}\right)_6 = -\left(q_{z5,11}\right)_{k-1},$$

$$q_{z6,12} = (e)^{61}\left(a^{23}\right)_6 - \frac{2}{3}(e)^{63}\left(a^{21}\right)_6 = -\left(q_{z5,12}\right)_{k-1},$$

$$q_{z6,21} = (e)^{62}\left(a^{13}\right)_6 - \frac{2}{3}(e)^{63}\left(a^{12}\right)_6 = -\left(q_{z5,21}\right)_{k-1},$$

$$q_{z6,22} = (e)^{62}\left(a^{23}\right)_6 - \frac{2}{3}(e)^{63}\left(a^{22}\right)_6 = -\left(q_{z5,22}\right)_{k-1},$$

$$q_{z6,31} = (e)^{61}\left(a^{11}\right)_6 + (e)^{62}\left(a^{12}\right)_6 + \frac{4}{3}(e)^{63}\left(a^{13}\right)_6 = -\left(q_{z5,31}\right)_{k-1},$$

$$q_{z6,32} = (e)^{61}\left(a^{21}\right)_6 + (e)^{62}\left(a^{22}\right)_6 + \frac{4}{3}(e)^{63}\left(a^{23}\right)_6 = -\left(q_{z5,32}\right)_{k-1}.$$

## References


Antal, S.P., et al.: Development of a next generation computer code for the prediction of multi-component multiphase flows. In: Int. Meeting on Trends in Numerical and Physical Modeling for Industrial Multiphase Flow, Cargese, France (2000)

Brackbill, J.U., Kothe, D.B., Zeinach, C.: A continuum method for modelling surface tension. Journal of Computational Physics 100, 335 (1992)

Gregor, C., Petelin, S., Tiselj, I.: Upgrade of the VOF method for the simulation of the dispersed flow. In: Proc. of ASME 2000 Fluids Engineering Division Summer Meeting, Boston, Massachusetts, June 11-15 (2000)

Harlow, F.H., Amsden, A.A.: Numerical calculation of multiphase flow. Journal of Computational Physics 17, 19–52 (1975)

Hirt, C.W.: Volume-fraction techniques: powerful tools for wind engineering. J. Wind Engineering and Industrial Aerodynamics 46-47, 327 (1993)

Hou, S., Zou, Q., Chen, S., Doolen, G., Cogley, A.C.: Simulation of cavity flow by the lattice Boltzmann method. J. Comput. Phys. 118, 329 (1995)

Jamet, D., Lebaigue, O., Courtis, N., Delhaye: The second gradient method for the direct numerical simulation of liquid-vapor flows with phase change. Journal of Comp. Physics 169, 624–651 (2001)

Kolev, N.I.: IVA4: Modeling of mass conservation in multi-phase multi-component flows in heterogeneous porous media. Kerntechnik 59(4-5), 226–237 (1994)

Kolev, N.I.: The code IVA4: Modelling of momentum conservation in multi-phase multi-component flows in heterogeneous porous media. Kerntechnik 59(6), 249–258 (1994)

Kolev, N.I.: The code IVA4: Second law of thermodynamics for multi phase flows in heterogeneous porous media. Kerntechnik 60(1), 1–39 (1995)

Kolev, N.I.: Comments on the entropy concept. Kerntechnik 62(1), 67–70 (1997)

Kolev, N.I.: On the variety of notation of the energy conservation principle for single phase flow. Kerntechnik 63(3), 145–156 (1998)

Kolev, N.I.: Conservation equations for multi-phase multi-component multi-velocity fields in general curvilinear coordinate systems, Keynote lecture. In: Proceedings of ASME FEDSM 2001, ASME 2001 Fluids Engineering Division Summer Meeting, New Orleans, Louisiana, May 29-June 1 (2001)

Kothe, D.B., Rider, W.J., Mosso, S.J., Brock, J.S., Hochstein, J.I.: Volume tracking of Interfaces having surface tension in two and three dimensions. In: AIAA 96-0859 (1996)

Kumbaro, A., Toumi, I., Seignole, V.: Numerical modeling of two-phase flows using advanced two fluid system. In: Proc. of ICONE10, 10th Int. Conf. On Nuclear Engineering, Arlington, VA, USA, April 14-18 (2002)

Lahey Jr, R.T., Drew, D.: The analysis of two-phase flow and heat transfer using a multidimensional, four field, two-fluid model. In: Ninth Int. Top. Meeting on Nuclear Reactor Thermal-Hydraulics (NURETH-9), San Francisco, California, October 3-8 (1999)

Miettinen, J., Schmidt, H.: CFD analyses for water-air flow with the Euler-Euler two-phase model in the FLUENT4 CFD code. In: Proc. of ICONE10, 10th Int. Conf. On Nuclear Engineering, Arlington, VA, USA, April 14-18 (2002)

Nakamura, T., Tanaka, R., Yabe, T., Takizawa, K.: Exactly conservative semi-Lagrangian scheme for multi-dimensional hyperbolic equations with directional splitting technique. J. Comput. Phys. 147, 171 (2001)

Nourgaliev, R.R., Dinh, T.N., Sehgal, B.R.: On lattice Boltzmann modelling of phase transition in isothermal non-ideal fluid. Nuclear Engineering and Design 211, 153–171 (2002)

Osher, S., Fredkiw, R.: Level set methods and dynamic implicit surfaces. Springer-Verlag New York, Inc., Secaucas (2003)

Rider, W.J., Kothe, D.B.: Reconstructing volume tracking. Journal of Computational Physics 141, 112 (1998)

Staedke, H., Franchello, G., Worth, B.: Towards a high resolution numerical simulation of transient two-phase flow. In: Third International Conference on Multi-Phase, ICMF 1998, June 8-12 (1998)

Sussman, M., Smereka, P., Oslier, S.: A level set approach for computing solutions to incompressible two-phase flow. Journal of Computational Physics 114, 146 (1994)

Swthian, J.A.: Level set methods. Cambridge University Press, Cambridge (1996)

Takewaki, H., Nishiguchi, A., Yabe, T.: The Cubic-Interpolated Pseudo Particle (CIP) Method for Solving Hyperbolic-Type Equations. J. Comput. Phys. 61, 261 (1985)

Takewaki, H., Yabe, Y.: Cubic-Interpolated Pseudo Particle (CIP) Method-Application to Nonlinear Multi-Dimensional Problems. J. Comput. Phys. 70, 355 (1987)

Tomiyama, A., et al.: (N+2)-Field modelling of dispersed multiphase flow. In: Proc. of ASME 2000 Fluids Engineering Division Summer Meeting, Boston, Massachusetts, June 11-15 (2000)

Toumi, I., et al.: Development of a multi-dimensional upwind solver for two-phase water/steam flows. In: Proc. of ICONE 8, 8th Int. Conf. On Nuclear Engineering, Baltimore, MD USA, April 2-6 (2000)

Tryggavson, G., et al.: A front tracking method for the computations of multiphase flows. Journal of Comp. Physics 169, 708–759 (2001)

Verschueren, M.: A difuse-interface model for structure development in flow, PhD Thesis, Technische Universitteit Eindhoven (1999)

van Wijngaarden, L.: Hydrodynamic interaction between gas bubbles in liquid. J. Fluid Mech. 77, 27–44 (1976)

Yabe, T., Takei, E.: A New Higher-Order Godunov Method for General Hyperbolic Equations. J. Phys. Soc. Japan 57, 2598 (1988)

Xiao, F., Yabe, T.: Completely conservative and oscillation-less semi-Lagrangian schemes for advection transportation. J. Comput. Phys. 170, 498 (2001)

Xiao, F., Yabe, T., Peng, X., Kobayashi, H.: Conservation and oscillation-less transport schemes based an rational functions. J. Geophys. Res. 107, 4609 (2002)

Xiao, F.: Profile-modifiable conservative transport schemes and a simple multi integrated moment formulation for hydrodynamics. In: Amfield, S., Morgan, P., Srinivas, K. (eds.) Computational Fluid Dynamics, p. 106. Springer, Heidelberg (2003)

Xiao, F., Ikebata, A.: An efficient method for capturing free boundary in multi-fluid simulations. Int. J. Numer. Method in Fluid 42, 187–210 (2003)

Yabe, T., Wang, P.Y.: Unified Numerical Procedure for Compressible and Incompressible Fluid. J. Phys. Soc. Japan 60, 2105–2108 (1991)

Yabe, T., Aoki, A.: A Universal Solver for Hyperbolic-Equations by Cubic Polynomial Interpolation. Comput. Phys. Commun. 66, 219 (1991)

Yabe, T., Ishikawa, T., Wang, P.Y., Aoki, T., Kadota, Y., Ikeda, F.: A universal solver for hyperbolic-equations by cubic-polynomial interpolation. II. 2-dimensional and 3-dimensional solvers. Comput. Phys. Commun. 66, 233 (1991)

Yabe, T., Xiao, F., Utsumi, T.: Constrained Interpolation Profile Method for Multiphase Analysis. J. Comput. Phys. 169, 556–593 (2001)

Yabe, T., Tanaka, R., Nakamura, T., Xiao, F.: Exactly conservative semi-Lagrangian scheme (CIP-CSL) in one dimension. Mon. Wea. Rev. 129, 332 (2001)

Yabe, T., Xiao, F., Utsumi, T.: The constrained interpolation profile method for multiphase analysis. J. Comput. Phys. 169, 556 (2001)