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Part 1:

Theoretical Basis: Conservation and State Equations, Numerics.

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Abstract

The IVA3 computer code is developed for numerical simulation of flows consisting of air, steam, water, microscopic solid particles which can be carried only by water, and "liquid metal" – immiscible with water. The "liquid metal" is considered to be either in liquid state, in equilibrium liquid – solid state, or in solid state in form of macroscopic solid particles. The flow is transient and three dimensional. The geometry confining the flow is an arbitrary technical geometry, characterized by obstacles etc. In this geometry, there may be relatively large volumes not occupied by technical structures (pool flow) and/or volumes occupied partially by technical structures, considerably influencing the flow (flow in confined geometry). Within the definition space the flow interacts with (a) walls, and/or (b) with a nuclear reactor core, and/or (c) with boundary conditions applied at the boundary of the definition space. The geometrical obstacles may change with time modelling closing or opening flow cross sections as prescribed functions of time.

This work contains description of the physical and mathematical basis on which the IVA3 computer code relies.

After describing the state of the art of the 3D modeling for transient multiphase flows, the model assumptions and the modeling technique used in IVA3 are described. Starting with the principles of conservation of mass, momentum, and energy, the non averaged conservation equations are derived for each of the velocity fields which consist of different isothermal components. Thereafter averaging is applied and the working form of the system of 21 partial differential equations is derived. Special attention is paid to the strict consistence of the modeling technique used in IVA3 with the second principle of thermodynamics. The entropy concept used is derived starting with the unaveraged conservation equations and subsequent averaging. The source terms of the entropy production are carefully defined and the final form of the averaged entropy equation is given ready for direct practical applications. The idea of strong analytical thermodynamic coupling between pressure field and changes of the other thermodynamic properties, which is used for the first time in 3D multi fluid modeling, is presented in detail.

After obtaining the working form of the conservation equations, the discretization procedure and the reduction to algebraic problems is presented. The mathematical solution method together with some information about the architecture of IVA3 including the local momentum decoupling and accuracy control is presented too.

Ein Drei–Feld Modell der transienten 3D Multiphasen Drei–Komponenten Strömung für das Rechenprogramm IVA3

Teil 1: Theoretische Basis: Erhaltungs– und Zustandsgleichungen. Numerik

Kurzfassung

Das Computerprogramm IVA3 wurde für die numerische Simulation von Strömungen bestehend aus Luft, Wasserdampf, Wasser, mikroskopischen festen Partikeln, die vom Wasser getragen werden können, und "Metallen", die nicht im Wasser aufgelöst werden können, entwickelt. Die "Metalle" können entweder flüssig, oder im

Zweiphasengleichgewichtszustand, oder fest in der Form von makroskopischen Partikeln sein. Die Strömung ist transient und dreidimensional. Die Geometrie, in der die Strömung stattfindet, ist eine beliebige technische Geometrie, die durch Strömungshindernisse etc. charakterisiert wird. In dieser Geometrie können relativ große Volumina, die frei von technischen Strukturen sind (Poolströmungen) und/oder Volumina, die teilweise von technischen Strukturen ausgefüllt sind (Kanalströmungen), vorhanden sein. Innerhalb des Defintionsbereiches erfährt die Strömung Wechselwirkung mit (a) Wänden, und/oder (b) mit der Spaltzone eines Kernreaktors, und/oder (c) mit Randbedingungen, die an den Rändern des Integrationsbereiches wirken. Die geometrischen Strömungshindernisse können veränderlich sein und Schließen oder Öffnen von Strömungsquerschnitten als vorgeschriebene Zeitfunktionen modellieren.

Diese Arbeit beinhaltet eine Beschreibug der physikalischen und mathematischen Grundlagen, auf denen das Computerprogramm IVA3 basiert. Nach Beschreibung des derzeitigen Standes der Modellierung der dreidimensionalen transienten Mehrphasenströmungen werden die Modellannahmen und die Herangehensweise in IVA3 dargestellt. Beginnend mit den Prinzipien der Erhaltung von Masse, Impuls und Energie werden die nicht gemittelten Erhaltungsgleichungen für jedes Geschwindigkeitsfeld bestehend aus mehrkomponentigen isothermen Mischungen hergeleitet. Nach einer Mittelung wird die Arbeitsform des Systems aus 21 partiellen Differentialgleichungen hergeleitet. Spezielle Aufmerksamkeit wird der strikten Übereinstimmung mit dem zweiten Hauptsatz der Thermodynamik geschenkt. Das in IVA3 verwendete Entropiekonzept wird hergeleitet beginnend mit nichtgemittelten Erhaltungsgleichungen und nachfolgender Mittelung. Die Quellterme der Entropieproduktion werden sorgfältig definiert and eine endgültige Form der gemittelten Entropiegleichung, welche fertig für direkte praktische Anwendung ist, wird hergeleitet. Die Idee der strengen analytischen thermodynamischen Koppelung zwischen dem Druckfeld und den Änderungen der anderen thermodynamischen Größen, welche hier zum ersten Mal in der 3D Modellierung von Mehrphasenströmungen angewendet wurde, wird im Detail dargestellt.

Nach der Erhaltung der Arbeitsform der Erhaltungsgleichungen wird die Diskretisierungsprozedur und die Reduktion der partiellen Differentialgleichungen auf ein algebraisches Problem beschrieben. Das mathematische Lösungsverfahren sowie einige Informationen über die Architektur von IVA3, die lokale Kräfteabkoppelung und die Genauigkeitskontrolle während der Integration werden diskutiert.

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1. INTRODUCTION

Several processes in environment and industrial equipment are associated with transient three–dimensional flows consisting of micro–, and macroscopic particles, liquid and gas mixtures. The increasing importance of the environment protection topics and the optimization of 3D technological processes needs sophisticated methods for the mathematical description of multiphase flows. Computer simulation of physical problems is now widely accepted as the third method of investigation in science – besides theory and experiment. In computer aided analysis of accidental processes in power plants with water cooled nuclear reactors, the safety engineer has frequently to do with flows consisting of mixtures of air, water, water steam, microscopic solid particles and liquid metals. The complexity of such multiphase flows is mainly due to the big variety of combinations of the three aggregate states and chemical components, and even for simple mixtures consisting of one, two or three chemical components, it is due to the variety of flow patterns. In addition the situation is further complicated by the complexity of the geometry of the technical equipment confining the flow. So the interesting dilemma arises: on one hand the desire (a) to establish basic conservation equations relying on rational mechanics, (b) to develop the needed closure relations for multiphase flows, (c) to prove theorems for uniqueness and stability of the numerical solutions, and (d) to create a versatile computer code architecture relying on this results; on the other, the daily need to analyze such kind of flow for practical design and licensing before the previous task is completely solved. As the experience with the development of computer models for one– and twophase flows shows, there is a straightforward feed back between the above discussed steps. Moreover, without interaction between the four steps non of them can successfully be finished. That is why we decided to start the development of the IVA computer codes, modeling 3D flows consisting of air, water, water steam, microscopic solid particles and molten metal, it being clear that only the interaction of the above mentioned steps will bring us ahead in our understanding of this complicated physical phenomenon.

The computer code IVA3 can be applied for modeling flows in many branches of science and industrial equipment design as e.g. nuclear technology, meteorology, lava–water interaction, chemical equipments etc.

The purpose of this paper is to present a brief summary of this development. Full documentation of the code is under preparation and will be published in the near future.

1.1 SUBJECT OF IVA3

The IVA3 computer code is developed for numerical simulation of flows consisting of air, steam, water, microscopic solid particles which are only carried by water, and "liquid metal" which immiscible with water. The "liquid metal" is considered to be either in liquid state, or in equilibrium liquid – solid state, or in solid state in form of macroscopic solid particles. The flow is transient and three dimensional. The geometry confining the flow is an arbitrary technical geometry, characterized by obstacles etc. In this geometry, there may be relatively large volumes not occupied by technical structures (pool flow) and/or volumes occupied partially by technical structures which considerably influence the flow (flow in confined geometry). Within the definition space, the flow interacts with (a) walls, and/or (b) with a nuclear reactor core, and/or (c) with boundary conditions applied at the boundaries of the definition space. The geometrical obstacles may change with time modelling closing or opening flow cross sections as prescribed functions of time.

1.2 STATE OF THE ART

Particular interest in modelling of multiphase flows arises with the necessity to model numerically accidental processes in high energy converting components of power plants. One started 30 years ago with three–point models, arriving today at models using several thousand points in the discretization network. If we talk today about *mathematical models of multiphase flows*, we think of *computer codes* of sizes of 1 000 FORTRAN statements for one dimensional flow and up to 50 000 statements for three–dimensional flow or flow in quasi one–dimensional networks. Thus, as *model elements* we count

1. *Systems of partial differential equations* (PDEs) reflecting the global *conservation principles*, transformed in proper form for numerical integration, the so called *working form* of the system;

2. Approximations for the *thermodynamic properties* of the chemical components;

3. *Initial and boundary conditions*;

4. Mathematical *methods for integration of the system of PDEs*, and a strategy of coupling them with the constitutive equations;

5. Systems of equations reflecting the micro conservation laws for mass, momentum and energy conservation on geometrical surfaces dividing the phases from each other or the flow from structures, frequently called *constitutive equations.*

In the following we use the term "multiphase flow model" having in mind its five above mentioned components.

The only universal way known to us at present time to transfer the empirical experience gained in small– and semi–scale experiments to design full scale industrial machines is the use of mathematical models of the controling physical phenomena.

Thus, are there models reported in the literature with the characteristics summarized in the the previous Chapter ?

The development of *one–phase models* by Amsden and Harlow [1] (1964), Hirt and Harlow [2] (1967), Harlow and Amsden [3] (1968), Hirt [4] (1968), Harlow and Amsden [5] (1971), Kobayashi and Namathame [6] (1975), Takeuchi [7] (1979 – MULTIFLEX), Amsden and Harlow [8] (1980 – SMAC), Chen et al. [9] (1980 – BODYFIT – 1FE), Hall [10] (1982 – DUVAL), Gay and Gloski [11] (1983 – GFLOW), Domanus et al., [12] (1990 – COMMIX–1C), Sakai [13] (1990 – COMMIX–2(V)) among many others has been a prerequisite for the development of two–phase models.

Equilibrium models of one–component flow were reported by Hall and Porshing [14] (1981 – DUVAL, non–homogeneous), Van der Vorst and Singhal [15] [1981 – SWIRL, non–homogeneous, (r,θ,z)], Bottoni [16] (1984 – COMMIX – SM) etc. Carver and Calcudean [17] developed in 1986 the steady state FAITH computer code using two velocity fields for modeling of incompressible two–component flow in a toroidal coordinate system (3D).

On the basis of *drift–flux five–equation models*, the computer program SOLA–DF was developed in 1979 by Hirt et al. [18]. The steam was assumed to be saturated. Moessinger [19] (DRIX–2D) introduces "*turbulent viscosity*" in the code SOLA–DF.

Six– and more–equation models have been used in practical application since 1974, for example Amsden and Harlow [20] (KACHINA). Each of the two velocity fields used by these authors was assumed to consist of two components: gas and liquid. Thermal nonequilibrium was assumed for the two velocity fields. This simulation technique was improved further by Rivard and Torrey [21] (K–FIX 1976). In each velocity field only one component was considered, but the source terms were taken into account implicitly in the numerical solution. In both codes separated momentum equations were used. The next step was made by Liles et al. for TRAC–P1 [22] (1978), TRAC–PD2 [23] (1981) and by Kelly et al. [24] for (THERMIT–2 1981). The three models are coupled with models of nuclear reactor internals. The THERMIT–2 model takes into account the turbulent twophase transport, which is not considered in the TRAC codes. All of the above mentioned models describe one–component flows.

The need for extension of the 3D – flow description which uses two velocity fields to more sophisticated models, using three velocity fields for modeling of one component flows was recognized in the earlier 80–ies. Kelly and Kohrt [25] (1983) succeeded in developing the first one–component, 3D, three velocity field model for the COBRA–TF code, in which the droplets and the continuous liquid are supposed to be in thermal equilibrium. This family of codes was extended further by Thurgood et al. [26] (1983) with COBRA–TF/TRAC. In COBRA–NC [27] (1984), a noncondensing gas component and turbulent diffusion were taken into account.

A further parallel activity has been the PHOENICS code development by Spalding et al. [28] (1982). The PHOENICS code employs *two velocity fields with four chemical components in each field*, respectively.

A *fourth velocity field* was introduced by Williams and Liles [29] (1984) in a one–component model of a vapour field, a continuous liquid field, and two dispersed droplet fields. A successful one–dimensional comparison was made with an experiment of Lehigh University for post–critical heat transfer. Relying on the TRAC code development, Dearing (Oct. 1985) [30] reported the conservation equations for a two–dimensional four–field model of gas mixture of steam and hydrogen, liquid water, and solid and molten nuclear reactor core material.

The author developed a *three–field model of a two–component nonequilibrium flow* [31] (1977). A further solid phase was introduced to extend equilibrium and nonequilibrium models from two to *three components using two velocity fields* [32] (1986).

In the soviet literature, Nigmatulin & Ivandeev [33], Ivandeev & Nigmatulin [34] (1977) used three velocity fields for describing steady state critical one–component two–phase flow, assuming non compressible liquid and considering the steam as a perfect gas.

There are only few attempts to model transient multi–dimensional three–phase flows known to the author. They will be shortly discussed next.

Bankoff and Hadid [35] (1984) used the capabilities of the PHOENICS computer code [28] (1981) to model twophase flow by means of two velocity fields. They modelled with one velocity field the solid particles and with the other the equilibrium mixture of steam and liquid, assuming it to be homogeneous. A 2D geometry was used.

Similarly, Abolfadl and Theofanous [36] (1987) used the two velocity field code K–FIX [21] (1977) dropping the assumption of thermodynamic equilibrium of the vapor –

liquid system.

The lumping of vapor and liquid into one velocity field is appropriate only for fast running processes driven by considerable pressure differences. For processes with relatively slow pressure changes, the pressure difference driven separation of the "vapor – liquid – solid particles" mixture is important and cannot be neglected.

The author developed the computer code IVA2, describing three–phase flows in porous structures with arbitrary internals e.g. a nuclear reactor core by means of three velocity fields [37–42] (1985–86). The first velocity field consists of steam and a noncondensible gas, the second of continuous liquid and solid particles, and the third of discrete liquid and solid particles. IVA2 employs a diffusion form of the mixture momentum equations for each direction. The differences between the center of mass velocity of the mixture and the field velocities are computed using empirical correlations obtained from steady state experiments. The three velocity fields are in thermodynamic nonequilibrium in general. The constitutive packet describes pool flow as well as flow in confined geometry.

In 1988, Amarasooriya and Theofanous [44] extended the K–FIX solution scheme to 2D two–component three velocity field flow. The first field is vapor, the second water, and the third solid particles. In 1989, Medhekar et al. [45] extended this code further including microscopic inert particles homogeneously mixed with the liquid field as already done in IVA2. In addition, a constitutive relationship describing the triggering mechanism was introduced in order to describe the production rate of microscopic particles from the macroscopic solid particle field.

In the same year Thyagaraja and Fletcher [46] published a model describing 2D flow consisting of solid particles, liquid, and steam by means of three velocity fields. The authors confine themselves to noncompressible flow, letting the densities constant. Nevertheless they published a successful comparison with a small scale premixing experiment with a pressure change of 2 bar and applied their code to large scale mixing calculations [47]. Recently, Fletcher in his review paper [48] (1989) envisaged the development of computer codes which should relax the above mentioned restrictions.

Bohl et al. [49] (1988), developed an advanced 2D fluid dynamics model for pool flow consisting of three velocity fields and three chemical components, where the first one is gas, the second can be either liquid or gas and the third can be either in solid, in liquid, or in gaseous state.

Conclusion: up to now there is no computer code solving the task discussed in Chapter 2 in variable 3D geometry.

1.3 MODELING TECHNIQUE AND MODEL ASSUMPTIONS

IVA3 models a transient (τ – without index), three–dimensional (r,θ,z) flow passing through a porous body. The volume porosity γ_v in the immediate neighborhood of the point (r,θ,z) is defined as the ratio of the flow volume to the total volume of the computational cell i.e. $1 - \gamma_v$ part of the total cell volume is occupied by structure. We define flow in cells with $\gamma_v < 1$ as flow in confined geometry and flow in cells with $\gamma_v=1$ as pool flow. Surface permeability (γ_n, $n = r, \theta, z$) is similarly defined as the ratio of the surface area in the n direction available to the flow to the total surface area in the same direction. Note the difference between surface permeability defined here and the permeability coefficients usually used to define the resistance of the porous structure in the mechanics of flows in porous body. Surface permeabilities within the computational region remain unchanged per definition unless a special condition is imposed defining particular surface permeabilities as prescribed functions of time.

To model the physical picture described in Chapter 2 needs several decisions to formalize it, i.e. to divide it into several subproblems. We start with the so–called velocity fields. The velocity field "l" in IVA3 is an abstract, α_l – part of the total flow volume in the computational cell having its own temperature T_l and velocity V_l. After analyzing the possible flow topologies and flow patterns we define in IVA3 three such velocity fields, $l = 1, l_{max}$, where $l_{max} = 3$. The fields interact with each other (ml, $m \neq l$) and with structures through their surfaces.

Now we describe the correspondence between the abstract velocity fields "l" and the substances participating in the flow.

The gas is associated with the first velocity field ($l = 1 \equiv$ gas). In each computational cell this field can be either continuous, or discrete (bubbles). The gas consists of air and steam denoted with "n1" and "M1", respectively. The air is called inert component and is not allowed to change the state of aggregate, while the steam, called non inert component, may condense. The gas phase obeys the Dalton law. The noncondensing gas component "n1" is assumed to be a perfect gas.

The water is associated with the second and, under certain circumstances, with the third velocity field. In each computational cell the water in the second velocity field can be: (a) either continuous or discrete (droplets) for pool flow, or (b) only continuous for flow in confined geometry (channel flow). The water in the second velocity field is carrying microscopic solid particles with a prescribed diameter. These particles, denoted with "n2", are called the inert component of the second velocity field – inert because they are not allowed to change the state of aggregate whereas the water, the non inert component of the second velocity field which is denoted by "M2", may evaporate. For flows in confined geometry the second velocity field may be entrained i.e. transported to the third velocity field.

The third velocity field is associated with: (a) water droplets in confined geometry or (b) with "liquid metal" in pool flow. In the case of flows in confined geometry, microscopic solid particles of the same chemical substance as in the second velocity field having the same previously prescribed particle diameter are carried with the water droplets in the third velocity field. These solid particles, denoted with "n3", are called inert component of the third velocity field, because they are not allowed to change their state of aggregate, whereas the water droplets, denoted with "M3", the non inert component of the third velocity field, may evaporate. In confined geometry the droplets may be deposited into the continuous liquid of the second velocity field.

Finally, in case of pool flow in a cell, the third velocity field is associated with "liquid metal" of the same chemical substance as the solid particles of the second velocity field. In this case the third velocity field is immiscible with the others and consists of the inert component "n3" only. The liquid metal is allowed to freeze and to form solid particles. There are no heat sources in the liquid metal.

We see that there is one common feature of the velocity fields "l", namely all of them are considered as homogeneous mixtures of an inert and a noninert component, denoted with "nl" and "Ml", respectively, having the same temperature as the velocity field l, $T_{nl} = T_{Ml} \equiv T_l$.

No high order effects of the surface curvature on all terms in the basic equations are taken into account (e.g. the pressures of all of the three velocity fields are equal to the system pressure).

The concentration of microscopic solid particles in liquid–gas mixtures is of particular interest in many applications, e.g. radioactivity transport, environment pollution etc. Small impurities in the classical two phase flow theory are usually neglected due to their negligible effect on flow mechanics. In contrast with the mechanical influence, the thermodynamic influence on metastable liquids and gases can be substantial. Microscopic solid particles substantially increase the bubble nuclei generation and consequently the flashing initiation and flashing itself which has an enormous impact on the mechanical behavior of the system. Therefore considering microscopic particles is a step forward in the sophistication of modeling of twophase flows. Now let us answer the question: why the proposed association with the velocity fields? Small movements of the microscopic components "nl" within the field "l" can be successfully described by diffusion inside the field "l" or neglected. It saves the introduction of an additional velocity field, and therefore modelling costs. In contrast, the macroscopic structures are strongly heterogeneous, and therefore they must be associated with a separate velocity field.

Zemansky [50] p.566 defines "a phase as a system or a portion of the system composed of any number of chemical constituents satisfying the requirements (1) that it is homogeneous and (2) that it has a definite boundary" In this sense we are attempting to mathematicaly describe 5 phases at the maximum.

2. SYSTEM OF PARTIAL DIFFERENTIAL EQUATIONS DESCRIBING THE FLOW

We start with the presumption that the system of all equations describing the macroscopic behavior of the flow has to be solved *numerically.* Therefore we discuss some details that are important for the integration at the very beginning of the derivation of the equations.

The flow is described by means of a vector of variables depending upon space and time. Writing the conservation equations for mass, momentum, and energy for a given control volume at a given time, *local instantaneous formulation*, one can describe in general the flow if the time scale of the integration and the length scale of the space discretization resolve all frequencies and wave lengths inherent to the studied phenomenon, i.e. the time scale of the parameter changes is comparable to the integration time step and the structural length scale is comparable to the available discretization size – *direct simulation.*

The local instantaneous conservation laws can be formulated in different ways. In what follows some of them will be discussed briefly.

(1) The most popular way is to formulate the conservation laws as being valid only for the space occupied by the velocity field in the so–called separated flow models. In this case, the local instantaneous conservation equations for *single phase flow* are applied to each of the velocity fields and therefore the generated equations are valid for the time and space dependent volume occupied by the particular velocity field only. In addition, local instantaneous balances of mass, momentum and energy are formulated at the interfaces as boundary conditions – *sometimes called jump conditions* – e.g. Ishii [65] (1975). The jump conditions are valid at the interfaces only. *Both groups of local instantaneous conservation equations are not valid for all of the space and time domains under consideration.*

(2) Another way is to formulate the local instantaneous conservation laws as being valid *everywhere* in the space and time domains under consideration, i.e. in the bulk of the velocity field, at the interfaces, and outsides of the velocity field. This means that the equations for each particular velocity field are defined in a control volume equal to or larger than the subvolume possibly occupied by the velocity field under consideration. The equations generated in this manner are called local instantaneous field conservation equations – see Bedereaux et al [86] (1976), Kataoka [126] (1985).

(3) A third group of local instantaneous equations can be formulated for an *observable control volume*. The word observable is used here in the sense that the control volume possesses a size comparable to the size of the sensors of the measuring instruments, i.e., has a finite size.

The local instantaneous volume fraction of the velocity field is equal to one, $\alpha_l = 1$, in the first formulation for the regions occupied by the velocity field of interest. The volume averaged instantaneous volume fraction arises after a volume averaging.

In the second formulation, the control volume is divided into an *infinite* number of *nonuniform* subvolumes so as to define in each of them the local instantaneous phase volume fraction, α_l, as a *velocity field existence function* being zero for nonexisting velocity field, and one for existing velocity field. The volume averaged instantaneous volume fraction arises after a volume averaging. Subsequent time averaging defines the volume and time averaged volume fraction. Performing time averaging, the local volume fraction is easily obtained.

In the third formulation the control volume is divided into a *finite* number of *uniform* subvolumes. In this case the local instantaneous volume fraction assumes *continuous* values between zero and one in the control volume. Again, different kinds of averaging lead to time and/or volume averaged local volume fractions.

For practical applications all of the three above discussed formulations lead to useful results. The first approach formulated for the first time the local surface conservation equations (sometimes called *jump conditions*) and after averaging the averaged interface conservation equations and the averaged macroscopic quantities. The second resolved the criticism that the local instantaneous equations defined by the first formalism are not field equations. The second formalism provides local instantaneous conservation field equations valid in all the space and time domains of interest. The subsequent averaging leads to the same averaged interface conservation equations and macroscopic quantities. The third formulation is very practicable for *free surface modelling* allowing all wave lengths and frequencies, for deriving *nonlinear jump conditions resulting from the interface curvature* – see Ramshaw and Trap [93] (1978), Zuber [102] (1979), Banerjee [103] (1984) among others, or for *direct simulation* of multiphase flows with future computers.

In the authors view, there are no arguments against the *simultaneous* interpretation of the local instantaneous volumetric fraction in the sense of the three above discussed formulations:

– equivalent to "one" only for the regions occupied by the velocity field under consideration,

– equivalent to the "velocity field existence function" that is defined in the total time and space domain under consideration and takes values of 0 or 1, and finally

– identical to the heterogeneous local volumetric fraction in finite volume formulations.

We call further this interpretation the *triple interpretation* of the local instantaneous volume fraction of the velocity field l.

Usually for practical applications the time scales of integration and the length scales of discretization are much larger than the system characteristics due to the limitations of the present day computers. So in order to be practically useful, the instantaneousaneous conservation equations should be appropriately *averaged*. The averaging is required also in order to *interpret measurements* which provide observations of some averaged flow properties. Two different approaches are known to express averages of the products as products of averages in the conservation equations: (a) definition of distribution coefficients or tensors (requires large numbers of constitutive relations); (b) weighted averages (introduces new dependent variables, retains the dimensions of the problem). There is a lot of literature published from the community searching for appropriate averaging procedures. The proposed averaging schemes can be classified as follows:

I. *Time and/or volume averaging*:

(a) *Cross section spatial averaging* (simple kind of volume averaging, reduce dimensions of the problem): see Zuber [51] (1964), Zuber and Findlay [52] (1965), Wallis [53] (1977), Yadigaroglu and Lahey [54] (1964), Panton [55] (1968) and for rigorously derivation Delhaye [56] (1976) and Delhaye and Achard [57] (1977).

(b) *Time averaging* – the most popular: In three fundamental papers Teletov [58, 59] (1945, 1957) and later in [60] (1958) formulated the instantaneousaneous and the averaged equations of conservation of mass, momentum and energy for a twophase one–component flow (preceded by the two–fluid super fluidity Helium 2 model of Landau [61] (1941)). Teletov's equations – today sometimes called unfounded "ad hoc equations" – are later being used in thousands of publications concerning different aspects of twophase flows. More rigorous time averaging for one–component twophase flow is given in Rahmatulin [62] (1956), Drew [63] (1971), Frenkel [64] (1973), Ishii [65] (1975), Delhaye [66, 67] (1976) and Delhaye and Achard [57] (1977).

(c) *Volume averaging* – the averaging volume length scale is much smaller then the length scale of the macroscopic changes: for rigorous derivation see Nigmatulin [68, 69] (1977, 1978) (further information in Dobran [70–73] (1983–85), Iwanga and Ishihara [74] (1980) among many others).

Time and volume averaged equation have virtually identical form but different interpretations of the averaged terms.

(d) *Combinations of space and time averaging*: Delhaye and Achard [57] (1977), Drew [63] (1971), Bataille [75] (1981), Bataille and Kestin [76] (1981) among many others. For example Bataille [77] (1988) classified the existing combinations of *averaging procedures* in two groups: In the first group *the distance between the particles* ($=n^{-1/3}$, n being the number of particles per unit volume of the mixture) *is much less than the heterogeneity of the continuous phase* without discrete impurities. For this case it is advisable to average first in a control volume with characteristic sizes much less than the heterogeneity and much bigger than the characteristic particle size, and to perform thereafter averaging in a time interval much less than the characteristic time constant of the process studied. In the second group *the distance between the particles is much bigger than the heterogeneity of the continuous velocity field.* The fluctuations of both structures are influencing each other. In this case, a time or statistical averaging is advisable. Although the equations resulting from the two kinds of averaging look very similar, they contain important and different information as to the procedure to formalise different phenomena, and how to measure them.

II. *Ensemble averaging*:

The ensemble averaging is in fact the determination of all possible realizations of the system parameters, determination of the probability distribution over all the possible realizations, and a probability weighted average over all possible realizations – Buyevich [78] (1966) Batchelor [79] (1970), Buyevich [80] (1966), Selesnev [81] (1976), Buyevich and Shchelchova [82] (1978). The closure conditions for the resulting averaged equations are difficult to constitute.

Unfortunately the rigorous ensemble averaging and some combinations of the above mentioned types of averaging results in very complicated equations and need large numbers of up to now not defined constitutive closure relations. The discussion about which of the above techniques is most rigorous and in the same time practicable is not closed and having in mind the development of turbulence research in one–phase fluid mechanics in the last 50 years it cannot be foreseen when this discussion will be completed. And even having the final form of one "well established" set of averaged equations the problem with the practical application is not solved automatically. One needs appropriate integration methods for any given class of initial and boundary conditions. It is well known that even for simple twophase flows there are no universal theorems for uniqueness and stability of the solutions. So, apparently the dilemma arises: on one hand to stop the application and wait until the above circle of problems is solved, which is not serious; or, on the other hand, to make "compromises" in the application using solvable systems and available closure relations, developing and sophisticating the solution methods for the so obtained set of equations in order to be helpful in the daily need to analyze such kinds of flows for practical design and licensing and at the same time to provide experience with the numerical methods and constitutive relationships integrated into the model. Even the latter is much easier to say than to do for multiphase flows. Fortunately the division of the existing methods into two basic groups is conditional because the solution of the system of the resulting equations is not possible without concretization of the actual flow pattern or topology. The latter is nothing else but replacing the ensemble averaged systems with time and volume averaged systems – see the discussion in Deich and Phillipov [83] (1981) p.36. That is why we prefere in this work to follow the Teletov–Ishii–Delhaye scheme of deriving the conservation equations under consideration of the porosity of the space:

1. Write the equations representing the local instantaneous conservation principles.
2. Perform time averaging.
3. Perform volume averaging.

The local instantaneous *equations* obtained as a result of the first step are valid on the micro scale being of order of the smallest flow observation that we can make, but on a scale much larger than the molecular scale, i.e. they *average the motion of individual molecules* and operate with macroscopic parameters like pressure, temperature, density and velocities representative for large ensembles of molecules. Thus the first step of averaging leads to *loss of information of the thermodynamic behavior* of the system. The lost information must be provided by the first group of constitutive relationships, namely the *equations of state*. The equations of state provide the relationships between the microscopic molecular motion and the macroscopic parameters.

The time averaging introduces new terms in the equations describing the *turbulent* *pulsation* of the flow parameters. If we neglect these terms, we filter the high frequencies of the oscillations of the flow parameters. If we are interested in this information, we need additional *constitutive relations for the describing of the turbulent flow behavior*. In addition, time averaging means that *all source terms* of the equations obtained are representative for the integration time step. Consequently, the *source terms* must not be local instantaneous values at the beginning of the time step but *time averaged* values taking into account the *unknown* changes of the driving forces during the time step which needs additional care when formulating the closure constitutive relations.

The volume averaging enables us to operate with parameters representative of control volumes larger than the characteristic length of the largest structural characteristics e.g. bubble or droplet diameters, surface wave lengths, etc. At this stage of the averaging, if we proceed to work with the volume averaged parameters only, we will lose information on the spectral *distribution of the characteristic structural dimensions and wave lengths*. In many cases this information is very important in order to determine the *flow structure and topology*. Therefore it should be provided again by constitutive relationships or additional differential equations and constitutive relationships. Again, like withy the time averaging, the *source terms* for the resulting equations must be *volume averaged* over the spectral characteristics of the length scale of the flow structure.

2.1 PRINCIPLE OF CONSERVATION OF MASS

The purpose of the following chapter is to present the mathematical form of the principle of conservation of mass for each velocity field and for each inert component inside each particular field. Thereafter we will show an alternative notation of the same principle for dispersed inert solid particles with equal diameters carried by a continuum. Using the same idea, we will derive an equation describing the conservation of the number of nuclei for spontaneous evaporation or condensation and show the relationship between this equation and the equation describing the conservation of the number of the originating droplets or bubbles (discrete phase).

The principle of conservation of mass for plane geometry and one–phase flow has been formulated for a first time in the form of a partial differential equation by Jean le Round d'Alambert in the pioneer papers Traite...des fluides (1744) and Theorie generale des vents (1745), and was generalized to its contemporary form in a few papers by Euler in 1757.

Having this forerunner and following the Teletov – Ishii – Delhaye – Kataoka concept it is a straightforward step to write the local instantaneous mass conservation equation of the velocity field "l" for the situation schematically presented in Figure 2. The size of the region of interest, called *computational region*, is much larger than the size of the local structure D_d. Consider a control volume dVol, placed inside the computational volume. The size of the control volume is much larger than the molecular free path length. The control volume is the smallest possible observable volume, which means that its size is comparable with the size of the sensors of the measuring instruments as shown in Fig. 2 a) trough d). Fig. 1 shows the control volume in more detail. The control volume dVol is occupied partially by non movable structures. The geometry of the structures inside dVol is described as follows:

(a) γ_v is the part of dVol available for the flow. γ_v is called local volumetric porosity in the following. The part of dVol occupied by structures is therefore $1 - \gamma_v$;

(b) γ^n belongs to the n–th of the six surfaces dF^n defining the control volume dVol. γ^n is the part of the surface dF^n available to the flow. The γ^n's are called surface permeabilities in the following. Note the difference from the permeability coefficients usually used for description of the pressure drop in porous media. The part of the surfaces occupied by nonmovable structures is therefore $1 - \gamma^n$.

Inside the volume available for the flow, $dVol_{flow}$ (within dVol) we assume that three velocity fields exist. Each of the velocity fields is designated with l, where l = 1, 2, 3. The instantaneous geometry of the velocity field is defined in a similar way as the nonmovable structure:

(a) α_l is the part of γ_vdVol available to the velocity field l. α_l is called local instantaneous volume fraction of the velocity field l in the following.

(b) α_l^n belongs to the n–th of the six surfaces defining the control volume. $\alpha_l^n \gamma^n dF^n$ is the part of the surface available to the velocity field l. The α^n are called heterogeneous volume fractions in the following.

We define the macroscopic density ρ_l only within the space of dVol occupied by velocity field l. Outsides velocity field l the density ρ_l is not defined. The macroscopic density obeys some law expressed by the macroscopic equation of state. The equation of state describes the interdependence between macroscopic density, called simply density in the following, pressure in the control volume and temperature of the velocity field l.

The above definitions are sufficient to compute the following:

The part of the control volume dVol occupied by the velocity filed l is

$$\alpha_l \gamma_v dVol \tag{2.1.1}$$

and the mass within this volume is

$$\rho_l \alpha_l \gamma_v dVol. \tag{2.1.2}$$

The mass of the larger computational volume that is designated by Vol, and consists of many control volumes dVol, is simply the sum of the masses of the control volumes dVol, namely

$$\iiint_{Vol} \rho_l \alpha_l \gamma_v dVol. \tag{2.1.3}$$

The change of this mass of the velocity field l per unit time inside the computational volume Vol in kg/s

$$\frac{\partial}{\partial \tau} \iiint_{Vol} \rho_l \alpha_l \gamma_v dVol. \tag{2.1.4}$$

is due to two reasons:

(a) convectional mass transfer through the surface F defining the computational volume Vol;

(b) convectional mass transfer trough the surfaces separating the velocity field l from the neighboring velocity field designated with m. We call this mass transfer component interfacial mass transfer in the following.

Next we compute these two components (a) for the control volume dVol and (b) for the larger computational volume Vol.

Consider each of the six surfaces dF^n defining dVol. Define the normal velocity of the velocity field l, V_l^n, pointing outwards from the control volume dVol. With this definition the mass flow in kg/s of the velocity field l through the surface dF^n is

$$\alpha_l^n \rho_l V_l^n \gamma^n dF^n. \tag{2.1.5}$$

Sum this mass flow over all six surfaces. The result

$$\sum_{n=1}^{6} \alpha_l^n \rho_l V_l^n \gamma^n dF^n \tag{2.1.6}$$

is the mass change of the velocity field l in kg/s for the control volume dVol due to mass transfer across the surfaces dF^n. Now consider the computational volume Vol consisting of many dVol's. Sum all mass flows across the surfaces dF^n for all dVol's. The mass flows at the common surfaces between neighboring dVol's cancel. What remains is the net mass flow at the surface F defining the volume Vol

$$\iint_F \alpha_l^n \rho_l V_l^n \gamma^n dF. \tag{2.1.7}$$

Thus if there is no interfacial mass transfer across the interfaces between velocity field l and the neighboring velocity field m, the change of the mass of the velocity field l within the computational volume Vol with time in kg/s equals the net mass flow of the field l through the surface F

$$\frac{\partial}{\partial \tau} \iiint_{Vol} \rho_l \alpha_l \gamma_v dVol + \iint_F \alpha_l^n \rho_l V_l^n \gamma^n dF^n = 0. \tag{2.1.8}$$

Next we introduce the effect of the interface mass transfer. The interface mass transfer can be caused by evaporation, condensation, entrainment, deposition or external sources. External refers to the regions outsides the computational region Vol.

The interface in m^2 belonging to the control volume dVol and separating the velocity field l from the neighboring fields is designated with dF_{li}. Here, i refers to interface. Define for dVol some representative normal velocity V^n_{li}. V^n_{li} points outwards from the velocity field l. We call this velocity in the following interfacial mass transfer velocity. It has notting to do with the normal interface velocity. V^n_{li} is the velocity with which the mass leaves field l across the interface due to evaporation, condensation etc. With this definitions we can compute the interfacial mass flow in kg/s leaving the velocity field l within the control volume dVol across the surface dF_{li}

$$\rho_l V^n_{li} dF^n_{li}. \tag{2.1.9}$$

Consequently the mass flow leaving the velocity field l due to evaporation, condensation etc. within the computational volume Vol consisting of many dVol's is simply the sum of the mas flows over all surfaces dF_{li}

$$\iint_{F_{li}} \rho_l V^n_{li} dF^n_{li}. \tag{2.1.10}$$

Here F_{li} is the interface of the velocity field l being insides the computational volume Vol.

It is customary in twophase flow theory to introduce the local interface density of the velocity field l as the interface of the velocity field l per unit flow volume $dVol_{flow}$ belonging to our control volume dVol

$$a_{il} = dF_{li}/dVol_{flow}. \tag{2.1.11}$$

With this definition the mass flow leaving the velocity field l due to evaporation, condensation etc. within the computational volume Vol consisting of many dVol's can be simply rewritten as the sum of the mass flows over all surfaces dF_{li} belonging to all dVol's.

$$\iint_{F_{li}} \rho_l V^n_{li}\, dF_{li} = \iiint_{Vol_{flow}} \rho_l V^n_{li} a_{li}\, dVol_{flow} = \iiint_{Vol} \rho_l V^n_{li} a_{li} \gamma_v\, dVol = - \iiint_{Vol} \mu_l \gamma_v\, dVol. \tag{2.1.12}$$

The product

$$\mu_l = - \rho_l V^n_{li} a_{li} \tag{2.1.13}$$

is the mass transferred into the velocity field l per unit time and unit mixture flow volume $dVol_{flow}$. We call this term local instantaneous mass source density in $kg/(m^3s)$ of the velocity field l. Note the difference between the mass source per unit volume of the flow, μ_l, and the mass source per unit of the control volume dVol, $\mu_l\gamma_v$.

Thus with the above definitions and considerations we can finally write the mass balance for a computational volume Vol, namely: The change of the mass of the velocity field l within the computational volume Vol with time in kg/s equals the net mass flow of the field l through the surface F and the interface of the velocity field F_{li}

$$\frac{\partial}{\partial\tau}\iiint\limits_{Vol}(\rho_l\alpha_l-\mu_l)\gamma_v dVol + \iint\limits_{F}\alpha_l^n\rho_l V_l^n\gamma^n dF^n = 0. \tag{2.1.14}$$

The convective term

$$\iint\limits_{F}\alpha_l^n\rho_l V_l^n\gamma^n dF^n \tag{2.1.15}$$

can be used in practical applications with different degrees of simplification. The most important thing here are

(a) the relationships between the heterogeneous volume fractions α_l^n and local instantaneous volume fraction α_l,

$$f_\alpha(\alpha_l, \alpha_l^n) = 0 \tag{2.1.16}$$

and

(b) the relationships between the surface permeabilities γ^n and the local volume porosity γ_v

$$f_\gamma(\gamma_l, \gamma_l^n) = 0. \tag{2.1.17}$$

The simplifications used in IVA3 are described below.

Define indices n of the surfaces dF_n belonging to dVol as shown in Fig. 1. Introduce

$$\lim_{dVol\to\epsilon^3}(\alpha_l^n) = \alpha_l, \quad \text{for } n = 1...6, \tag{2.1.18}$$

$$\lim_{dr\to\epsilon}(\gamma^1, \gamma^2) = \gamma_r, \tag{2.1.19}$$

$$\lim_{rd\theta\to\epsilon}(\gamma^3, \gamma^4) = \gamma_\theta, \tag{2.1.20}$$

$$\lim_{dz \to \epsilon} (\gamma^5, \gamma^6) = \gamma_r. \tag{2.1.21}$$

where ϵ is chosen so as to satisfy the inequality:

$$\text{size of dVol} >> \epsilon >> \text{molecular free path length.} \tag{2.1.22}$$

With this simplification and after defining the vector γ as follows

$$\gamma = \begin{vmatrix} \gamma_r \\ \gamma_\theta \\ \gamma_z \end{vmatrix}, \tag{2.1.23}$$

we can apply the Gauss – Ostrogradsky theorem to the convective term as follows

$$\iint_F \alpha_1^n \rho_1 V_1^n \gamma^n \, dF = \iiint_{Vol} \nabla.(\alpha_1 \rho_1 V_1 \gamma) \, dVol. \tag{2.1.24}$$

Here V_1 is the velocity vector with components (u_1, v_1, w_1) in (r, θ, z) direction, respectively, and $V_1\gamma$ is the vector with components $(u_1\gamma_r, v_1\gamma_\theta, w_1\gamma_z)$ in (r, θ, z) direction, respectively, and ∇ is the Nabla operator.

Next we discuss the important consequences of this approach.

Definition 2.1.18 means that only the local instantaneous volume fraction is needed to describe the flow under the assumption of homogenezation (mechanical nonequilibrium retained) of the phases insides dVol, which is of course a very strong simplification that introduces unphysical diffusion that has nothing to do with numerical diffusion. It influences the modeling of disperse flow pattern less than free surface modeling. This problem is already recognized and a way to improve it shown by Hirt and Nichols [130] (1981) is also applicable to multiphase mechanics.

Generally speaking, at all of the surfaces 1, 3 and 5 of the control volume dVol three surface permeabilities in the three main direction can be defined. Therefore the surface permeabilities defined in this way form a tensor which is obviously symmetric for infinitesimal dVol's. All γ^n's can be computed as space functions in Vol knowing this tensor. In fact for the practical application six surface permeabilities need to be defined. In IVA3 we define three of them and in addition rules for the computation of the residual three (harmonically weighting). In many technical applications the functional relationship 2.1.17 is known and the introduction of the volume porosity must be consistent with this relationship. We use only its diagonal elements in the derivation of the mass and energy balances. Further we use the vector γ as defined in 2.1.23 containing the three diagonal elements of this tensor.

Thus the simplification with respect to the geometry definition of the nonmovable structures is less restrictive than the simplification concerning the volume fractions.

Note that for technical structures the introduction of the local volume porosity is a convenient formalism to describe the real distances between the flow volumes and to retain the mathematical description of acoustic processes unaffected by the geometry description.

Using Eq. 2.1.24 we rewrite 2.1.14 as follows

$$\iiint_{Vol} [\frac{\partial}{\partial\tau}(\alpha_1\rho_1\gamma_v) + \nabla.(\alpha_1\rho_1 V_1 \gamma) - \gamma_v\mu_1]\, dVol = 0 \qquad (2.1.25)$$

which represents the mass conservation equation of the velocity field l in the volume Vol consisting of many dVol's and consists of a simple sum of the mass conservation applied per unit volume of each of the control volumes dVol

$$\frac{\partial}{\partial\tau}(\alpha_1\rho_1\gamma_v) + \nabla.(\alpha_1\rho_1 V_1 \gamma) = \gamma_v\mu_1. \qquad (2.1.26).$$

The dimension of Eq. 2.1.25 is in kg/s and that of Eq. 2.1.26 in kg/s per m^3 of the control volume dVol.

The triple interpretation of the local instantaneous volume fraction α_1 is preferred here rather then only one of the above discussed three interpretations in order to retain the freedom to use this form for different applications.

For convenience of the numerical integration the source term μ_1 is split in two non negative groups of terms

$$\mu_1 = \sum_{m=1}^{l_{max}, A} (\mu_{ml} - \mu_{lm}). \qquad (2.1.27)$$

The source terms having two subscripts are non–negative. The two successive subscripts denote the direction of the mass transfer. For instance μ_{ml} denotes the *transferred mass per unit time and unit volume of the flow* from velocity field "m" to velocity field "l". As a consequence of this definition, the source terms with two identical subscripts are equal to zero ($\mu_{mm} = \mu_{imm} = 0$). We denote with A the region "outside of the flow". For instance μ_{Al} means mass transport from exterior source into the velocity field l. For the mass transport among the velocity fields and between the exterior sources and the velocity fields we assume that *the mass convectively leaving the velocity field has its concentrations of the inert components (the mass entering the field has the concentrations of the donor field, respectively).*

Performing time and volume averaging and omitting the averaging signs for simplicity of the further discussion we obtain the same form as 2.1.1 but with different interpretation of all of its terms, which now contain products of time and volume averaged variables.

The local instantaneous mass conservation equation of the microscopic component "il" in the velocity field "l" *(inside the part of the control volume filled with the component "il", the net mass flow of the component "il" must equal the rate of increase of mass of the component "il")* is:

$$\frac{\partial}{\partial \tau}(\alpha_{il}\rho_{il}\gamma_v) + \nabla.(\alpha_{il}\rho_{il}V_{il}\gamma) = \gamma_v\mu_{il} \equiv \gamma_v \sum_{m=1}^{l_{max}, A} (\mu_{iml}-\mu_{ilm}) \tag{2.1.28}$$

Note that for gas mixture $\alpha_{il} = \alpha_l$, whereas for mixtures consisting of liquid and macroscopic solid particles $\alpha_{il} \neq \alpha_l$.

It is convenient for the description of the transport of the microscopic component "il" in the velocity field "l" to replace the velocity component V_{il} by the sum of the *averaged centre of mass* (c.m.) velocity of the particular field, V_l, and the *deviation from the c.m. velocity* or the so–called *diffusion velocity*, δV_{il}, of the inert component with respect to the c.m. velocity of the field, as suggested by Reynolds

$$V_{il} = V_l + \delta V_{il}. \tag{2.1.29}$$

Fick [84] (1855) noticed, that the *mass flow rate of the microscopical impurity with respect the mass flow rate of the continuous mixture including the impurity is proportional to the gradient of the concentration of this impurity*

$$\alpha_{il}\rho_{il}\delta V_{il} = - \alpha_l\rho_l D_{il}^l \nabla C_{il}, \tag{2.1.30}$$

where

$$C_{il} = \alpha_{il}\rho_{il}/(\alpha_l\rho_l) \tag{2.1.31}$$

is the mass concentration of the inert component "i" in the velocity field "l". The coefficient of proportionality, D_{il}^l [m^2/s], is called *coefficient of molecular diffusion*. The diffusion mass flow rate is directed from regions with higher concentration to regions with lower concentration, which is reflected by the minus sign in the assumption made by Fick, called later *Fick's law*, because many processes in nature and industrial equipments are successfully described mathematically by the above approach – *diffusion processes*. Substituting 2.1.30, 2.1.31 in 2.1.28 gives

$$\frac{\partial}{\partial \tau}(\alpha_l\rho_l C_{il}\gamma_v) + \nabla.(\alpha_l\rho_l C_{il} V_l \gamma) - \nabla.(\alpha_l\rho_l D_{il}^l \gamma \nabla C_{il}) = \gamma_v\mu_{il} \tag{2.1.31}$$

Molecular diffusion has *microscopic* character, being caused by the endless molecular interactions. There are special theoretical treatments of how to determine the molecular diffusion constant in multi–component mixtures which will not be discussed here.

The diffusion can have also *macroscopic* character, being caused by the macroscopic strokes between large eddies, having dimensions considerably larger than the molecular dimensions – *turbulent diffusion*. In a mixture at rest the first phenomenon is the only mechanism driving diffusion. In real flows both mechanisms are observed. The higher the velocity of the flow, the higher the effect of the turbulent diffusion. The c.m. velocity of the velocity field can be expressed as an averaged c.m. velocity and a pulsation component

$$V_l = V_l + V_l'. \tag{2.1.32}$$

Replacing in Eq. 2.1.31, performing time and volume averaging and omitting any averaging signs for simplicity of the further discussion we obtain

$$\frac{\partial}{\partial\tau}(\alpha_l\rho_l C_{il}\gamma_v) + \nabla.(\alpha_l\rho_l C_{il} V_l \gamma) + \nabla.(\alpha_l\rho_l C_{il} V_l' \gamma) - \nabla.(\alpha_l\rho_l D_{il}^l \gamma \nabla C_{il}) = \gamma_v \mu_{il}. \tag{2.1.33}$$

O. Reynolds assumes

$$\alpha_l\rho_l C_{il} V_l' = -\alpha_l\rho_l D_{il}^t \nabla C_{il}, \tag{2.1.34}$$

where the *coefficient of the turbulent diffusion* D_{il}^t *is proportional to the coefficient of the turbulent kinematic viscosity* (this is not valid for turbulence of electro–conductive liquids in a strong magnetic field):

$$D_{il}^t = \nu_{il}^t / Sc^t, \tag{2.1.35}$$

where the proportionality is determined by the turbulent *Schmidt number* (e.g. $Sc^t = 0.77$ if no other information available). This coefficient is *not a thermodynamic property of the material* as the molecular coefficient is, but a *property of the flow.* Thus, having for the total diffusion coefficient

$$D_{il}^* = D_{il}^l + D_{il}^t. \tag{2.1.36}$$

we obtain finally

$$\frac{\partial}{\partial\tau}(\alpha_l\rho_l C_{il}\gamma_v) + \nabla.[\alpha_l\rho_l\gamma(V_l C_{il} - D_{il}^* \nabla.C_{il})] = \gamma_v \sum_{m=1}^{l_{max}, A} (\mu_{iml} - \mu_{ilm}) \equiv \gamma_v \mu_{il} \tag{2.1.37}$$

After differentiation of the first two terms of the above equation and comparing with the averaged Eq. 2.1.26 we obtain the *non–conservative form*

$$\alpha_l\rho_l(\gamma_v \frac{\partial C_{il}}{\partial\tau} + V_l\gamma.\nabla C_{il}) - \nabla[\alpha_l\rho_l D_{il}^*\gamma\nabla C_{il}] = \gamma_v(\mu_{il} - C_{il}\mu_l). \tag{2.1.38}$$

The simplicity of this equation is the reason for the choice of C_{il} as elements of the *dependent variables vector* describing the flow. As a consequence of this choice the *equation of state* of the multi–component mixture, $\rho_l = \rho_l(p, T_l, \text{all } C_{il})$, has to be derived from the equation of state of the elementary components of the mixture, $\rho_{il} = \rho_{il}(p_{il}, T_l)$. This will be a subject of Chapter 2.5.

We denote with μ_l and μ the time and volume averaged *mass sources per unit time and unit volume of the flow.*

The non–conservative form of the concentration Eq. 2.1.16 for the velocity fields 2 and 3 can be written in another way. Suppose the solid particles of the n–th component of the velocity field l, have a diameter D_{nl}. After dividing the mass of this component being in unit volume of the velocity field $\rho_l C_{nl}$, by the mass of one particle $\rho_{nl}\frac{4}{3}\pi D_{nl}^3$, we get the number of the particles of the component "n" in unit volume of the velocity field "l"

$$n_{nl} = \rho_l C_{nl}/(\rho_{nl}\frac{4}{3}\pi D_{nl}^3). \tag{2.1.39}$$

We see that the denominator is a constant. Dividing Eq. 2.1.15 and using Eq. 2.1.17 we obtain

$$\frac{\partial}{\partial\tau}(\alpha_l n_{nl}\gamma_v) + \nabla.[\alpha_l\gamma(V_l n_{nl} - D_{nl}^*\nabla.n_{nl})] = \gamma_v\frac{\mu_{nl}}{\rho_{nl}\frac{4}{3}\pi D_{nl}^3}. \tag{2.1.40}$$

This form illustrates the idea how to obtain the equation for the *conservation of the number of nuclei per unit volume of the continuous liquid field,*

$$n_1^* = \sum_n n_{n2} + n_1^k \tag{2.1.41}$$

initiating flashing if the field becomes thermodynamically *unstable*, namely

$$\frac{\partial}{\partial\tau}(\alpha_2 n_1^*\gamma_v) + \nabla.[\alpha_2\gamma(V_2 n_1^* - \frac{\nu_2^t}{Sc^t}\nabla.n_1^*)] = \gamma_v(\Sigma\frac{\mu_{n2}}{\rho_{n2}\frac{4}{3}\pi D_{n2}^3} + \alpha_2\dot{n}_1^k). \tag{2.1.42}$$

Subtracting the equation describing the solid particles transport, from the equation of the total number of nuclei, we obtain the *equation describing the transport of the number of the kinetics nuclei* only

$$\frac{\partial}{\partial\tau}(\alpha_2 n_1^k\gamma_v) + \nabla.[\alpha_2\gamma(V_2 n_1^k - \frac{\nu_2^t}{Sc^t}\nabla.n_1^k)] = \gamma_v\alpha_2\dot{n}_1^k, \tag{2.1.43}$$

where with

$$\alpha_2 \dot{n}_1^k = f_{1w} \frac{4}{D_{hy}} n''_{1w} + \alpha_2 f_{n2}\, \Sigma\, n_{n2} + \alpha_2(\dot{n}_{1h}+\dot{n}_{1d}) - \dot{n}_{1kin} \qquad (2.1.44)$$

we denote the number of nuclei generated per unit time and unit volume of the continuous liquid. The particular components of the right hand side are:

f_{1w}	*Frequency of the nuclei* generation from one activated seed on the channel wall;
n''_{1w}	Number of the *activated seeds* on unit area of the wall;
$f_{1w} \frac{4}{D_{hy}} n''_{1w}$	Number of the *nuclei generated* from the wall per unit time and unit volume of the flow (wall cavity nucleation rate);
D_{hy}	Hydraulic diameter (4 times cross sectional area / perimeter);
f_{n2}	Frequency of the nuclei generated from one *activated seed on the particle* belonging to the second velocity field;
$\alpha_2 f_{n2} \Sigma n_2$	Number of the *nuclei generated from the solid particles* homogeneously mixed with the second velocity field per unit time and unit volume of the flow;
$\dot{n}_{1h}+\dot{n}_{1d}$	Bulk liquid nucleation rate.
$\dot{n}_{1h}$	Number of the nuclei generated by *homogeneous nucleation* in the second velocity field per unit time and unit volume of the flow;
$\dot{n}_{1d}$	Number of the nuclei generated from the *dissolved gases* in the second velocity field per unit time and unit volume of the flow;
$\dot{n}_{1kin}$	Number of the *nuclei transformed into bubbles* per unit time and unit volume of the flow;

Because the nuclei have microscopic dimensions, they can be transported not only by convection, but by *turbulent diffusion* too. The Eq. 2.1.43 has a physical meaning only if the second velocity field exists, $\alpha_2 > 0$, and, of course, if there is liquid in the field, which can evaporate, $C_{M2} > 0$. In case of missing gas phase, $\alpha_1 = 0$, the initial value of the number of the bubbles in unit volume of the mixture is $n_1 = \alpha_2 n_1^*$.

If one is not particularly interested in the number of the nuclei, only Eq.2.1.13 should be used having in mind that

$$\dot{n}_{1kin} = f_{1w} \frac{4}{D_{hy}} n''_{1w} + \alpha_2 f_{n2}\, \Sigma\, n_{n2} + \alpha_2(\dot{n}_{1h} + \dot{n}_{1d}). \qquad (2.1.45)$$

In case of flashing or evaporation, the balance of the bubble number density can be described by the following Equation

$$\frac{\partial}{\partial\tau}(n_1\gamma_v) + \nabla.[(n_1 V_1 - \frac{\nu_1^t}{Sc^t} \nabla n_1)\gamma] = \gamma_v(\dot{n}_{1kin} - \dot{n}_{1col} + \dot{n}_{1sp}) \quad \text{for} \quad \alpha_1 > 0,$$

(2.1.46)

where

$\dot{n}_{1col}$	is the number of the bubbles disappearing due to *coalescence* per unit time and unit volume of the flow;
$\dot{n}_{1sp}$	is the number of the bubbles arising due to the hydrodynamic bubble *splitting* (disintegration) per unit time and unit volume of the flow;
$-\frac{\nu_1^t}{Sc^t}$	is the diffusive flux of bubble number density due to the fact that the bubbles are in "random motion" in the presence of a void fraction gradient.

In accordance with Batchelor [79] (1988)

$$-\frac{\nu_1^t}{Sc^t} \approx \mathrm{const}\ D_1[V_1'V_1']^{1/2} = \mathrm{const}\ D_1 \Delta V_{12}[H(\alpha_1)]^{1/2} \tag{2.1.47}$$

where const ≈ 1,

$$H(\alpha_1) \approx \frac{\alpha_1}{\alpha_{1m}}\left(1 - \frac{\alpha_1}{\alpha_{1m}}\right) \tag{2.1.48}$$

and $\alpha_{1m} \approx 0.62$ is the limit of the closest packing of bubbles.

If in one time step $\Delta\tau$, void arises (for τ, $\alpha_{1a} = 0$, and for $\tau + \Delta\tau$, $\alpha_1 > 0$) or void already exists (for τ, $\alpha_{1a} > 0$, and for $\tau + \Delta\tau$, $\alpha_1 > 0$) , the expression

$$\dot{n}_{1kin} = (\alpha_2 n_1^k)_a / \Delta\tau \tag{2.1.49}$$

reflects the assumption, that all nuclei in the second velocity field become bubbles within the time step $\Delta\tau$.

In a similar way we write the *conservation equation for the condensation nuclei in the vapour component*

$$\frac{\partial}{\partial\tau}(\alpha_1 n_3^k \gamma_v) + \nabla.\left[\alpha_1 \gamma\left(V_1 n_3^k - \frac{\nu_1^t}{Sc^t} \nabla.n_3^k\right)\right] = \gamma_v \alpha_1 \dot{n}_3^k \tag{2.1.50}$$

valid for, $C_{M1} > 0$, $\alpha_1 > 0$, and the *conservation equation for the droplet number density*

$$\frac{\partial}{\partial\tau}(n_3 \gamma_v) + \nabla.\left[\left(n_3 V_3 - \frac{\nu_3^t}{Sc^t} \nabla n_3\right)\gamma\right] = \gamma_v(\dot{n}_{3kin} - \dot{n}_{3col} + \dot{n}_{3sp}) \quad \text{for } \alpha_3 > 0.$$

(2.1.51)

$-\frac{\nu_3^t}{Sc^t}$ is the diffusive flux of droplet number density due to the fact that the droplets are in "random motion" in the presence of a gradient of the voloumetric fraction of the droplets.

Again following Batchelor [79] (1988) we write

$$-\frac{\nu_3^t}{Sc^t} \approx \text{const } D_3 \, [V_3'V_3']^{1/2} = \text{const } D_3 \Delta V_{13} \, [H(\alpha_3)]^{1/2} \tag{2.1.52}$$

where const ≈ 1,

$$H(\alpha_3) \approx \frac{\alpha_3}{\alpha_{3m}}(1 - \frac{\alpha_3}{\alpha_{3m}}) \tag{2.1.53}$$

and $\alpha_{3m} \approx 0.52$ is the limit of the closest packing of droplets.

Again, if one is not particularly interested in the number of the nuclei, only Eq.2.1.34 should be used.

A comparison of nonequilibrium model predictions with experimental data for flashing in Laval nozzles, carried out by the author [38] (1985), shows that the numerical simulation of the nucleation density, and of the discrete particle (bubbles or droplets) density is the right way to obtain a more accurate prediction than with the widespread approach of assuming an almost arbitrary number density inside the range of $10^9 \div 10^{13}$. Deich and Philippov [83] (1981) analysed the pressure and temperature distribution inside the eddies of subcooled steam, and came to the conclusion, that *eddies* with proper dimensions *serve as a nuclei for condensation*, which is an additional argument advocating the above discussed method.

If we multiply the bubble number density, n_1, by the surface energy of one bubble, $\pi D_1^2 \sigma_2$, we will obtain the surface energy per unit mixture volume. The conservation equation for this energy is similar to Eq. 2.1.46. It is interesting to note that the surface energy is transported by the convection and diffusion of the *discrete* velocity fields but the terms supplying the change of this energy (kinetic origination, collision, splitting) are on account of the energy of the surrounding *continuous* liquid.

2.2 MOMENTUM PRINCIPLE

Fluid dynamics was first envisaged as a systematic science in Johann Bernoulli's Hydrodynamics (1737), and Daniel Bernoulli's Hydrodynamique (1738). The ideas expounded in these books were formulated mathematically as *local* instantaneous partial differential equations by Euler in two pioneer papers (1752, 1755). In these equations no dissipation terms like $\eta \nabla^2 V$ are present. These terms are introduced first by Navier in 1825 on molecular arguments. Later in 1845, Stokes proposed independently the same mathematical theory of fluids. This theory uses the concept of a stress tensor, introduced by Cauchy a decade earlier. The work of Stokes popularized this fruitful idea in fluid mechanics.

Our purpose in this Chapter is to extend the Teletov – Ishii – Delhaye formulation for l_{max} velocity fields in a porous body and to define the actual form of the source terms taking into account the interaction between the separated velocity fields, as well as between the walls confining the flow and the velocity fields. Thereafter we will discuss the relationship between the deformations of the velocity fields and the viscous stress.

2.2.1 NON AVERAGED MOMENTUM EQUATIONS

The time rate of change of momentum of a body equals the net force exerted on it (Newton). We applied this principle for *each velocity field* in a control volume

$$\frac{\partial}{\partial \tau}(\alpha_l \rho_l V_l \gamma_v) + \nabla.[\alpha_l(\rho V\, V + \tau)_l \gamma] + \alpha_l \gamma \nabla p + (\alpha_l \rho_l g + f_l)\gamma_v$$

$$= \gamma_v[\mu_{Al} V_{Al} - \mu_{lA} V_l + \sum_{m=1}^{l_{max}} (\mu_{ml} V_m - \mu_{lm} V_l)] \qquad (2.2.1.1)$$

and for each of the three space directions. The scalar notation of the above equation needed for the construction of the numerical solution is given in Appendix 1. When formulating the momentum transport resulting from the mass transfer among the velocity fields and between external sources and the velocity fields, we assume that *the mass leaving one and entering another velocity field has the same velocity as the donor field.*

The inertial momentum of rotation around an arbitrary oriented axis of a control volume of continuum is proportional to the 5th power of the linear volume dimension and the volume itself is proportional to the 3rd power of the linear dimension. From the mechanical equilibrium condition for all angular momenta around an axis for vanishing dimensions of the control volume, one obtains the *symmetry of the components of the viscous stress tensor* (see Schlichting [87] p.50): $\tau_{r\theta}=\tau_{\theta r}$, $\tau_{rz}=\tau_{zr}$, $\tau_{\theta z}=\tau_{z\theta}$.

Each velocity component can be decomposed in Taylor series. The *linear part* of this decomposition corresponds to small movements of a control volume. The linear part can be properly rearranged, and one sees that each small movement of the continuum consists of *deformation, translation,* and *rotation.* In the *classical mechanics for Newtonian fluids,* one looks for a *relationship* between the *deformation of the velocity field and the stress.* Usually the heuristic approach proposed by Helmholtz and Stokes is used. This approach contains three main hypotheses (see Schlichting [87] p.58), namely:

(a) the *viscous stresses are caused only by deformations* of the velocity field (Navier–Stokes) (change of the form of the volume for constant volume, or change of the volume itself for constant mass in the initial volume, or both simultaneously),

(b) the *viscous stresses are linearly dependent on the deformations* of the velocity field (Newton),

(c) this dependence is *invariant to the chosen orientation of the directions of the axes* of the coordinate system.

The mathematical notation of this hypotheses is

$$\tau = \eta\,[\nabla.V + (\nabla.V)^T] + \frac{2}{3}\,\eta\,(\mathrm{div}\ V)\ \delta \qquad (2.2.1.2)$$

where τ is the second order tensor for the momentum flux, $\nabla.V$ is the dyadic product of the Nabla – operator and the velocity vector, $(\nabla.V)^T$ is $\nabla.V$ transposed, div V is the divergence of the velocity vector and δ is the unit tensor whth diagonal elements equal to one and non–diagonal elements equal to zero. The viscous stress components needed for the construction of the numerical solution are given in Appendix 2.

It is important to emphasise that inspite of the fact that several processes in fluid dynamics are successfully described by the above hypotheses, that they are *only hypotheses*, which are not derived from experiment, neither proven by abstract arguments.

Lets us repeat the background conditions: (a) *continuum,* (b) *small velocity changes,* (c) *only the linear part of the Taylor series is taken into account,* and therefore (d) *linear dependence between stresses and velocity deformations.*

This limitation of the hypotheses has to be borne in mind during practical applications.

2.2.2 AVERAGED EQUATIONS

Equation 2.2.1.1 is local instantaneous. Usually in practical applications *averaged properties* of the flow are of interest. That is why averaging of this equation in a characteristic time interval and in a given control volume is necessary.

We replace the instantaneous values of the velocities V by the sum of the *averaged value* $\overline{V}$ and the *pulsation components* V' with respect to the averaged values $V=\overline{V}+V'$, perform *time averaging* in a time interval much less than the characteristic time constant of the process considered (Reynolds) and thereafter averaging in a space volume, and obtain the following momentum equation (the averaging symbols are dropped again for simplicity)

$$\frac{\partial}{\partial \tau}(\alpha_l \rho_l V_l \gamma_v) + \nabla.\{\alpha_l[\rho\,(V\,V + V'\,V')+\tau]_l \gamma\} + \alpha_l \gamma\,\nabla p + (\alpha_l \rho_l g + f_l)\gamma_v$$

$$= \gamma_v[\mu_{Al} V_{Al} - \mu_{lA} V_l + \sum_{m=1}^{l_{max}} (\mu_{ml} V_m - \mu_{lm} V_l)], \qquad (2.2.2.1)$$

The scalar notation of the averaged momentum equations needed for the construction of the numerical solution is given in Appendix 3. In reality, the velocity pulsations depend on the pulsations of the volumetric concentrations too. Thus to obtain a more general form of the averaged equations needs the introduction of $\alpha_1=\bar{\alpha}_1+\alpha_1'$, $\rho_1=\bar{\rho}_1+\rho_1'$ etc. This leads to very complicated systems, because additional variables are introduced that characterize the turbulence and for which no information is now available on how they can be calculated. For this reason, we confine our attention to the above described much simplified approach. This approach describes correctly the case of missing dispersed phase.

The reader can find further development of the theory for the case of dispersed flow of droplets and gas without viscous terms by Besnard and Harlow [88] (1985).

2.2.3 REYNOLDS STRESSES OF TURBULENT PULSATIONS

We see from Eq. 2.2.2.1 that *the products of the pulsation velocity components,* called *Reynolds stresses, act on the flow introducing additional macroscopic cohaesion inside the velocity field.* The search for a proper way of a quantitative estimation of the Reynolds stresses for multiphase flows is in its initial stage. One of the possible ways for its formulation is the use of the analogy with one–phase fluids. Such a variant is the use of the *Boussinesq hypothesis* (1877) for the *turbulent eddy viscosity* inside the velocity field, namely:

$$\rho V'V' = \eta^t[\nabla.V + (\nabla.V)^T] + \frac{2}{3}\eta^t(\text{div } V + k)\,\delta, \tag{2.2.3.1}$$

where k is the *kinetic energy of the turbulent pulsations of the velocity component,*

$$k = \frac{1}{2}(u'u' + v'v' + w'w'). \tag{2.2.3.2}$$

The scalar notation of the components of the Reynolds stress tensor needed for the construction of the numerical solution is given in Appendix 4. After replacing the Reynolds stresses in the averaged momentum equations with their counterparts from Eqs. 2.2.3.1 the terms containing k are absorbed by the pressure gradient, because the system pressure is formed by the molecular as well as by the turbulent pulsations. The Boussinesq hypothesis does not solve the problem of the turbulence description in the velocity field. It simply transferres it into the search for a formalism for estimating the so called *turbulent dynamic viscosity coefficient* η^t.

2.3 ENERGY PRINCIPLE (FIRST LAW OF THERMODYNAMICS)

Euler has considered the flow density as a function of the pressure $\rho = \rho(p)$ only and did not need an equation of conservation of energy to describe the flow completely. Later with further development of thermodynamics, it became clear that fluid density depends not only on the pressure but on the temperature $\rho = \rho(p,T)$ as well. The German physician R. J. Mayer in 1842 and the English scientists J. P. Joule in 1843 to 1867 have shown through their experiments that mechanical work or kinetic energy can be transformed into internal energy of the fluid in a closed system by compression or viscous dissipation. Both scientists stated that the energy can be neither created nor destroyed: it can only change in form. This fundamental principle is contained in the first law of thermodynamics. Thus the need arises to formulate the energy principle for a flowing continuum. Probably B. de Saint Venant 1839 was the first to use a simple form of a one–dimensional equation of conservation of the energy. B. Riemann (1826–1866) [97] has used (probably for first time) a transient equation of conservation of energy in a perfect gas. With time the energy conservation equations for open systems became more complicated, taking into account more possibilities of energy transformation from one form to another including phase changes. When writing the energy equation for the velocity field l, our task is reduced to the extension of the Teletov–Ishii analysis, which is for two velocity fields and one–component twophase flow to a formulation for l_{max} velocity fields describing three–phase, three component flow in porous body.

The energy principle formulated for each velocity field is: *The sum of the rate of heat added to the velocity field inside the control volume from the surroundings plus the rate of work done on the velocity field inside the control volume is equal to the rate of change of the energy of the velocity field as it flows through the control volume.* Thus the instantaneous energy conservation equation for unit flow volume is

$$\frac{\partial}{\partial\tau}\{[\sum_{i=1}^{i_{max}} \alpha_{il}\rho_{il}(e_{il} + \frac{V_{il}^2}{2})]\gamma_v\} + \gamma_v(\sum_{i=1}^{i_{max}} p_{il}\frac{\partial\alpha_{il}}{\partial\tau})$$

$$+ \nabla.\{[\sum_{i=1}^{i_{max}} \alpha_{il}\rho_{il}(e_{il} + p_{il}/\rho_{il} + \frac{V_{il}^2}{2})V_{il}]\gamma\}$$

$$+ \nabla.[(\alpha_l\tau_l.V_l)\gamma] - \nabla.[(\alpha_l\lambda_l^l\,\nabla T_l)\gamma] + \gamma_v[\alpha_l\rho_l(g.V_l) + f_l.V_l] =$$

$$\gamma_v\{\dot{q}_l''' + \sum_n(\mu_{nAl}h_{nAl} - \mu_{nlA}h_{nl}) + \mu_{MAl}h_{MAl} - \mu_{MlA}h_{Ml}$$

$$+ \sum_n(\mu_{nAl}\frac{V_{nAl}^2}{2} - \mu_{nlA}\frac{V_{nlA}^2}{2}) + \mu_{MAl}\frac{V_{MAl}^2}{2} - \mu_{MlA}\frac{V_{MlA}^2}{2}$$

$$+ \sum_{m=1}^{l_{max}}[\mu_{Mml}(h_{Mml}^* + V_{Mm}^2/2) - \mu_{Mlm}(h_{Ml} + V_{Ml}^2/2)$$

$$+ \sum_n(\mu_{nml}(h_{nl} + V_{nm}^2/2) - \mu_{nlm}(h_{nl} + V_{nl}^2/2))]\}, \qquad (2.3.1)$$

where i=n, M. We denote here with * the specific enthalpies of saturated steam or water after evaporation or condensation, respectively. For instance μ_{M21} enters the gas phase with $h_{M21}^*=h''(p)$ or μ_{M12} enters the liquid phase with $h'(p_{Ml})$, where $h''(p)$ is the steam saturation enthalpy as a function of system pressure and $h'(p_{Ml})$ is the water saturation enthalpy as a function of steam partial pressure.

In order to ensure consistency with the second law of thermodynamics we take into account in the energy equations the power of *all acting forces* that are considered in the momentum equations – see Kolev [37] (1985) p.6, Kolev [39] (1986) p.5 or in Arnold [104] (1988) p.258.

2.4 ENTROPY PRINCIPLE (SECOND LAW OF THERMODYNAMICS)

The purpose of the present Chapter is to *derive the entropy equations from the mass, momentum and energy conservation equations* presented in the previous Chapters.

2.4.1 NON AVERAGED EQUATIONS

We transform the energy Eq. 2.3.1 through the following steps:

– Express the specific internal energies of the components by

$$e_{il} = h_{il} - p_{il}/\rho_{il}, \tag{2.4.1.1}$$

and obtain

$$\frac{\partial}{\partial\tau}\{\sum_{i=1}^{i_{max}} \alpha_{il}\rho_{il}(h_{il} + V_{il}^2/2)\gamma_v\} - \gamma_v(\sum_{i=1}^{i_{max}} \alpha_{il}\frac{\partial p_{il}}{\partial\tau})$$

$$+ \nabla.\{[\sum_{i=1}^{i_{max}} \alpha_{il}\rho_{il}(h_{il} + V_{il}^2/2).V_{il}]\gamma\}... \tag{2.4.1.2}$$

After differentiating the first and the third terms, and comparing with the mass conservation equations of the inert components nl, and of the noninert components Ml in the velocity field l, we obtain

$$\sum_{i=1}^{i_{max}} [\alpha_{il}\rho_{il}(\gamma_v\frac{\partial h_{il}}{\partial\tau} + V_{il}\,\gamma.\nabla h_{il})] - \gamma_v(\sum_{i=1}^{i_{max}} \alpha_{nl}\frac{\partial p_{nl}}{\partial\tau}).. \tag{2.4.1.3}$$

We multiply each of the momentum equations with one of the corresponding velocity components u_l ,v_l ,w_l, respectively, and subtract them from the corresponding energy equation. The result is

$$\sum_{i=1}^{i_{max}} [\alpha_{il}\rho_{il}(\gamma_v\frac{\partial h_{il}}{\partial\tau} + V_{il}\gamma.\nabla h_{il})] - [\sum_{i=1}^{i_{max}} \alpha_{il}(\gamma_v\frac{\partial p_{il}}{\partial\tau} + V_{il}\gamma.\nabla p_{il})] + \alpha_l\gamma.(\tau:\nabla V)_l$$

$$-\nabla.[(\alpha_l\lambda_l^l\,\nabla T_l)\gamma] = \gamma_v\Big[\dot{q}_l''' + \sum_n \mu_{nAl}(h_{nAl} - h_{nl}) + \mu_{MAl}(h_{MAl} - h_{Ml})$$

$$+ \sum_n [\mu_{nAl}\,\frac{1}{2}\,(V_{nAl}-V_{nl})^2 - \mu_{nlA}\,\frac{1}{2}\,(V_{nlA} - V_{nl})^2]$$

$$+\mu_{MAl}\,\frac{1}{2}\,(V_{MAl}-V_{Ml})^2 - \mu_{MlA}\,\frac{1}{2}\,(V_{MlA}-V_{Ml})^2$$

$$+ \sum_{m=1}^{l_{max}} \{\mu_{Mml}[h^*_{Mml} - h_{Ml} + \frac{1}{2}\,(V_{Mm}-V_{Ml})^2]$$

$$+ \sum_n \mu_{nml}[h_{nm} - h_{nl} + \frac{1}{2}\,(V_{nm} - V_{nl})^2]\}\Big] \equiv \gamma_v q_l. \qquad (2.4.1.4)$$

In this case the *irreversible power of energy transformation due to the viscous dissipation* is

$$\alpha_l\gamma.(\tau:\nabla V)_l. \qquad (2.4.1.5)$$

A part of the dissipated power, i.e.

$$V_l.\nabla(\alpha_l\gamma.\tau_l) \qquad (2.4.1.6)$$

cancels after the subtraction.

At this place we make use of the Gibbs equation (the thermodynamic definitions of temperature and pressure are used here)

$$Tds = de + p\,dv. \qquad (2.4.1.7)$$

This is a differential equation of state which is extremely important in the thermodynamic theory of compressible substances. It relates the difference in entropy between any two infinitesimally separated states to the infinitesimal differences in internal energy and volume between those states. Note, that the Gibbs equation is valid only if "s" is a smooth function of "e" and "v" i.e. the differentials "de" and "dv" are uniquely defined (smooth equation of state). Using the definition of enthalpy (a mixture of thermodynamic and mechanical properties)

$$h = e + p\,v \qquad (2.4.1.8)$$

the Gibbs equation can be written as

$$T\rho\,ds = \rho\,dh - dp. \qquad (2.4.1.9)$$

After replacing "ds" in equation 2.4.1.4 with the Gibbs definitions of the *specific entropy* of the corresponding components

$$T_l\rho_{il}ds_{il} = \rho_{il}dh_{il} - dp_{il}, \qquad (2.4.1.10)$$

we obtain

$$T_l \left[\sum_{i=1}^{i_{max}} \alpha_{il}\rho_{il}\left(\gamma_v \frac{\partial s_{il}}{\partial \tau} + V_{il}\gamma.\nabla s_{il}\right)\right] - \nabla.[(\alpha_l\lambda_l^l \nabla T_l)\gamma] + \alpha_l\gamma.(\tau:\nabla V)_l = \gamma_v q_l.$$

(2.4.1.11)

Using the equations for conservation of mass for each component

$$\frac{\partial}{\partial \tau}(\alpha_{il}\rho_{il}\gamma_v) + \nabla.(\alpha_{il}\rho_{il}V_{il}\gamma) = \gamma_v\mu_{il}, \quad i = n,M,$$

this equation can be written in *conservative form*

$$T_l \left\{\frac{\partial}{\partial \tau}\left[\left(\sum_{i=1}^{i_{max}} \alpha_{il}\rho_{il}s_{il}\right)\gamma_v\right] + \nabla.\left[\left(\sum_{i=1}^{i_{max}} \alpha_{il}\rho_{il}V_{il}s_{il}\right)\gamma\right] - \gamma_v\left(\sum_{i=1}^{i_{max}} \mu_{il}s_{il}\right)\right\} - \nabla.[(\alpha_l\lambda_l^l \nabla T_l)\gamma]$$

$$+ \alpha_l\gamma.(\tau:\nabla V)_l = \gamma_v q_l. \quad (2.4.1.12)$$

After replacing the instantaneous values of the component velocities with the sums of the c.m. field velocities plus the deviations from the c.m. velocities

$$V_{il} = V_l + \delta V_{il}, \quad (2.4.1.13)$$

taking into account that the *specific mixture entropy* s_l *of the velocity field* can be calculated as follows

$$\alpha_l\rho_l s_l = \sum_{i=1}^{i_{max}} \alpha_{il}\rho_{il}s_{il}, \quad (2.4.1.14)$$

using Fick's law

$$\alpha_{il}\rho_{il}\delta V_{il} = -\alpha_l D_{il}^l \nabla \rho_{il} = -\alpha_l\rho_l D_{il}^l \nabla C_{il}, \quad (2.4.1.15)$$

and introducing the *Prandtl number*

$$Pr_l^l = \frac{\rho_l c_{pl}\nu_l^l}{\lambda_l^l}, \quad (2.4.1.16)$$

we obtain the following form of the local instantaneous entropy equations

$$T_l \left\{\frac{\partial}{\partial \tau}(\alpha_l\rho_l s_l\gamma_v) + \nabla.(\alpha_l\rho_l s_l V_l\gamma) - \gamma_v\left(\sum_{i=1}^{i_{max}} \mu_{il}s_{il}\right)\right\}$$

$$-\nabla.[\alpha_l\rho_l(c_{pl}\frac{\nu_l}{Pr_l}\nabla T_l + T_l\sum_{i=1}^{i_{max}} s_{il}D_{il}^l\nabla C_{il})\gamma] + \alpha_l\gamma.(\tau:\nabla V)_l = \gamma_v q_l.$$

(2.4.1.17)

2.4.2 AVERAGED EQUATIONS

After replacing the instantaneous values of the field velocities with the sums of the time averaged field velocities plus the fluctuation components

$$V_l = \overline{V}_l + V_l' \qquad (2.4.2.1)$$

and averaging the so obtained equations, we obtain the following form of the entropy equations (for simplicity we drop the averaging signs)

$$T_l\,\{\frac{\partial}{\partial\tau}(\alpha_l\rho_l s_l\gamma_v) + \nabla.(\alpha_l\rho_l s_l V_l\gamma) - \gamma_v(\sum_{i=1}^{i_{max}}\mu_{il}s_{il}) + \nabla.(\alpha_l\rho_l s_l V_l'\gamma)\}$$

$$-\nabla.[\alpha_l\rho_l(c_{pl}\frac{\nu_l}{Pr_l}\nabla T_l + T_l\sum_{i=1}^{i_{max}} s_{il}D_{il}^l\nabla C_{il})\gamma] + \alpha_l\gamma.(\tau:\nabla V)_l + \alpha_l\gamma.(\tau:\nabla V)_l' = \gamma_v q_l.$$

(2.4.2.2)

In the next Chapter we discuss the different terms of the above equation.

2.4.3 ENTROPY DIFFUSION

For the practical applications of the entropy equation we need to define more accurately the term

$$\nabla.(\alpha_l\rho_l s_l V_l'\gamma). \qquad (2.4.3.1)$$

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

$$\nabla.(\alpha_l\rho_l s_l V_l'\gamma) \approx -\frac{1}{T_l}\,\nabla.(\alpha_l\rho_l c_{pl}\,\frac{\nu_l^t}{Pr_l^t}\,\nabla T_l) \qquad (2.4.3.2)$$

where

$$Pr_l^t = \frac{\rho_l c_{pl} \nu_l^t}{\lambda_l^t}, \tag{2.4.3.3}$$

is the *turbulent Prandtl number*, λ_l^t is the "*turbulent coefficient of thermal conductivity*" or "*eddy conductivity*". Note that the *thermal diffusion* ν_l^l/Pr_l is a *thermodynamic property* of the continuum l, and ν_l^t/Pr_l^t is a *mechanical property of the flowing field l* [$Pr_l^t \cong 0.7 \div 0.9$ in channels, whereas for flow in jets (i.e., in "free turbulence") the value is more nearly 0.5 –see Bird et al [98] (1960), $Pr_l^t \cong 0.5 \div 2.5$ for water, air and steam – see Hammond [99] (1985)].

Defining the total entropy diffusion coefficient D_l^s by

$$D_l^s.\nabla s_l = c_{pl}\left(\frac{\nu_l}{Pr_l} + \frac{\nu_l^t}{Pr_l^t}\right) \nabla T_l + T_l \sum_{i=1}^{i_{max}} s_{il} D_{il}^l \nabla C_{il}$$

$$= \left[c_{pl}\left(\frac{\nu_l}{Pr_l} + \frac{\nu_l^t}{Pr_l^t}\right) \left(\frac{\partial T_l}{\partial s_l}\right)_{p,C_{il}} + T_l \sum_{i=1}^{i_{max}} s_{il} D_{il}^l \left(\frac{\partial C_{il}}{\partial s_l}\right)_{p,T_l}\right] \nabla s_l$$

$$= T_l \left[\frac{\nu_l}{Pr_l} + \frac{\nu_l^t}{Pr_l^t} + \sum_{i=1}^{i_{max}} s_{il} D_{il}^l / \left(\frac{\partial s_l}{\partial C_{il}}\right)_{p,T_l}\right] \nabla s_l \tag{2.4.3.4}$$

we can write finally the following form of the entropy equations

$$T_l \left\{\frac{\partial}{\partial \tau}(\alpha_l \rho_l s_l \gamma_v) + \nabla.(\alpha_l \rho_l s_l V_l \gamma) - \gamma_v\left(\sum_{i=1}^{i_{max}} \mu_{il} s_{il}\right)\right\} - \nabla.[(\alpha_l \rho_l D_l^s.\nabla s_l)\gamma]$$

$$+ \alpha_l \gamma.(\tau:\nabla V)_l + \alpha_l \gamma.(\tau:\nabla V)_l' = \gamma_v q_l. \tag{2.4.3.5}$$

2.4.4 SOURCE TERMS

In order to obtain the turbulent part of the source terms in the entropy equations we make analogous transformations to those made in the previous Chapter. Replacing the instantaneous velocities by $V_{Al} = V_{Al} + V_{Al}'$, $V_{lA} = V_{lA} + V_{lA}'$, $V_m = V_m + V_m'$, $V_l = V_l + V_l'$, in the quadratic terms and averaging in time we obtain (for simplicity we drop the averaging signs)

$$q_l = \dot{q}_l''' + \sum_{i=1}^{i_{max}} \mu_{iAl}(h_{iAl}-h_{il}) + \sum_{m=1}^{l_{max}} [\mu_{Mml}(h_{Ml}^{*}-h_{Ml}) + \sum_n \mu_{nml}(h_{nm} - h_{nl})]$$

$$+ \mu_{Al}\,\frac{1}{2}\,(V_{Al}-V_l)^2 - \mu_{lA}\,\frac{1}{2}\,(V_{lA}-V_l)^2] + \sum_{m=1}^{l_{max}} \mu_{ml}\,\frac{1}{2}\,(V_m-V_l)^2 + q_l^t, \tag{2.4.4.1}$$

where

$$q_l^t = \mu_{Al}\,\frac{1}{2}\,(V'_{Al}-V'_l)^2 - \mu_{lA}\,\frac{1}{2}\,(V_{lA} - V'_l)^2] + \sum_{m=1}^{l_{max}} \mu_{ml}\,\frac{1}{2}\,(V'_m-V'_l)^2. \tag{2.4.4.2}$$

We see that the mass transfer between the velocity fields and between the fields and external sources causes additional entropy transport, because of the different pulsation characteristics of the donor and acceptor fields.

The question arises how to estimate V'. From the definition of the specific energy of the turbulent pulsations

$$k_l^2 = \frac{1}{2}\,V_l'^2 = \frac{1}{2}\,(u_l'^2 + v_l'^2 + w_l'^2), \tag{2.4.4.3}$$

we see that V'_l is of the order of magnitude of k_l. For k_l we have information either from algebraic models or from the k–ϵ model of turbulence.

Another possibility to describe the turbulence anisotropy is by introducing *anisotropy coefficients* of turbulence $F_{rl} = u_l'^2/(2k_l^2)$, $F_{\theta l} = v_l'^2/(2k_l^2)$, $F_{zl} = w_l'^2/(2k_l^2)$, in addition to the k–ϵ model. Wang et al. [100] (1987) report that for a vertical bubble flow with low gas concentration F_θ is nearly constant, $F_{\theta 2} \cong 0.25$, and for the other coefficients the authors give a table with empirical constants. There is a conceptual problem in this approach because the k–equation is derived under the assumption of isotropic turbulence.

2.4.5 VISCOUS DISSIPATION

Next we compute the *irreversible power caused by the viscous forces due to deformation of the mean values of the velocities in the space*:

$$-\alpha_l\rho_l P_{kl} \equiv \alpha_l \gamma.(\tau:\nabla V)_l = \nabla.(\alpha_l \tau_l.V_l \gamma) - V_l.\nabla.(\alpha_l \tau_l \gamma) =$$

$$= \alpha_l\{\gamma_r(\tau_{rrl}\,\frac{\partial u_l}{\partial r} + \tau_{r\theta l}\,\frac{\partial v_l}{\partial r} + \tau_{rzl}\,\frac{\partial w_l}{\partial r})$$

$$+\gamma_\theta[\tau_{\theta rl}(\frac{1}{r\kappa}\frac{\partial u_l}{\partial\theta}-\frac{\kappa}{r}v_l)+\tau_{\theta\theta l}(\frac{1}{r\kappa}\frac{\partial v_l}{\partial\theta}+\frac{\kappa}{r}u_l)+\tau_{\theta zl}\frac{1}{r\kappa}\frac{\partial w_l}{\partial\theta}]$$

$$+\gamma_z(\tau_{zrl}\frac{\partial u_l}{\partial z}+\tau_{z\theta l}\frac{\partial v_l}{\partial z}+\tau_{zzl}\frac{\partial w_l}{\partial z})\} \qquad (2.4.5.1)$$

For a symmetrical stress tensor $\tau_{r\theta l}=\tau_{\theta rl}$, $\tau_{\theta zl}=\tau_{z\theta l}$, $\tau_{zrl}=\tau_{rzl}$, we have

$$-\alpha_l\rho_l P_{kl}=\alpha_l[\gamma_r\tau_{rrl}\frac{\partial u_l}{\partial r}+\gamma_\theta\tau_{\theta\theta l}(\frac{1}{r\kappa}\frac{\partial v_l}{\partial\theta}+\frac{\kappa}{r}u_l)+\gamma_z\tau_{zzl}\frac{\partial w_l}{\partial z}$$

$$+\tau_{r\theta l}[\gamma_r\frac{\partial v_l}{\partial r}+\gamma_\theta(\frac{1}{r\kappa}\frac{\partial u_l}{\partial\theta}-\frac{\kappa}{r}v_l)]+\tau_{rzl}(\gamma_r\frac{\partial w_l}{\partial r}+\gamma_z\frac{\partial u_l}{\partial z})+\tau_{\theta zl}(\gamma_\theta\frac{1}{r\kappa}\frac{\partial w_l}{\partial\theta}+\gamma_z\frac{\partial v_l}{\partial z})]$$

$$(2.4.5.2)$$

Now replacing the stress tensor components using the Helmholtz and Stokes hypotheses, Eq. 2.2.1.4, we obtain the final expression

$$-\alpha_l\rho_l P_{kl}=-\alpha_l\eta_l\{2[\gamma_r(\frac{\partial u_l}{\partial r})^2+\gamma_\theta(\frac{1}{r\kappa}\frac{\partial v_l}{\partial\theta}+\kappa\frac{u_l}{r})^2+\gamma_z(\frac{\partial w_l}{\partial z})^2]$$

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

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

$$+(\frac{1}{r\kappa}\frac{\partial w_l}{\partial\theta}+\frac{\partial v_l}{\partial z})(\gamma_\theta\frac{1}{r\kappa}\frac{\partial w_l}{\partial\theta}+\gamma_z\frac{\partial v_l}{\partial z})]$$

$$-\frac{2}{3}[\frac{\partial u_l}{\partial r}+(\frac{1}{r\kappa}\frac{\partial v_l}{\partial\theta}+\frac{\kappa}{r}u_l)+\frac{\partial w_l}{\partial z}][\gamma_r\frac{\partial u_l}{\partial r}+\gamma_\theta(\frac{1}{r\kappa}\frac{\partial v_l}{\partial\theta}+\frac{\kappa}{r}u_l)+\gamma_z\frac{\partial w_l}{\partial z}]\}.$$

$$(2.4.5.3)$$

We see that as for one–phase flow, the *viscous dissipation* P_{kl} (a) *is a positive quadratic form,* $P_{kl}\geq 0$, (b) *the mathematical description does not depend on the rotation of the coordinate system* [see Zierep [101] (1983)], *and* (c) *contains no derivatives of the viscosity.*

The *turbulent pulsations* irreversibly dissipate power in the viscous fluid, i.e.

$$\alpha_l\gamma.(\tau:\nabla V)_l'=-\alpha_l\rho_l\epsilon_l, \qquad (2.4.5.4)$$

where

$$\epsilon = \nu \{ 2 \overline{[\gamma_r (\frac{\partial u_l'}{\partial r})^2 + \gamma_\theta (\frac{1}{r^\kappa} \frac{\partial v_l'}{\partial \theta} + \kappa \frac{u_l'}{r})^2 + \gamma_z (\frac{\partial w_l'}{\partial z})^2}$$

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

$$+ \overline{(\frac{\partial w_l'}{\partial r} + \frac{\partial u_l'}{\partial z})(\gamma_r \frac{\partial w_l'}{\partial r} + \gamma_z \frac{\partial u_l'}{\partial z})}$$

$$+ \overline{(\frac{1}{r^\kappa} \frac{\partial w_l'}{\partial \theta} + \frac{\partial v_l'}{\partial z})(\gamma_\theta \frac{1}{r^\kappa} \frac{\partial w_l'}{\partial \theta} + \gamma_z \frac{\partial v_l'}{\partial z})]}$$

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

(2.4.5.5)

In fact, this is the *definition equation for the viscous dissipation of the turbulent kinetic energy* k_l. We see again that ϵ_l (a) *is a positive quadratic form,* $\epsilon_l \geq 0$, (b) *the mathematical description does not depend on the rotation of the coordinate system,* (c) *and contain no derivatives of the viscosity.*

We obtain an estimate for the value of ϵ in a given point in space and time from algebraic turbulence models or from the ϵ–equation in the k–ϵ model.

Thus, we can write the following form of the *entropy equations*

$$\alpha_l \rho_l (\gamma_v \frac{\partial s_l}{\partial \tau} + V_l \gamma . \nabla s_l) - \nabla . (\alpha_l \rho_l D_l^s \gamma . \nabla s_l) + \gamma_v \mu_l s_l = \gamma_v D s_l^*,$$

(2.4.5.6)

where

$$D s_l^* = \frac{1}{T_l} [\alpha_l \rho_l (P_{kl} + \epsilon_l) + q_l] + \sum_n \mu_{nl} s_{nl} + \mu_{Ml} s_{Ml} = \frac{1}{T_l} [\alpha_l \rho_l (P_{kl} + \epsilon_l) + \dot{q}_l'''$$

$$+ \sum_{m=1}^{l_{max}, A} \mu_{ml} \frac{1}{2} (V_m - V_l)^2 - \mu_{lA} \frac{1}{2} (V_{lA} - V_l)^2 + q_l^t]$$

$$+ \sum_{i=1}^{i_{max}} \mu_{iAl} \left(s_{il} + \frac{h_{iAl}-h_{il}}{T_l}\right) - \sum_{i=1}^{i_{max}} \mu_{ilA}\left(s_{il} + \frac{h_{il}-h_{il}}{T_l}\right)$$

$$+ \sum_{m=1}^{l_{max}} \left[\mu_{Mml}\left(s_{Ml} + \frac{h^*_{Ml}-h_{Ml}}{T_l}\right) + \sum_n \mu_{nml}\left(s_{nl} + \frac{h_{nm}-h_{nl}}{T_l}\right) - \sum_{i=1}^{i_{max}} \mu_{ilm}\left(s_{il} + \frac{h_{il}-h_{il}}{T_l}\right)\right]$$

$$= \frac{1}{T_l}\left[\alpha_l\rho_l(P_{kl} + \epsilon_l) + \dot{q}_l''' + \sum_{m=1}^{l_{max},A} \mu_{ml}\, \frac{1}{2}\, (V_m-V_l)^2 - \mu_{lA}\, \frac{1}{2}\, (V_{lA}-V_l)^2 + q_l^t\right]$$

$$+ \sum_{i=1}^{i_{max}} (\mu_{iAl}s_{iAl} - \mu_{ilA}s_{il}) + \sum_{m=1}^{l_{max}} \left[\sum_n (\mu_{nml}s_{nm} - \mu_{nlm}s_{nl}) + \mu_{Mml}s^*_{Ml} - \mu_{Mlm}s_{Ml}\right].$$

Having in mind that

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

and

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

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

$$\mu_l^+ s_l = \left(\sum_{i=1}^{i_{max}} C_{il}s_{il}\right) \sum_{\substack{m=1\\ m\neq l}}^{l_{max},A} \mu_{ml},$$

$$\mu_l^- s_l = \left(\sum_{i=1}^{i_{max}} C_{il}s_{il}\right) \sum_{\substack{m=1\\ m\neq l}}^{l_{max},A} \mu_{lm},$$

we obtain the *final semi conservative form of the entropy equation*

$$\alpha_l\rho_l\left(\gamma_v \frac{\partial s_l}{\partial \tau} + V_l\gamma\cdot\nabla s_l\right) - \nabla\, (\alpha_l\rho_l D_l^s\gamma\cdot\nabla s_l) + \gamma_v\mu_l^+ s_l = \gamma_v Ds_l,$$

$$(2.4.5.7)$$

in which

$$Ds_l = \frac{\dot{q}_l'''}{T_l} + \sum_{\substack{m=1\\ m\neq l}}^{l_{max},A} \Big[\sum_n \mu_{nml} s_{nm} + \mu_{Mml} s^*_{Mml} + \sum_{i=1}^{i_{max}} s_{il}(\mu_{lm} C_{il} - \mu_{ilm})\Big]$$

$$+ \frac{1}{T_l}\Big[\alpha_l \rho_l (P_{kl} + \epsilon_l) + \sum_{\substack{m=1\\ m\neq l}}^{l_{max},A} \mu_{ml} \frac{1}{2} (V'_m - V'_l)^2 - \mu_{lA} \frac{1}{2} (V'_{lA} - V'_l)^2$$

$$+ \sum_{\substack{m=1\\ m\neq l}}^{l_{max},A} \mu_{ml} \frac{1}{2} (V_m - V_l)^2 - \mu_{lA} \frac{1}{2} (V_{lA} - V_l)^2\Big], \qquad (2.4.5.7)$$

where for lm ≡ 23, 32, lA (mechanical transport),

$\mu_{nlm} = \mu_{lm} C_{nl}$,

$\mu_{Mlm} = \mu_{lm} C_{Ml}$,

otherwise (evaporation or condensation)

$\mu_{nlm} \neq \mu_{lm} C_{nl}$,

$\mu_{Mlm} \neq \mu_{lm} C_{Ml}$,

and

$m = A$, $s^*_{Mml} = s_{Mm}$.

This equation reflects very interesting physical phenomena. We see that velocity gradients cause energy dissipation $P_{kl} \geq 0$, which generates turbulent kinetic energy. The turbulent kinetic energy increases the turbulent viscosity by the Prandtl–Kolmogorov law and helps to reduce the velocity gradients. The irreversible dissipation of kinetic energy caused by the turbulent pulsation increases the specific internal energy of the continuum field $\epsilon_l \geq 0$. This dissipation decreases the specific turbulent kinetic energy directly.

If the equation is applied to a single velocity field in a closed system without interaction with external mass, momentum or energy sources, the change of the specific entropy of the system will be non–negative, because the sum of the dissipation terms $P_{kl}+\epsilon_l$ is non–negative. This expresses the *second law of thermodynamics.* The second law tells us in what direction a process will develop in nature. *The process will proceed in a direction such that the entropy of the system always increases, or at best stays the same* (P_{kl}

$+ \epsilon_l=0)$ – *entropy principle.* This information is not contained in the first law of thermodynamics. It results only after combining the three conservation principles (mass, momentum and energy). In a way it generalises these principles.

In the case of steady–state one–phase, $\alpha_l = 1$, incompressible, $\nabla V_l = 0$, isentropic, $P_{kl} + \epsilon_l = 0$, flow with equal velocity gradients in all directions, Taylor [119] (1935) noticed that $\epsilon_l \approx \frac{1}{2} 15 \, \nu_l \left(\frac{\partial w_l}{\partial z}\right)^2$. In this case the turbulence does not depend on the spatial direction – isentropic turbulence.

This equation is not only very informative, but very convenient for numerical integration because of its *simplicity* compared to the primitive form of the energy principle – Eq. 2.3.1. This is the reason why we chose the *specific entropies* of the velocity fields together with the concentrations of the inert component C_{nl} as *components of the dependent variables* vector as already mentioned in Chapter 2.1. This unique combination of the dependent variables simply *minimizes the computational work* during the numerical integration and therefore makes the computer code *faster* and the analysis *cheaper.* Moreover, it makes the code architecture simple and allows us to include more other physical phenomena in a general flow model.

Note that the three forms of the same equation, conservative, non conservative, and semi conservative are mathematically identical. *The introduction of the semi conservative form is perfectly suited for numerical integration because it ensures proper initialization of the value of the entropy in a computational cell in which a previously not existing field just originates.*

The flow modelling concept which makes use of the specific entropies of the velocity fields as components of the dependent variables vector, is called "*entropy concept*" in the following.

It might be useful for the understanding of the final form of the averaged entropy equation if it can be compared with the frequently used form written in terms of specific internal energy. That is why we give this form in Appendix 8.

2.5 THE MIXTURE VOLUME CONSERVATION EQUATION

Any numerical method in fluid mechanics must provide correct coupling between pressure changes and velocity changes. A very effective approach is to replace one of the mass conservation equations by a particular combination of all of them, i.e. the mixture volume conservation equation (MVCE). This equation can be directly discretized and incorporated into the numerical scheme. Another possibility is to follow the same scheme as if deriving the MVCE analytically but starting with already discretized mass conservation equations. The purpose of this section is to derive the analytical form of the MVCE, to discuss the physical meaning of every single term and finally to show what makes this equation so appropriate for use by constructing numerical schemes for complicated multiphase flows:

The MVCE was obtained as follows:

– Differentiate the mass conservation equations using the chain rule.

– Divide each equation by its particular density. The resulting equitations have dimensions $m^3/(m^3 s)$. They reflect the volume change balance of each velocity field per unit time and per unit mixture volume.

– Substitute the density derivatives using the differential form of the equation of state of each velocity field.

– Compare the so obtained equations with the concentration and the entropy equations and replace the groups

$$\alpha_l \rho_l \left(\gamma_v \frac{\partial s_l}{\partial \tau} + V_l \gamma . \nabla s_l \right) = Ds_l^N \tag{2.5.1}$$

$$\alpha_l \rho_l \left(\gamma_v \frac{\partial C_{nl}}{\partial \tau} + V_l \gamma . \nabla C_{nl}\right) = DC_{nl}^N \tag{2.5.2}$$

where

$$Ds_l^N = \nabla . (\alpha_l \rho_l D_l^s \gamma \nabla s_l) + \gamma_v (Ds_l - \mu_l^+ s_l), \tag{2.5.3}$$

$$DC_{nl}^N = \nabla . [\alpha_l \rho_l D_{nl}^* \gamma \nabla C_{nl}] + \gamma_v (\mu_{nl} - \mu_l C_{nl}). \tag{2.5.4}$$

– Add the so obtained volume conservation equations and use the fact that $\Sigma\ \alpha_l = 1$ and $\Sigma\ d\alpha_l = 0$ to cancel the sum of the time derivatives of the volume concentrations.

The final form of the MVCE is:

$$\frac{\gamma_v}{\rho a^2} \frac{\partial p}{\partial \tau} + \sum_{l=1}^{3} \frac{\alpha_l}{\rho_l a_l^2} V_l \gamma \nabla p + \nabla . \left(\sum_{l=1}^{3} \alpha_l V_l \gamma \right) = \sum_{l=1}^{3} D\alpha_l, \tag{2.5.5}$$

where

$$D\alpha_l = \gamma_v \frac{\mu_l}{\rho_l} - \frac{1}{\rho_l^2} \left(\frac{\partial \rho_l}{\partial s_l} Ds_l^N + \frac{\partial \rho_l}{\partial C_{nl}} DC_{nl}^N \right) \tag{2.5.6}$$

and

$$\frac{1}{\rho a^2} = \sum_{l=1}^{3} \frac{\alpha_l}{\rho_l a_l^2} = \frac{1}{p} \sum_{l=1}^{3} \frac{\alpha_l}{\kappa_l} = \frac{1}{\kappa p}. \tag{2.5.7}$$

is the definition equation of the velocity of sound of the "homogeneous" mixture of three velocity fields.

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

$$\frac{\gamma_v}{\kappa p}\frac{\partial p}{\partial \tau} + \sum_{l=1}^{3} \frac{\alpha_l}{\kappa_l p} V_l \gamma . \nabla p + \nabla . (\sum_{l=1}^{3} \alpha_l V_l \gamma) = \sum_{l=1}^{3} D\alpha_l , \tag{2.5.8}$$

or

$$\frac{\gamma_v}{\kappa}\frac{\partial}{\partial \tau} \ln p + \sum_{l=1}^{3} \frac{\alpha_l}{\kappa_l} V_l \gamma . \nabla \ln p + \nabla . (\sum_{l=1}^{3} \alpha_l V_l \gamma) = \sum_{l=1}^{3} D\alpha_l \tag{2.5.9}$$

or some integrated forms, where

$$\kappa = \rho a^2 / p, \tag{2.5.10}$$

$$\kappa_l = \rho_l a_l^2 / p \tag{2.5.11}$$

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

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

(a) the convective specific volume change $\nabla .(\Sigma\ \alpha_l V_l \gamma)$ of the control volume;

(b) the change of the specific volume of the mixture associated with the net specific volume change of the mixture due to the mass sources $\gamma_v \Sigma\ \mu_l / \rho_l$;

(c) density change due to the spatial pressure, entropy and concentration changes of the particular velocity fields.

For the case of negligible diffusion

$$\nabla\ [\alpha_l \rho_l D_{nl}^{*} \gamma \nabla C_{nl}] \approx 0 \tag{2.5.12}$$

$$\nabla\ (\alpha_l \rho_l D_l^{s} \gamma\ \nabla s_l) \approx 0, \tag{2.5.13}$$

the RHS of the MVCE contains no differential terms

$$D\alpha_l = \gamma_v \{ \frac{\mu_l}{\rho_l} - \frac{1}{\rho_l^2} \left[\frac{\partial \rho_l}{\partial s_l} (Ds_l - \mu_l^{+} s_l) + \frac{\partial \rho_l}{\partial C_{nl}} (\mu_{nl} - \mu_l C_{nl}) \right] \}. \tag{2.5.14}$$

This means that during the numerical integration the influence of the changes of entropies and concentrations on the creation of the pressure field can be taken into account in only one step (without outer iterations). This simplifies the program architecture extremely, speeds up the numerical integration, and therefore makes it cheaper, compared to any other approach. This is the reason to choose the MVCE equation in IVA code series instead of one of the three mass conservation equations.

This is an important difference between the entropy concept presented here that is used in the IVA code series and the concept used in all other computer codes (e.g. TRAC series [22, 23, 25, 26] (1981–1985), AFDM [49] (1990) etc.)

For completeness of the theory we give the MVCE equation in case of steady state noncompressible flow

$$\nabla.(\sum_{l=1}^{3} \alpha_l V_l \gamma) = \sum_{l=1}^{3} D\alpha_l, \quad \text{or} \quad \nabla.(J\gamma) = \sum_{l=1}^{3} D\alpha_l, \tag{2.5.16}$$

where

$$J = \sum_{l=1}^{3} \alpha_l V_l = \sum_{l=1}^{3} j_l \tag{2.5.17}$$

is the *volumetric mixture flow rate*, and

$$j_l = \alpha_l V_l \tag{2.5.18}$$

are the volumetric flow rates of the particular velocity fields. In case of neglected diffusion and no mass exchange among the velocity fields or between the flow and external sources, we have

$$\nabla.(J\gamma) = 0 \tag{2.5.19}$$

or

$$J\gamma = \text{const.} \tag{2.5.20}$$

Let us emphasise one specific property of this equation. The term

$$\sum_{l=1}^{3} \frac{\alpha_l}{\rho_l a_l^2} V_l \gamma.\nabla p \tag{2.5.21}$$

represents the dimensionless change of the density. This fact allows to use for instance *up–wind* discretization even of the pressure terms (*donor–cell* concept), because one practically discretizes the dimensionless density change in the intervals (Δr, $r\Delta\theta$, Δz).

The above–mentioned feature of this equation makes it very suitable for its coupling with the momentum equations, for derivation of one equation valid for the mixture, similar to the Poisson equation for one phase flow.

3. EQUATION OF STATE

The averaged governing equations are derived from the instantaneous equations. As already mentioned the averaging of the motion of the individual molecules by the instantaneous equations leads to loss of information on the thermodynamic behavior of the system. The lost information must be provided by the state and transport equations.

3.1 THERMODYNAMIC AND TRANSPORT PROPERTIES OF "SIMPLE" CONSTITUENTS

IVA3 uses a set of analytical approximations of the following "simple" substances: air, water, steam, uranium dioxide in solid liquid and equilibrium solid–liquid state. Alternatively, instead of approximations for the uranium dioxide properties the analytical approximations for stainless steel or corium can be used in IVA3.

For air, the Irvine and Liley [105] (1984) approximations of ρ, c_p, $h = f(T)$ and $s=s(T,p=const)$ are used where the influence of the pressure on the entropy, $-R \ln(p/p_0)$ is added, where p_0 is some reference pressure (e.g. 10^5) and R is the gas constant of air. For steam, the Irvine and Liley [105] (1984) approximations of ρ, c_p, s, $h = f(T,p)$ are used. For water, the Rivkin and Kremnevskaya [106] (1977) approximations of ρ ,c_p , $h = f(T,p)$ are used. For the metastable water, the above mentioned analytical properties of Rivkin and Kremnevskaya [106] (1977) are extrapolated taking into account the discussion by Scripov et al. [110] (1980). The water entropy as a function of temperature and pressure is computed as follows. First the saturation entropy as a function of liquid temperature is computed, $s' = s'[p'(T)]$, using analytical approximations proposed by Irvine and Liley [105] (1984) and thereafter the pressure correction $s = s(s',p'-p)$ is imposed as proposed by Gerland and Hand [113] (1989).

The Irvine and Liley [105] (1984) analytical approximations for the steam – water saturation line, $p' = p'(T)$ and $T' = T'(p)$, are used in IVA3. Consequently the Clausius – Clapeyron equation for dp'/dT was obtained by taking the first derivative of the analytical approximation with respect to the temperature.

The steam – water saturation properties are computed as a function of p and $T'(p)$ using the above mentioned approximations.

Analytical approximations to the properties ρ_l, c_p, s, $h = f(T)$ of solid and liquid uranium dioxide as proposed by Fischer, Chawla et al., Fink et al. [112, 114, 116] (1981 – 1990) are used.

We use for the solid stainless steel properties ρ, c_p ,s , $h = f(T)$ the analytical approximations proposed Chawla et al. [114] (1981) and for the liquid stainless steel properties ρ , c_p, s, $h = f(T)$ the approximations proposed by Chawla et al., Touloukian and Makita [114, 115]. For solid and liquid corium properties we modify the above mentioned two sets in order to obtain a set that is based on a mixture of UO_2 and stainless steel.

For the solid–liquid two–phase region of "liquid metal" we use the assumption of thermodynamic equilibrium within the velocity field and compute the properties as explained in Kolev [111] (1990) Ch.IV.C.

The derivatives $(\partial h/\partial p)_T$, $(\partial \rho/\partial T)_p$, $(\partial \rho/\partial p)_T$ are easily obtained by differentiating the corresponding analytical approximations.

The transport properties of the "simple" substances are computed as follows. Thermal conductivity and dynamic viscosity of air, and steam $\lambda = \lambda(T)$ – Irvine and Liley [105] (1984). The water thermal conductivity $\lambda = \lambda(T, p)$ is computed using the Rivkin and Alexandrov [108] (1975) approximation and the water dynamic viscosity $\eta = \eta(T, p)$ and surface tension $\sigma = \sigma(T)$ using the TRAC approximation, Liles et al. [109] (1981). The thermal conductivity of solid and liquid uranium dioxide and stainless steel, as well as the dynamic viscosity and surface tension of liquid uranium dioxide and steel are computed using the Chawla et al. [114] (1981) approximations. For the corium set of properties we use the transport properties of uranium dioxide.

3.2 THERMODYNAMIC PROPERTIES OF THE VELOCITY FIELDS

The velocity fields of IVA3 are by definition binary mixtures of inert and noninert components. The main assumption made in Section 1.3 is that in case of gas mixture the air and the steam possess the same field temperature T_l and obey the Dalton's law. For the binary mixture of water and microscopic solid particles, the microscopic character of the particles allows to neglect the temperature difference with respect to the surrounding water and to assume that the water and the solid particles possess the same field temperature. The solid particles in this mixture are incompressible. The needed equation of state and their derivatives $(\partial \rho_l/\partial p)_{s_l,C_{nl}}$, $(\partial \rho_l/\partial s_l)_{p,C_{nl}}$, $(\partial \rho_l/\partial C_{nl})_{p,s_l}$, $(\partial s_l/\partial p)_{T_l,C_{nl}}$, $(\partial s_l/\partial T_l)_{p,C_{nl}}$, $(\partial s_l/\partial C_{nl})_{p,T_l}$ and $(\partial T_l/\partial p)_{s_l,C_{nl}}$, $(\partial T_l/\partial s_l)_{p,C_{nl}}$, $(\partial T_l/\partial C_{nl})_{p,s_l}$ etc. are expressed as functions of p, T_l and C_{nl} by using the equation of state of the "simple" substances. Details of the general derivation for mixtures of n components are already published by the author in [111] (1990) and will not be repeated here. It is only noted that the expressions used in IVA3 are the simple cases for two components of the general expressions presented in [111] (1990) for n components.

Thermal conductivity and dynamic viscosity of the air steam mixture are computed using the mole weight method of Wilke [117] (1950).

In the framework of the entropy concept we have values of p, s_l and C_{nl} in each computational cell after each integration step. The corresponding temperature T_l is easily computed by iterations

$$T_l = T_l^{old} \exp\{[s_l - s_l^{old}(T_l^{old}, p, C_{nl})]/c_{pl}\} \qquad (3.2.1)$$

for p and C_{nl} = const. For velocity fields that have existed in the previous time level the iteration (old) starts with the old time level temperature $T_l^{old} = T_{la}$ and for just originating fields with appropriate initial values (e.g. if liquid or steam is presented – with the saturation temperature $T_l^{old} = T'(p)$). Convergence is garanteed unless one operates beyond the validity of the analytical approximations. Alternatively a method is provided in IVA3 to compute the temperature from the linearized equation of state

$$T_l = T_{la} + \left(\frac{\partial T_l}{\partial s_l}\right)_{p,C_{nl}}(s_l - s_{la}) + \left(\frac{\partial T_l}{\partial p}\right)_{s_l,C_{nl}}(p - p_a) + \left(\frac{\partial T_l}{\partial C_{nl}}\right)_{p,T_l}(C_{nl} - C_{nla}) \tag{3.2.2}$$

except in cases in which the velocity fields just originate. This possibility saves computer time.

Having the temperature, the system pressure, and the inert mass concentration we compute the steam partial pressure by means of Newton iterations

$$p_{Ml}^{new} = p_{Ml}^{old} - \frac{p - p_{Ml}^{old} - \frac{C_{nl}}{1-C_{nl}} R_{nl} T_l \rho_{Ml}}{-1 - \frac{C_{nl}}{1-C_{nl}} R_{nl} T_l \left(\frac{\partial \rho_{Ml}}{\partial p_{Ml}}\right)_{T_l}} \tag{3.2.3}$$

where

$$\rho_{Ml} \text{ and } \left(\frac{\partial \rho_{Ml}}{\partial p_{Ml}}\right)_{T_l} = f(p_{Ml}^{old}, T_l) \tag{3.2.4}$$

starting with the value

$$p_{Ml}^{old} = p \frac{1-C_{nl}}{1-C_{nl}\left(1-\frac{R_{nl}}{R_{Ml}}\right)}. \tag{3.2.5}$$

The pressures of the second and the third velocity fields are equal to the system pressure p by definition. Thus we have all what we need to compute all thermodynamic and transport properties of the "simple" constituents and consequently all mixture properties.

At different places of our development we use the following form of the equation of state

$$d\rho_l = \left(\frac{\partial \rho_l}{\partial p}\right)_{s_l,C_{nl}} dp + \left(\frac{\partial \rho_l}{\partial s_l}\right)_{p,C_{nl}} ds_l + \left(\frac{\partial \rho_l}{\partial C_{nl}}\right)_{p,s_l} dC_{nl}. \tag{3.2.6}$$

So one important group of the closure equations for IVA3 is complete.

4. NUMERICAL METHOD

4.1 WORKING FORM OF THE CONSERVATION EQUATIONS USED IN IVA3

The IVA3 models is based (a) on two of the three mass conservation equations for each velocity field, (b) on the MVCE, (c) on the three inert mass concentration equations, (d) on the three particle number density conservation equations, and finally (e) on the nine momentum equations for each velocity field and each of the three space directions. The set of the resulting 21 partial differential equations is integrated numerically under the following additional simplifying assumptions:

(1) Neglect the diffusion terms $\nabla.(\alpha_l\rho_l D^*_{nl}\gamma\nabla C_{nl})$, $\nabla.(\alpha_l\rho_l D^s_l\gamma\, \nabla s_l)$, and $\frac{\nu_l}{Sc}\nabla n_l$.

(2) Neglect the lift forces in cases of dispersed structure.

(3) Neglect the spatial part of the virtual mass forces.

(4) Neglect the turbulence effects on momentum transport.

It is simple matter to remove the first three simplifying assumptions in the code. Removing of simplification (4) needs probably long years effort from the multiphase community to provide adequate transport equations (like k–ϵ, etc, e.g. [100] (1987)) and a reliable set of closure relationships for 3D three–phase flows.

4.2 FORMULATION OF THE MATHEMATICAL PROBLEM

Let us formulate the mathematical problem to be solved:

a) The *system of* 21 *nonlinear nonhomogeneous partial differential equations with variable coefficients* describing the transient flow has to be integrated in the *three–dimensional region* R.

b) The *vector of dependent variables* is

$$U^T = (\alpha_1, \alpha_2, s_l, C_{nl}, n_l, p, u_l, v_l, w_l), \tag{4.2.1}$$

where l = 1, 2, 3.

c) The *independent variables* are the three *space coordinates* (r,θ,z) and the *time* τ

$$U=U(\tau, r, \theta, z). \tag{4.2.2}$$

d) The definition region R is *divided* through the *permeabilities* in the three directions

$(\gamma_r,\gamma_\theta,\gamma_z)$=functions of (r,θ,z), (4.2.3)

where

$0 \le (\gamma_r,\gamma_\theta,\gamma_z) \le 1$ (4.2.4)

and through the *volume porosities*

$\gamma_v=\gamma_v(r,\theta,z)$, (4.2.5)

where

$0 < \gamma_v \le 1.$ (4.2.6)

into a number of *subregions* $R_{i,j,k}$.

e) The *surface permeabilities* and the *volume porosities* are *not smooth* functions of the space coordinates in the region R.

f) *Inside the subregions* $R_{i,j,k}$, the *dependent variables are smooth functions of time and space.*

g) *Boundary conditions act on the outer boundary surfaces of the definition region as functions of time.*

h) In order to construct numerical solutions it is essential that the following sets of closure equations are defined: (1) approximations for the state and transport properties and thermodynamic derivatives, and (2) correlations modelling the heat, mass and momentum transport accross the surfaces dividing the separate velocity fields. We already provided the information needed for modeling the first group of properties in Section 3. Part II is devoted on the second group of models.

4.3 IVA3 INTEGRATION PROCEDURE

The integration procedure of IVA3 is a logical sequence of steps needed to obtain a set of dependent variables for each computational cell satisfying the conservation equations for each time step under the introduced simplifying assumptions and working hypothesis for any given class of initial and boundary conditions. We found the following procedure leading to unconditionally stable solutions:

1. Read:

(a) Logical control information;
(b) Geometry;
(c) Initial conditions;
(d) Boundary conditions;
(e) External sources;
(f) Variable permeabilities;

2. Perform:

(a) Impose actual geometry;
(b) Store old time level information;
(c) Impose boundary conditions;
(d) Impose structure heat sources;
(e) Address non–mechanical constitutive equations;

– Compute thermophysical and transport properties for simple constituents and for binary mixtures;
– Recognize the flow pattern;
– Compute energy and mass source terms for each particular cell corresponding to the recognized flow pattern;

(f) Address mechanical constitutive equations:

– Recognize flow pattern for staggered cell;
– Compute drag and virtual mass forces;

(g) Compute coefficients of the discretized momentum equations;
(h) Decouple the field momentum equations for each direction;
(k) Estimate velocities based on the old time level pressures;
(l) Impose cyclic boundary conditions in case of closed cylindrical geometry;
(m) Outer iterations:

– Estimate new $\approx s_l$, $\approx C_{nl}$, $\approx \alpha_l$; Repeat this step as many times as necessary to satisfy with prescribed accuracy all entropy and concentration equations and two of the three mass conservation equations. This step in addition to the outer iteration complex makes the IVA3 methods fully implicit.
– Compute the coefficients of the pressure equation;
– Solve the pressure equation for $\tau+\Delta\tau$;
– Perform convergence, accuracy and time step control;
– Compute velocities for $\tau+\Delta\tau$;
– Impose cyclic boundary conditions;
– Compute s_l, C_{nl}, α_l for $\tau+\Delta\tau$;
– Control convergence;
– Control general accuracy requirements, if not fulfilled perform the next outer iteration; if no convergence is achieved reduce time step, recover the old time level situation and repeat the outer iterations until convergence is achieved;

– Perform the next outer iterations until all general accuracy requirements are satisfied;

(n) Perform temperature inversion;
(o) Optimize time step for the next integration step;
(p) Perform as many time steps as required to reach the prescribed process time;

3. Write restart information for prescribed step frequency, before prescribed CPU time is reached, and at the end of the simulation.

Next we describe the discretization of the system of 21 partial equations and the analytical reduction to the linearized pressure equation.

4.3.1 SPACE DISCRETIZATION, LOCATION OF THE DISCRETE VARIABLES AND DISCRETIZATION IF THE MASS CONSERVATION EQUATIONS

The *flow is defined in the domain* shown in Figure 3. The (IM+2)(JM+2)(KM+2) elementary cells have the form depicted in Figure 4. We introduce the following integer indices for r direction, i = 1, IM+2, for θ direction, j = 1, JM+2, and for z direction k = 1, KM+2 denoting the location of the variables used. The *cell boundaries* are defined by the following coordinates r_h, θ_h, z_h. The *dimensions of the elementary cells* Δr, $\Delta\theta$, Δz are a result of a *non–uniform space discretization.* The *cell centres have the coordinates* r, θ, z. The *distances between the cell centres* are Δr_h, $\Delta\theta_h$, Δz_h. The *dependent variables* (α_l, C_{nl}, s_l, p, n_l,), the *state and the transport properties* T_l, ρ_l, ν_l, λ_l etc., and the *volumetric porosity are located in the cell centres.*

To achieve a simple and transparent code architecture, we use the usual *layer of surrounding fictitious cells* (see Fig. 3): i=1 and i=IM+2; j=1 and j=JM+2; k=1 and k=KM+2. The *boundary conditions* as time functions are applied in these cells. This practice ensures a *uniform* integration procedure per time step for the inner cells.

The *surface permeabilities* γ_r, γ_θ, γ_z, and the *velocity components* u_l, v_l, w_l *are located in the walls* as shown in Fig. 4. So all dependent field variables are defined at the cell center and all flow variables are defined at the surface at the cell. This forms the so–called staggered grid system that is extensively used in fluid mechanics. The reader can find the considerations leading to the definition of the pressure and velocities in different space locations for instance by Issa in [118] (1983). For the example of the limiting case of the steady state momentum equation having convective and diffusion terms and a pressure gradient, Issa shows that the location of the above mentioned variables at the same point and the use of discretization schemes of the first order of accuracy leads to unphysical (chequer–board) oscillations. The staggered grid system is not necessarily needed if high order discretization methods are used.

Note, that the *surface permeability is a tensor* with nine components. γ_r, γ_θ and γ_z are its diagonal elements. For the construction of numerical schemes the other 6 components are needed too. For this purpose the definition of the surface permeabilities γ_r^c, γ_θ^c and γ_z^c in the centre of the elementary cell, shown in Fig. 4, is necessary.

If the surface permeability between two neighbouring cells is equal to zero, no mass can be transferred between them in the direction perpendicular to the surface.

As a consequence of the definition of the velocity location on the cell surface and the homogeneization of the other properties inside the cell, *the mass leaving the cell has the properties of the cell.* This is called further *donor–cell concept* – Harlow [5] (1971).

All field variables have three indices, i, j and k. For simplicity, we omit writing the indeces except in the case where one of them is to be distinguished from i,j,k. For example $p_{i,j,k+1}$ is replaced by p_{k+1}.

The *old time variables* obtain an index "a". The time variables not indicated with "a" are either in the *new time plane* or are the best available guesses for the new time plane.

Further we denote with m=1 through 6 the cells i+1, i–1, j+1, j–1, k+1 and k–1, respectively, surrounding the cell (i,j,k).

For convenience of the notation we define the normal velocities to the surfaces of each computational cell as follows

$$(V_1^n)^T = (u_1, -u_{1,i-1}, v_1, -v_{1,j-1}, w_1, -w_{1,k-1}). \qquad (4.3.1.1)$$

These velocities are positive defined if directed from the control volume to the environment.

4.3.2 FINITE DIFFERENCES APPROXIMATIONS OF THE EQUATIONS DESCRIBING THE TRANSPORT OF THE FIELD PROPERTIES

The purpose of this Section is to show *how to compute the scalar properties of each velocity field*, except the pressure, *in the new time level knowing the corresponding properties in the old time level.*

There are several methods for discretizing the *equations of convection–diffusion type*. The reader can find valuable ideas in the publications of Chow et al. [120] (1984), Patel et al. [121] (1985), Patel et al. [122] (1986). For *multiphase flows* we use one of the widely used methods: the *donor–cell* method. Thise method is *numerically unconditionally stable.*

As already shown in the previous Chapters the *conservative* form of the conservation equations contain terms like

$$\ldots\frac{\partial}{\partial z}(F\,\Phi - \Gamma\,\frac{\partial \Phi}{\partial z}) = \ldots \qquad (4.3.2.1)$$

for each of the three space coordinates. F is the *mass flow* of the field in z direction. We denote with Φ generally *some qualitative characteristics* of the flow. Γ reflects the *diffusion* properties of the field. Remember, that differentiating the convective terms and comparing them with the corresponding field mass conservation equation multiplied by Φ, leads to a considerably simpler form

$$\ldots\, F\,\frac{\partial \Phi}{\partial z} - \frac{\partial}{\partial z}(\Gamma\,\frac{\partial \Phi}{\partial z})\ldots \quad [\equiv \ldots\frac{\partial}{\partial z}(F\,\Phi - \Gamma\,\frac{\partial \Phi}{\partial z}) - \Phi\,\frac{\partial F}{\partial z}]. \qquad (4.3.2.2)$$

The subject of our further consideration is the discretization of the above combination of terms. In order to use the definition location of F, i.e. the boundary of the elementary cell, we discretize the primary form

$$\ldots\,\frac{\partial}{\partial z}(F\,\Phi - \Gamma\,\frac{\partial \Phi}{\partial z}) - \Phi\,\frac{\partial F}{\partial z}. \qquad (4.3.2.3)$$

For this purpose we need an *assumption* for the *profile form of $\Phi=\Phi(z)$ along the space coordinate z.* The *linear profile of Φ is the simplest possible assumption* for the character of this function. In this case after having discretized the *convective* terms by means of the *donor–cell* principle – Courant et al. [123] (1952), and the *diffusion* terms by means of *central finite differences*

$$\frac{1}{\Delta z}[F_6\{\tfrac{1}{2}[1+\text{sign}(F_6)]\Phi \;+ \tfrac{1}{2}[1-\text{sign}(F_6)]\Phi_{k+1}\} - \frac{\Gamma_6}{\Delta z_h}(\Phi_{k+1}-\Phi)]$$

$$-\frac{1}{\Delta z}[F_5\{\tfrac{1}{2}[1+\text{sign}(F_5)]\Phi_{k-1} + \tfrac{1}{2}[1-\text{sign}(F_5)]\Phi \;\} - \frac{\Gamma_5}{\Delta z_{h,k-1}}(\Phi-\Phi_{k-1})]$$

$$-\frac{1}{\Delta z}\Phi(F_6-F_5)\ldots \tag{4.3.2.4}$$

and taking into account

$$\tfrac{1}{2}[1+\text{sign}(F)]-1=-\tfrac{1}{2}[1-\text{sign}(F)] \tag{4.3.2.5}$$

$$\tfrac{1}{2}[1-\text{sign}(F)]-1=-\tfrac{1}{2}[1+\text{sign}(F)] \tag{4.3.2.6}$$

we obtain

$$-\frac{1}{\Delta z}[-F_6\{\tfrac{1}{2}[1-\text{sign}(F_6)]+\frac{\Gamma_6}{\Delta z_h}\}(\Phi_{k+1}-\Phi)$$

$$-\frac{1}{\Delta z}[\;F_5\{\tfrac{1}{2}[1+\text{sign}(F_5)]+\frac{\Gamma_5}{\Delta z_{h,k-1}}\}(\Phi_{k-1}-\Phi)$$

$$= (b_{k+1} + b_{k-1})\,\Phi - b_{k-1}\,\Phi_{k-1} - b_{k+1}\,\Phi_{k+1}. \tag{4.3.2.7}$$

Note an important property of the linearized coefficients b_{k-1}, b_{k+1}, namely that they are *not negative* $b_{k-1}\ge 0$, $b_{k+1}\ge 0$. Therefore: (a) Increasing of $\Phi_{k\pm1}$ in the locations neighbouring to k leads to increasing of Φ and vice versa; (b) If the coefficients $b_{k\pm1}$ are equal to zero (e.g. due to $\gamma_{z,k\pm1}=0$), the gradient $\Phi_{k\pm1}-\Phi$ cannot influence the value of Φ.

The coefficient b contains information for the *time constant of the propagation of a disturbance of* Φ, namely $\Delta\tau \approx \Delta z/$(convective + diffusion velocity). Therefore the *limitation of the time step* is associated with the *material velocity* of the quality Φ.

The above method is appropriate in cases, where the condition

$$Pe = \frac{F\Delta z_h}{\Gamma} < 2, \quad \text{Patankar [124] (1980)} \tag{4.3.2.8}$$

is satisfied. The local grid *Peclet number*, Pe, is the *ratio* of the amounts of the property Φ transported by *convection* and *diffusion*, respectively. Large values of Pe, e.g. $|Pe| > 10$, mean predominating convection and small values mean predominating diffusion. For onedimensional processes without sources of Φ and with predominant convection, the linearization of the profile lead to overestimation of the diffusion component of the flow. This is characteristic for *coarse meshes*, leading to $|Pe| > 10$. This consideration leads some investigators to look for a more realistic profile of the function $\Phi = \Phi(z)$ as a base for construction of discretization schemes without a strong upper limitation of the mesh size.

It is beyond of the scope of this paper to discuss all existing methods from one–phase fluid mechanics that are potential candidates for solving the problem discussed here. We confine ourselves to first–order donor–cell for the convective terms for the following reasons:

(a) Consistency in the high order discretization needs weighted averaging of the source terms along a prescribed number of cells, which is an extremely complicated matter in multiphase flow due to the possibility of existence of different flow patterns in different cells at the same time.

(b) During the IVA–Code development the numerics was kept simple deliberately in order to concentrate attention on the related physical models.

Now we discretize the mass conservation equation for each velocity field using the donor–cell concept and introduce some abbreviations which will be used in the following

$$\frac{\alpha_l\rho_l\gamma_v-(\alpha_l\rho_l\gamma_v)_a}{\Delta\tau}+\sum_m[b_{lm+}\alpha_l\rho_l-b_{lm-}(\alpha_l\rho_l)_m]-\gamma_v\mu_l=0, \qquad (4.3.2.9)$$

where

$$b_{lm+}=\beta_m\xi_{lm+}V^n_{lm}\geq 0, \qquad (4.3.2.10)$$

$$b_{lm-}=-\beta_m\xi_{lm-}V^n_{lm}\geq 0, \qquad (4.3.2.11)$$

$$\xi_{lm+}=\frac{1}{2}[1+\mathrm{sign}(V^n_{lm})], \qquad (4.3.2.12)$$

$$\xi_{lm-}=1-\xi_{lm+}. \qquad (4.3.2.13)$$

It is advisable to estimate the geometry coefficients

$$\beta_1=\frac{r_h^\kappa\gamma_r}{r^\kappa\Delta r},\ \beta_2=\frac{(r_h^\kappa\gamma_r)_{i-1}}{r^\kappa\Delta r},\ \beta_3=\frac{\gamma_\theta}{r^\kappa\Delta\theta},\ \beta_4=\frac{\gamma_{\theta,j-1}}{r^\kappa\Delta\theta},\ \beta_5=\frac{\gamma_z}{\Delta z},\ \beta_6=\frac{\gamma_{z,k-1}}{\Delta z},$$

once at the beginning of the actual simulation. If there is a change of the geometry during the time considered, it is advisable to perform corrections only for those elementary cells where this is necessary. Normally such cells are a small part of the whole cell number.

4.3.3 FORMULATION OF THE ALGEBRAIC PROBLEM FOR CONVECTION EQUATIONS

Now let us discretize the equation of the type of the entropy equation following the procedure already described in the previous Chapter

$$\alpha_{la}\rho_{la}\gamma_v\frac{s_l-s_{la}}{\Delta\tau}-\sum_m b_{lm}(s_{lm}-s_l)+\gamma_v\mu_l^+ s_l=\gamma_v Ds_l, \tag{4.3.3.1}$$

where

$$b_{lm}=b_{lm-}(\alpha_l\rho_l)_m.$$

Further for the simplicity of the notation we denote i+1, i–1, j+1, j–1, k+1, k–1 with 1...6, respectively.

The coefficients b_{11} through b_{16} consist of two characteristic components:

1) They contain a *geometrical* part $\beta_1...\beta_6$.

2) The *convective* part of the coefficients does not depend on whether we compute one of the variables s_l, C_{nl}. It is advisable in the general cycle to compute them once at the beginning of the cycle.

Flow convectively leaving the cell, $b_{lm}=0$, does not influence the specific properties (e.g. the entropy) of the velocity field in the donor cell. Only input flows, $b_{lm} > 0$, can influence the specific properties of the field in the acceptor cells (if they have specific properties different of those of the acceptor cell, $s_{ml} \neq s_l$).

4.3.4 PHYSICAL MEANING OF THE NECESSARY CONVERGENCE CONDITION FOR MULTIPHASE FLOW

Writing for each point (i,j,k) one algebraic equation 1 we obtain a *system of algebraic equations* for all s_l. This system has a special 7 diagonal symmetric structure. *The coefficients matrix is positive defined.* A possible method for its solution is the *iteration method of Gauss–Seidel* in one of its several variants. The *necessary condition for convergence* of this method is the *predominance of the elements on the main diagonal* compared to the other elements

$$|b_l| \geq \Sigma|b_{lm}| \quad \text{for all equations,} \tag{4.3.4.1}$$

$$|b_l| > \Sigma|b_{lm}| \quad \text{at least for one equation.} \tag{4.3.4.2}$$

This is the well known *Scarbourough criteron* [125] (1958). Because this is only a necessary condition, convergence is possible even if the criterion is *violeted.* But satisfaction of this condition gives the confidence, that this algebraic system can be solved *at least with one iteration method* [124] (1980). Having in mind that all of the elements of the sum

$$b = \gamma_v(\alpha_{1a}\rho_{1a}/\Delta\tau+\mu_1^+) + \sum_{m=1}^{6} b_{lm} \tag{4.3.4.3}$$

are not negative, the Scarbourough criterion is reduced to

$$\gamma_v(\alpha_{1a}\rho_{1a}/\Delta\tau+\mu_1^+) \geq 0 \quad \text{for all equations} \tag{4.3.4.4}$$

$$\gamma_v(\alpha_{1a}\rho_{1a}/\Delta\tau+\mu_1^+) > 0 \quad \text{at least for one equation.} \tag{4.3.4.5}$$

If $\alpha_{1a}>0$ at least for one elementary cell, the above conditions are always satisfied. If the velocity field 1 is missing in the integration domain, $\alpha_{1a}=0$ for all cells, it is necessary that $\mu_1^+ > 0$ at least for one single point.

Let us look at the Scarbourough criterion from another point of view. Supposing that the properties belonging to the flow leaving the cell are known in the new time level and that the properties belonging to the flow entering the cell are the best guesses for the new time level, and solving Eq. 4.3.316 with respect to s_l we obtain

$$s_l = \frac{\gamma_v(\alpha_{1a}\rho_{1a}s_{1a}/\Delta\tau+Ds_1) + \sum_{m=1}^{6} b_{lm}s_{lm}}{\gamma_v(\alpha_{1a}\rho_{1a}/\Delta\tau+\mu_1^+) + \sum_{m=1}^{6} b_{1m}}. \tag{4.3.4.6}$$

This result is similar to the use of the *point Jakobi method* for the solution of the above equation. This method consists of a successive visiting of all cells in the definition domain so many times as necessary to reduce the improvement of the solution from iteration to iteration below a prescribed small value. For a known space velocity distribution this method works without problem. Even though the method has the lowest convergence velocity compared to other existing methods, it illustrates an important feature, namely the *computation of the initial values of the field properties if the field occurs inside the actual time step,* $\alpha_{1a} = 0$, i.e.

$$s_l = \frac{\gamma_v Ds_1 + \sum_{m=1}^{6} b_{1m}s_{lm}}{\gamma_v\mu_1^+ + \sum_{m=1}^{6} b_{1m}}, \tag{4.3.4.7}$$

for

$$\gamma_v\mu_1^+ + \sum_{m=1}^{6} b_{lm} > 0. \tag{4.3.4.8}$$

Note that we do not need an initial value for s_{la} in this case. The velocity field can originate in several possible ways, e.g.

a) without convection and diffusion

$$s_l = Ds_l/\mu_l^+; \tag{4.3.4.9}$$

b) without source terms in the cell

$$s_l = \frac{\sum\limits_{m=1}^{6} b_{lm} s_{lm}}{\sum\limits_{m=1}^{6} b_{lm}}. \tag{4.3.4.10}$$

The *Scarbourough criterion is not satisfied if*

$$\gamma_v \left(\frac{\alpha_{la}\rho_{la}}{\Delta\tau} + \mu_l^+\right) + \sum_{m=1}^{6} b_{lm} = 0 \quad \text{for all cells.} \tag{4.3.4.11}$$

But in this case s_l is undefined in accordance with Eq. 4.3.4.6. With other words this criterion is an expression of the simple consideration that *if*

– the field does not exist in the entire integration domain and
– will not originate in the time step
its specific properties, like entropy etc., are undefined.

Remark: For the construction of the numerical method it is necessary to set the *initial values* of the field properties at least one time before starting the simulations in order to avoid multiplication with undefined numbers $\alpha_{la}\rho_{la}s_{la}/\Delta\tau$ in the computer. If during the transient the field disappears, it will retain its specific properties from the last time step. *If the field originates, its specific properties are obtained automatically by averaging the specific properties of the entering flows with weighting coefficients equal to the corresponding mass flow divided by the net mass flow into the cell, governed* by Eq. 4.3.4.6. In this case the old value of the specific properties (like s_{la} etc.) *does not influence the result.*

4.3.5 IMPLICIT TREATMENT OF THE MECHANICAL INTERACTION

Applying a spatial pressure difference on a multifield mixture with different field densities results in relative motion among the fields. The relative motion between two adjacent fields causes different forces on the interfaces. We postulate in IVA3 the following form of the drag and the virtual mass forces

$$f_{cd}^d = -(\alpha_d\rho_c\bar{c}_{cd}^d \tfrac{3}{4}/D_d)\,|\Delta V_{cd}|\,(V_c-V_d) = -c_{cd}^d\,(V_c-V_d) \tag{4.3.5.1}$$

$$f_{cd}^{vm} = -\alpha_d \rho_c \bar{c}_{cd}^{vm} \frac{\partial}{\partial \tau} (V_c - V_d) = -c_{cd}^{vm} \frac{\partial}{\partial \tau} (V_c - V_d) \tag{4.3.5.2}$$

where c stays for continuous and d for disperse. For convenience we define interaction coefficients having cd = 12, 21, 31, 13, 32, 23. Usually, to model a particular flow pattern needs only two of them greater than zero (e.g. bubble–liquid three phase flow, cd = 21, 23). To model the flow–structure interaction we postulate the following form of the force

$$f_{wc}^{d} = c_{wc}^{d} |V_c| V_c \tag{4.3.5.3}$$

where c=1,2,3. Usually, to model one particular flow pattern needs only one of them (e.g. bubble–liquid three phase flow, c = 2).

The coupling coefficients between the velocity fields correspond to each of the flow patterns modeled. For some of them the coupling is strong e.g. bubble–liquid in others not so strong, e.g. large diameters droplets–gas. In any case the coupling is nonlinear and after discretization must be resolved by iterations.

The way we do that in IVA3 is:

(a) Discretize the momentum equations.

(b) Linearize the nonlinear terms and write for each direction a system of three algebraic equations with respect to the field velocities.

(c) Solve with respect to the velocities.

(d) Use the so obtained three equations to construct the pressure–velocity coupling.

We call this method partial decoupling of the momentum equations (PDME). Note the difference between this procedure and the decoupling procedure used in COBRA–TF where the decoupling is performed with a lower degree of implicitness and solving for the directional mass flow rates instead for the velocities.

We demonstrate the method used in IVA3 in a simple example which will be extended later. We consider three momentum equations in r–directions neglecting all spatial derivatives except ∇p:

$$\alpha_l \rho_l \frac{\partial u_l}{\partial \tau} + \alpha_l \nabla p + \alpha_l \rho_l g_u - \sum_{\substack{m=1 \\ m \neq l}}^{3} [\bar{c}_{ml}^{d} (u_m - u_l) + \bar{c}_{ml}^{vm} \frac{\partial}{\partial \tau} (u_m - u_l) + \mu_{ml} (u_m - u_l)]$$

$$- \mu_{Al} (u_{Al} - u_l) - \mu_{lA} (u_{lA} - u_l) + c_{ul} |u_l| u_l = 0. \tag{4.3.5.4}$$

Note that by definition, if one velocity field does not exists, $\alpha_l = 0$, the coeffitions describing its coupling with the other fields are equal to zero, $\bar{c}_{lm}^{d} = 0$, $\bar{c}_{lm}^{vm} = 0$.

We discretize the time derivative an rewrite Eq. 4.3.5.4 in the following form

$$\left[\frac{\alpha_l \rho_l}{\Delta\tau} + c_{lu}|u_l| + a^*_{ll} - \sum_{\substack{m=1\\ m\neq l}}^{3} (a_{ml}-\mu_{ml})\right] u_l + \sum_{\substack{m=1\\ m\neq l}}^{3} (a_{ml}-\mu_{ml})\, u_m = b_l + b^*_l - \alpha_l \nabla p, \tag{4.3.5.5}$$

where

$$a^*_{ll} = \mu_{Al} - \mu_{lA}, \tag{4.3.5.6}$$

$$b^*_l = \mu_{Al} u_{Al} - \mu_{lA} u_{lA}, \tag{4.3.5.7}$$

and consider all velocities u_l in the new time plane (implicit formulation). We repeat this procedure for each of the velocity fields in the chosen direction. The so obtained system of algebraic equations with respect to the velocities $U^T=(u_1, u_2, u_3)$

$$A\, U = B - \alpha \nabla p, \quad \text{where} \quad \alpha^T = (\alpha_1, \alpha_2, \alpha_3) \tag{4.3.5.8}$$

can easily be solved with respect to the velocities provided $\det|A| \neq 0$. The result is

$$U = dU - RU\, \nabla p \tag{4.3.5.9}$$

where

$$dU = A^{-1} B \tag{4.3.5.10}$$

$$RU = A^{-1} \alpha. \tag{4.3.5.11}$$

Note an important property of the diagonal elements

$$\left[\frac{\alpha_l \rho_l}{\Delta\tau} + c_{lu}|u_l| + a^*_{ll} - \sum_{\substack{m=1\\ m\neq l}}^{3} (a_{ml}-\mu_{ml})\right] \tag{4.3.5.12}$$

of the matrix A: If the m–th diagonal element is zero this means that in that time the velocity field m does not exists and will not originate in the next time step. So the rank of the matrix is reduced by one. Even if the field m does not exist but just originates in the actual time step, the diagonal element is not zero and the initial velocity is induced properly.

One can easily extend this method even taking into account the spatial derivatives in the Eq. 4.3.5.5, extending the terms a^*_{ll} and b^*_l. The solution procedure is the same. Obviously, if one neglects all convective terms and mass sources no initial value for the not existing field can be defined.

In case of neglected convection, diffusion and mass source terms, the matrix A is symmetric and the expressions for the relative velocities are getting very simple.

4.3.6 DISCRETIZATION OF THE MOMENTUM EQUATIONS

The conservative form of the momentum equations without taking into acount turbulence effects, see Appendix 8 and Figure 5, can be simplified by differentiation of the convective terms and comparison with the mass conservation equations. Instead of discretizing the resulting system directly we derive the discretized working form of the momentum equations through the following steps:

1. Discretize the conservative form of the momentum equation (implicit).
2. Discretize the mass conservation equation for the same velocity field (implicit).
3. Multiply the thus obtained equation by u_l.
4. Subtract the thus obtained equation from the discretized momentum equation.

The result is given in Appendix 9 and rewriten in the following compact form here

$$\left[\frac{\alpha_{lau}\rho_{lau}}{\Delta\tau} + a^*_{ll} - \sum_{\substack{m=1\\ m\neq l}}^{l_{max}} (a_{ml}-\mu_{mlu})\right] u_l + \sum_{\substack{m=1\\ m\neq l}}^{l_{max}} (a_{ml}-\mu_{mlu})\, u_m =$$

$$b_l + b^*_l - \alpha_{lua}\frac{1}{\Delta r_h}\frac{\gamma_r}{\gamma_{vu}}(p_{i+1}-p). \tag{4.3.6.1}$$

We repeat this process for the chosen number of the velocity fields. The result is a system of algebraic equations with respect to the velocities with the same structure as that derived in the previous section. The a_l and b_l terms reflect the actions of the drag and of the added mass forces. The a^*_l and b^*_l terms reflect the actions of the spatial inertia and viscous forces. As in the previous section we solve this system with respect to each velocity and obtain finally

$$u_l = du_l - RU_l\,(p_{i+1}-p). \tag{4.3.6.2}$$

Again we emphasize the important property of the extended diagonal elements (multiplied by $\Delta\tau/\rho_{lau}$)

$$\alpha_{lau} + \left[a^*_{ll} - \sum_{\substack{m=1\\ m\neq l}}^{l_{max}} (a_{ml} - \mu_{mlu})\right] \Delta\tau/\rho_{lau} \tag{4.3.6.3}$$

of the matrix: If the m–th diagonal element is zero this means that in that time the velocity field does not exist and in the next time step will not originate. So the rank of the matrix is reduced by one. Even if the field does not exist but will originate in the next time step by convection, by mass transfer from the neighboring field, from other mass sources, or by an arbitrary combination of these three processes, the diagonal element is not zero and the initial velocity is induced properly.

As already mentioned we call this step of the IVA3 solution method partial decoupling of the momentum equations (PDME). The PDME is important for constructing a stable numerical algorithm even by first order donor cell discretization of the convective terms.

We derive the discretized working form of the momentum equations in the other two directions analogously to Eq. 3.4.6.1. The corresponding control volumes are shown in Figs. 6 and 7. The result is

$$v_l = dv_l - RV_l\,(p_{j+1}-p) \tag{4.3.6.4}$$

$$w_l = dw_l - RW_l\,(p_{k+1}-p). \tag{4.3.6.5}$$

This general structure of the Eq. 4.3.6.1 is perfectly suited for testing the code by introducing the mechanical effects step by step.

The thus obtained form of the momentum equations

$$V^n_{lm} = dV^n_{lm} - RVel_{lm}\,(p_m-p), \tag{4.3.6.6}$$

is further used to construct the algebraic problem for computing the pressure field. Here

$$(dV^n_l)^T = (du_l, -du_{l,i-1}, dv_l, -dv_{l,j-1}, dw_l, -dw_{l,k-1}), \tag{4.3.6.7}$$

$$(RVel_l)^T=(RU_l, RU_{l,i-1}, RV_l, RV_{l,j-1}, RW_l, RW_{l,k-1}). \tag{4.3.6.8}$$

Remember that the normal velocities

$$(V^n_l)^T=(u_l,-u_{l,i-1},v_l,-v_{l,j-1},w_l,-w_{l,k-1}), \tag{4.3.6.9}$$

are defined positive if directed from the control volume to the environment on each of the six surfaces (m) of the computational cell.

4.3.7 DERIVATION OF THE PRESSURE EQUATION

The mixture volume conservation equation, derived in Ch. 2.5 can be discretized directly using the donor–cell concept as already done in IVA2 [39] (1986).

In order to assure *full compatibility of the discretized pressure equation with the discretized mass conservation equations* we prefer here to derive the discretized pressure equation from the discretized mass conservation equations performing the same transformation as already described in Section 2.5. The result is

$$\gamma_v\,(\sum_l \frac{\alpha_l}{\rho_{la}a^2_{la}})\,\frac{p-p_a}{\Delta\tau} + \sum_l \frac{1}{\rho_{la}} \sum_m \beta_m[\xi_{lm+}\alpha_l\rho_l+\xi_{lm-}\alpha_{lm}\rho_{lm}]\,V^n_{lm} = \sum_l D\alpha_l - \frac{\gamma_v-\gamma_{va}}{\Delta\tau},$$

(4.3.7.1)

where

$$D\alpha_l = \frac{\gamma_v}{\rho_{la}} \{\mu_l - \alpha_l [(\frac{\partial \rho_l}{\partial s_l})_a \frac{s_l - s_{la}}{\Delta \tau} + (\frac{\partial \rho_l}{\partial C_{nl}})_a \frac{C_{nl} - C_{nla}}{\Delta \tau}]\}. \tag{4.3.7.2}$$

Replacing the normal velocities V^n_{lm} by means of the momentum equation we obtain finally the pressure equitation used in IVA3:

$$c\,p + \sum_m c_m p_m = d, \tag{4.3.7.3}$$

where

$$c = \frac{\gamma_v}{\Delta \tau} (\sum_l \frac{\alpha_l}{\rho_{la} a^2_{la}}) - \sum_m c_m , \tag{4.3.7.4}$$

$$c_m = -\beta_m \sum_l \frac{1}{\rho_{la}} [\xi_{lm+} \alpha_l \rho_l + \xi_{lm-} \alpha_{lm} \rho_{lm}]\, RVel_{lm}, \tag{4.3.7.5}$$

$$d = \frac{\gamma_v}{\Delta \tau} (\sum_l \frac{\alpha_l}{\rho_{la} a^2_{la}})\, p_a - \frac{\gamma_v - \gamma_{va}}{\Delta \tau} + \sum_l \{ D\alpha_l - \frac{1}{\rho_{la}} \sum_m \beta_m [\xi_{lm+} \alpha_l \rho_l + \xi_{lm-} \alpha_{lm} \rho_{lm}]\, dV^n_{lm}\}. \tag{4.3.7.6}$$

Writing this equation for each particular cell we obtain a system of (IM)(JM)(KM) algebraic equations with respect to the pressure in the new time plane. The coefficients matrix has the expected 7 diagonal (7 points) symmetric structure with garanteed diagonal dominance – see equation 4. The system coefficients are continuous nonlinear functions of the solutions of the system. Therefore the system is nonlinear. We solve this system by one of the 4 SOR methods built in the IVA3 code. The four methods in IVA3 differ in the volume of the computational work for the direct solution during the iterations. The first three methods solve directly the pressure equation plane by plane (rectangle, cylinder, circle) and the fourth performs strongly coupling between pressure and velocity along one line (line by line). Depending on the geometry of the problem which has to be simulated the user can choose one of the four methods.

4.3.8 COMPUTATION OF THE FIELD VOLUMETRIC FRACTIONS

After solving our general system with respect to the part of the dependent variable vector (s_l, C_{nl}, p, u, v, w), the *densities* can be easily calculated after the temperature inversion as shown in Section . Having the densities, it is a straightforward matter to update the *volume fractions* from the $l_{max}-1$ *independent mass conservation equations* . If we consider the field variables $\alpha_l\rho_l$ in the convective terms flowing out of the elementary cell in the new time plane and $\alpha_l\rho_l$ in the neighbouring cells as the best available guess in the new time plane during the iterative procedure, we can solve directly with respect to $\alpha_l\rho_l$.

$$\overline{\alpha_l\rho_l} = \mathrm{ALRZ}/\mathrm{ALRN}, \qquad (4.3.8.1)$$

where

$$\mathrm{ALRZ} = \gamma_{va}\,[\mu_l + \frac{(\alpha_l\rho_l)_a}{\Delta\tau}] + \sum_{m=1}^{6} b_{lm-}(\alpha_l\rho_l)_m, \qquad (4.3.8.2)$$

$$\mathrm{ALRN} = \frac{\gamma_v}{\Delta\tau} + \sum_{m=1}^{6} b_{lm+} > 0. \qquad (4.3.8.3)$$

The thus–obtained equation divided by the density ρ_l is

$$\overline{\alpha_l} = \overline{\alpha_l\rho_l}/\rho_l. \qquad (4.3.8.4)$$

As we already used the *sum of the mass conservation equations for the derivation of the pressure equation* only $l_{max}-1$ equations remain *independent.* Therefore we have to use only $l_{max}-1$ mass conservation equations for the computation of $l_{max}-1$ *volumetric fractions.* The simplest but the *worst* possible choice is the direct calculation

$$\alpha_m = \overline{\alpha_m} \qquad m = 1, l_{max} - 1 \qquad (4.3.8.5)$$

from the $l_{max} - 1$ mass equations. This problem, recognized by Spalding [127] (1981) for two velocity fields, was confirmed by the numerous numerical experiments made by the author during the development of the IVA2 three velocity field code. The reason is the similarity of the quantitative information contained in the pressure equation and in the gas mass conservation equation, due to the strong difference between the compressibilities of the gas and the other velocity fields. This is the reason for using such a combination of the mass equations, which differs from that already used for the derivation of the pressure equation. A possible choice could be

$$\alpha_m = c_m\overline{\alpha_m} + (1 - c_m)\,(1 - \sum_{l \neq m} \overline{\alpha_l}) \qquad (4.3.8.6)$$

Guidelines for choosing the multiplier c_m are based on physical reasoning. *c_m has to be chosen so as to allow the nonexistent velocity field to arise in the course of the calculation.* A good choice is

$$c_m = 1 - \alpha_m. \tag{4.3.8.7}$$

Even in case of $\alpha_m=0$, the m'th mass conservation equation is used to calculate α_m, so that the velocity field non–existing at the beginning of the time step can arise either by convection or diffusion through the elementary cell surfaces, or through mass transfer from the neighbouring velocity fields or by some combination of all mechanism. Substituting c_m from Eq. 4.3.8.7 into Eq. 4.3.8.6 and solving with respect to α_m, we obtain

$$\alpha_m = \overline{\alpha_m}/\Sigma\overline{\alpha_l}. \tag{4.3.8.8}$$

Setting $l_{max} = 2$ and $c_l = 1/2$, we get the method used by Carver [128] (1984), Carver and Salcudean [129] (1986), or $l_{max} = 2$ and $c_l = 1-\alpha_l$ the method used by Spalding [127] (1981). In fact the above equation generalizes the existing experience for two velocity fields and is useful for l_{max} velocity fields.

4.3.9 INITIAL AND BOUNDARY CONDITIONS

At the beginning of the integration of the system, all components of the dependent variables must be initialized. These may be previously calculated values describing a *steady state*. The practicing engineer usually creates his own library of such steady state solutions for the particular geometry studied before starting to simulate the processes of interest. There are many applications, where the steady state solution is of particular interest. Therefore, for the initial computation of the steady state itself *initial data* are needed which have to be *assigned explicitly*. In order to reach the steady state saving computer time, it is advisable to bear in mind the following two principles:

- No sudden changes of the dependent variables, e.g. shock waves etc., should be included in the initial conditions except in cases where they exist in the process studied, because the computer time needed to reach the steady state can be considerably greater than the computer time needed to simulate the transient process studied;

- If steady state has to be reached by time marching (simulation of a transient process), e.g. coolant acceleration by switching on of pumps, switching on of the heat source in the flow, for instance a nuclear reactor, etc., the boundary conditions have to be formulated with such time constants, which are characteristic for the real nature of the technical processes. Replacing them with step functions is only theoretically admissible. Nonrealistic boundary conditions can excite the dependent variables into states outsides of their definition regions, which means that further integration is impossible.

The *criteria for reaching the steady state* have to be economically reasonable with respect to the maximum achievable accuracy at all. For this purpose it is enough if the solution does not depend on time in the framework of the minimum achievable error band or if the solution reaches values quasi steadyly oscillating around a constant.

The definition of the geometrical structures through surface permeabilities and volumetric porosities is very convenient for the description even of complicated geometries. In this way particular volumes can be isolated from other volumes by nonpermeable surfaces (*walls*). We suggest that the velocity vector in such walls is zero, which means that its three components are zero (*non–slip condition*).

The *computation region is surrounded by a layer of fictitious auxiliary cells* I = 1, I = IM+2 K = 1 K = KM+2.

For their *dependent variables the values of the neighbouring inner cells are assigned* (if nothing else is prescribed).

The fictitious layers in the azimuthal direction J = 1 and J = JM+1 are *overlapping* with the layers J=JM+1 and J=2, respectively, so that the corresponding parameters are *directly assigned* from J=JM+1 and J=2 to J=1 and J=JM+2, respectively (*cyclic boundary condition*). A useful consequence of this strategy is the possibility to model symmetric sectors, where in the corresponding symmetry plane the surface permeabilities have simply to be set to zero.

Additional *boundary conditions* can be specified in the following way:

1. First the cells in which the boundary condition acts are defined by their integer indices. Next the type of the boundary condition is specified.

2. A physically meaningful combination of boundary conditions can be specified, for example (a) p, C_{nl}, α_l, T_l; (b) $u_l(v_l=0, w_l=0)$ or $v_l(u_l=0, w_l=0)$ or $w_l(u_l=0, v_l=0)$; (c) p; (d) $u_l=a$ (mixture sound velocity).

Boundary condition (a) can be used if one expects inflow into the computational region. This boundary condition must be completed with the boundary condition (b) if $u_l < 0$. Boundary condition (a) can be used alone in the case of outflow from the computational region to the outside. In this case, the flow has the parameter of the donor cell.

Only when boundary conditions (b) and (d) are used, we set the terms of the discretized momentum equations $du_l=u_{lRB}$, $RU_l=0$ in order to define $u_l=u_{lRB}$.

Useful ideas about how to use *nonconflicting combinations* of the boundary conditions can be found in the theory of the *method of characteristics* for integration of hyperbolic systems – see for instance Chapter 4 of Kolev [39] (1986).

4.3.10 TIME STEP AND ACCURACY CONTROL

A time step limitation dictated by the linear stability analysis for implicit donor–cell methods is used in IVA3

$$\Delta\tau_{CFL} < \max\left(\frac{\Delta r_h}{u_l}, \frac{r_h \Delta\theta_h}{v_l}, \frac{\Delta z_h}{w_l}\right) \text{ for all cells.} \tag{4.3.10.1}$$

This is the so called material Courant, Friedrichs and Levi (MCFL) criterion. Numerous numerical experiments show that the code can work in many cases with much higher time steps. Nevertheless the MCFL criterion is retained to ensure convergence in all cases. In addition to this limitation there are two reasons leading to further time step limits: (a) linearization limits, (b) definition limits for the dependent variables:

(a) Linearization limits:

While slow running physical processes are successfully simulated using only the MCFL criterion, for fast running processes more care is needed to ensure time step control leading to unconditional stability. That is why time step control leading to successful numerical integration of initial and boundary conditions leading to fast running processes with dramatical changes of the dependent variables can successfully handle also initial and boundary conditions leading to slow running processes. The opposite may, but must not be true.

The change of the dependent variables within an time step in each computational cell should not exceed a prescribed values

$$\Delta\tau^{p}_{max} < \frac{\gamma_v - \gamma_{va} + \gamma_v \left(\sum\limits_l \frac{\alpha_l}{\rho_{la} a_{la}^2}\right) \Delta p_{max}}{\sum\limits_l \{D\alpha_l - \ldots\} - \sum\limits_m c_m (p_{ma} - p_a)}, \tag{4.3.10.2}$$

$$\Delta\tau^{s}_{max} < \frac{\alpha_{la} \rho_{la} \Delta s_{lmax} \gamma_v}{\gamma_v [D s_l - \mu_l^{+} (s_{la} + \Delta s_{lmax})] + \sum\limits_{m=1}^{6} b_{lm} (s_{lam} - s_{la})}, \tag{4.3.10.3}$$

$\Delta\tau^{C}_{max}$ similar to the above equation.

These conditions are associated with the linearization of the strongly nonlinear system of 21 PDE's and the state equations for each time step, which is not considered in the classical von Neumann linear stability analysis of 1D numerical schemes for differential equations with constant coefficients.

From eq. 4.3.10.3 we see that for $\alpha_{la} \to 0$ any heat transfer from or to the velocity field leads to $\Delta\tau \to 0$ which hinders the further integration. This problem can be avoided if one simply defines a vector $\alpha_{\epsilon l}$ so that for $\alpha_l < \alpha_{\epsilon l}$ energy balance is no more used.

(b) Definition limits for the dependent variables:

The velocity field mass is non negative

$$\Delta\tau^{\alpha}_{\max} < \frac{\alpha^*_l \rho_l \gamma_v - (\alpha_l \rho_l \gamma_v)_a}{\gamma_v \mu_l - \sum\limits_m (b_{lm+} \alpha^*_l \rho_l - b_{lm-} (\alpha_l \rho_l)_m}, \qquad (4.3.10.4)$$

where $\alpha^*_l = 0$ for decreasing volumetric fraction, $\overline{\alpha_l} < \alpha_{la}$. For increasing volumetric fraction, $\overline{\alpha_l} > \alpha_{la}$ the volumetric fraction of the velocity field cannot exceed the value of one by definition, $\alpha^*_l = 1$.

Further we check the overall mass conservation as follows: After a successful number of outer iterations leading to convergence and reduction of the pressure and velocity increments below prescribed values, the densities computed after the temperature inversion together with the volume fractions are used to compute the mixture density $\rho = \Sigma\ \alpha_l \rho_l$. The mixture density ρ^* is computed from the mixture mass conservation equation

$$\frac{\rho^* \gamma_v - \rho_a \gamma_{va}}{\Delta\tau} \ldots = \ldots \qquad (4.3.10.5)$$

and thereafter the normalized error is estimated as

$$\Delta\rho = \frac{\rho - \rho^*}{\rho}.$$

The outer iterations are considered as successfully finished if pressure and velocity increments from iteration to iteration and the relative mass conservation error $\Delta\rho$ reach values smaller than the prescribed ones.

Additional time step optimization is imposed in order to have only a prescribed number of outer iterations, e.g. 6.

APPENDIX 1 Scalar Notation of the Momentum Equations.

In the scalar notation of the momentum equations, we use the universal form for Cartesian and cylindrical coordinates (κ=0 rectangular, κ=1 cylindrical).

r–direction:

$$\frac{\partial}{\partial\tau}(\alpha_l\rho_l u_l\gamma_v) + \frac{1}{r^\kappa}\frac{\partial}{\partial r}[r^\kappa\alpha_l(\rho uu+\tau_{rr})_l\gamma_r] + \frac{1}{r^\kappa}\frac{\partial}{\partial\theta}[\alpha_l(\rho vu+\tau_{\theta r})_l\gamma_\theta] + \frac{\partial}{\partial z}[\alpha_l(\rho wu+\tau_{zr})_l\gamma_z]$$

$$-\frac{\kappa}{r}\alpha_l(\rho vv+\tau_{\theta\theta})_l\gamma_\theta + \alpha_l\gamma_r\frac{\partial p}{\partial r} + (\alpha_l\rho_l g_r+f_{rl})\gamma_v = \gamma_v[\mu_{Al}u_{Al}-\mu_{lA}u_l+\sum_{m=1}^{l_{max}}(\mu_{ml}u_m-\mu_{lm}u_l)].$$

(A1.1)

θ–direction:

$$\frac{\partial}{\partial\tau}(\alpha_l\rho_l v_l\gamma_v) + \frac{1}{r^\kappa}\frac{\partial}{\partial r}[r^\kappa\alpha_l(\rho uv+\tau_{r\theta})_l\gamma_r] + \frac{1}{r^\kappa}\frac{\partial}{\partial\theta}[\alpha_l(\rho vv+\tau_{\theta\theta})_l\gamma_\theta] + \frac{\partial}{\partial z}[\alpha_l(\rho wv+\tau_{z\theta})_l\gamma_z]$$

$$+\frac{\kappa}{r}\alpha_l(\rho vu+\tau_{r\theta})_l\gamma_\theta + \alpha_l\gamma_\theta\frac{1}{r^\kappa}\frac{\partial p}{\partial\theta} + (\alpha_l\rho_l g_\theta+f_{\theta l})\gamma_v$$

$$=\gamma_v[\mu_{Al}v_{Al}-\mu_{lA}v_l+\sum_{m=1}^{l_{max}}(\mu_{ml}v_m-\mu_{lm}v_l)]. \tag{A1.2}$$

z–direction:

$$\frac{\partial}{\partial\tau}(\alpha_l\rho_l w_l\gamma_v) + \frac{1}{r^\kappa}\frac{\partial}{\partial r}[r^\kappa\alpha_l(\rho uw+\tau_{rz})_l\gamma_r] + \frac{1}{r^\kappa}\frac{\partial}{\partial\theta}[\alpha_l(\rho vw+\tau_{\theta z})_l\gamma_\theta] + \frac{\partial}{\partial z}[\alpha_l(\rho ww+\tau_{zz})_l\gamma_z]$$

$$+\alpha_l\gamma_z\frac{\partial p}{\partial z} + (\alpha_l\rho_l g_z+f_{zl})\gamma_v = \gamma_v[\mu_{Al}w_{Al}-\mu_{lA}w_l+\sum_{m=1}^{l_{max}}(\mu_{ml}w_m-\mu_{lm}w_l)].$$

(A1.3)

Note that in the scalar notation of the momentum equations in case of cylindrical coordinates the centrifugal and Coriolis forces arise. The *centrifugal force* = $\frac{\kappa}{r}\alpha_l\rho_l v_l v_l\gamma_\theta$ gives the effective force in r–direction resulting from fluid motion in the θ–direction, and the *Coriolis force* = $\frac{\kappa}{r}\alpha_l\rho_l v_l u_l\gamma_\theta$ is an effective force in the θ–direction when there is flow in both the r– and θ–directions. We see the components of the viscous stress tensor, $\tau_{\theta\theta l}$ and $\tau_{r\theta l}$ corresponding to these forces and acting in the opposite directions.

APPENDIX 2 Viscous Stress Components

$$\tau_{rr}=-\eta[2\frac{\partial u}{\partial r}-\frac{2}{3}(\nabla.V)], \qquad (A2.1)$$

$$\tau_{\theta\theta}=-\eta[2(\frac{1}{r^{\kappa}}\frac{\partial v}{\partial\theta}+\kappa\frac{u}{r})-\frac{2}{3}(\nabla.V)], \qquad (A2.2)$$

$$\tau_{zz}=-\eta[2\frac{\partial w}{\partial z}-\frac{2}{3}(\nabla.V)], \qquad (A2.3)$$

$$\tau_{r\theta}=\tau_{\theta r}=-\eta[r^{\kappa}\frac{\partial}{\partial r}(\frac{v}{r^{\kappa}})+\frac{1}{r^{\kappa}}\frac{\partial u}{\partial\theta}], \qquad (A2.4)$$

$$\tau_{\theta z}=\tau_{z\theta}=-\eta(\frac{\partial v}{\partial z}+\frac{1}{r^{\kappa}}\frac{\partial w}{\partial\theta}), \qquad (A2.5)$$

$$\tau_{zr}=\tau_{rz}=-\eta(\frac{\partial w}{\partial r}+\frac{\partial u}{\partial z}), \qquad (A2.6)$$

$$(\nabla.V)=\frac{1}{r^{\kappa}}\frac{\partial}{\partial r}(r^{\kappa}u)+\frac{1}{r^{\kappa}}\frac{\partial v}{\partial\theta}+\frac{\partial w}{\partial z}. \qquad (A2.7)$$

The first subscript of the components of the *viscous stress tensor* denotes the coordinate perpendicular to the plane where the stress is acting. The second subscript denotes the positive direction of the stress component itself.

APPENDIX 3 Scalar Notation of the Averaged Momentum Equations

r–direction

$$\frac{\partial}{\partial\tau}(\alpha_1\rho_1u_1\gamma_v)+\frac{1}{r^{\kappa}}\frac{\partial}{\partial r}[r^{\kappa}\alpha_1(\rho uu+\rho u'u'+\tau_{rr})_1\gamma_r]+\frac{1}{r^{\kappa}}\frac{\partial}{\partial\theta}[\alpha_1(\rho vu+\rho v'u'+\tau_{\theta r})_1\gamma_\theta]$$

$$+\frac{\partial}{\partial z}[\alpha_1(\rho wu+\rho w'u'+\tau_{zr})_1\gamma_z]-\frac{\kappa}{r}\alpha_1(\rho vv+\rho v'v'+\tau_{\theta\theta})_1\gamma_\theta+\alpha_1\gamma_r\frac{\partial p}{\partial r}+(\alpha_1\rho_1g_r+f_{r1})\gamma_v$$

$$=\gamma_v[\mu_{A1}u_{A1}-\mu_{1A}u_1+\sum_{m=1}^{l_{max}}(\mu_{m1}u_m-\mu_{1m}u_1)], \qquad (A3.1)$$

θ–direction

$$\frac{\partial}{\partial\tau}(\alpha_1\rho_1v_1\gamma_v)+\frac{1}{r^{\kappa}}\frac{\partial}{\partial r}[r^{\kappa}\alpha_1(\rho uv+\rho u'v'+\tau_{r\theta})_1\gamma_r]+\frac{1}{r^{\kappa}}\frac{\partial}{\partial\theta}[\alpha_1(\rho vv+\rho v'v'+\tau_{\theta\theta})_1\gamma_\theta]$$

$$+\frac{\partial}{\partial z}[\alpha_l(\rho wv+\rho w'v'+\tau_{z\theta})_l\gamma_z] + \frac{\kappa}{r}\alpha_l(\rho vu+\rho v'u'+\tau_{r\theta})_l\gamma_\theta + \alpha_l\gamma_\theta\frac{1}{r^\kappa}\frac{\partial p}{\partial \theta} + (\alpha_l\rho_l g_\theta+f_{\theta l})\gamma_v$$

$$=\gamma_v[\mu_{Al}v_{Al}-\mu_{lA}v_l+\sum_{m=1}^{l_{max}}(\mu_{ml}v_m-\mu_{lm}v_l)], \tag{A3.2}$$

z–direction

$$\frac{\partial}{\partial \tau}(\alpha_l\rho_l w_l\gamma_v) + \frac{1}{r^\kappa}\frac{\partial}{\partial r}[r^\kappa\alpha_l(\rho uw+\rho u'w'+\tau_{rz})_l\gamma_r] + \frac{1}{r^\kappa}\frac{\partial}{\partial \theta}[\alpha_l(\rho vw+\rho v'w'+\tau_{\theta z})_l\gamma_\theta]$$

$$+\frac{\partial}{\partial z}[\alpha_l(\rho ww+\rho w'w'+\tau_{zz})_l\gamma_z] + \alpha_l\gamma_z\frac{\partial p}{\partial z} + (\alpha_l\rho_l g_z+f_{zl})\gamma_v$$

$$=\gamma_v[\mu_{Al}w_{Al}-\mu_{lA}w_l+\sum_{m=1}^{l_{max}}(\mu_{ml}w_m-\mu_{lm}w_l)]. \tag{A3.3}$$

APPENDIX 4 Scalar Notation of the Components of the Reynolds Stress Tensor

$$\rho u'u'=-\eta^t[2\frac{\partial u}{\partial r}-\frac{2}{3}(\nabla.V+k)] \tag{A4.1}$$

$$\rho v'v'=-\eta^t[2(\frac{1}{r^\kappa}\frac{\partial v}{\partial \theta}+\kappa\frac{u}{r})-\frac{2}{3}(\nabla.V+k)] \tag{A4.2}$$

$$\rho w'w'=-\eta^t[2\frac{\partial w}{\partial z}-\frac{2}{3}(\nabla.V+k)] \tag{A4.3}$$

$$\rho u'v'=\rho v'u'=-\eta^t[r^\kappa\frac{\partial}{\partial r}(\frac{v}{r^\kappa})+\frac{1}{r^\kappa}\frac{\partial u}{\partial \theta}] \tag{A4.4}$$

$$\rho v'w'=\rho w'v'=-\eta^t(\frac{\partial v}{\partial z}+\frac{1}{r^\kappa}\frac{\partial w}{\partial \theta}) \tag{A4.5}$$

$$\rho w'u'=\rho u'w'=-\eta^t(\frac{\partial w}{\partial r}+\frac{\partial u}{\partial z}), \tag{A4.6}$$

APPENDIX 5 Scalar Components of the Drag Force

$$f_{ud}^d=-\alpha_d\rho_c\frac{1}{D_d}\frac{3}{4}c_{ud}^d(u_c-u_d)|u_c-u_d|, \tag{A5.1}$$

$$f^{d}_{vd}=-\alpha_{d}\rho_{c}\,\frac{1}{D_{d}}\,\frac{3}{4}c^{d}_{vd}(v_{c}-v_{d})|v_{c}-v_{d}|, \tag{A5.2}$$

$$f^{d}_{wd}=-\alpha_{d}\rho_{c}\,\frac{1}{D_{d}}\,\frac{3}{4}c^{d}_{wd}(w_{c}-w_{d})|w_{c}-w_{d}|. \tag{A5.3}$$

APPENDIX 6 Scalar Componets of the Lift Force

$$[[V_{d}-V_{c}]x[\nabla xV_{c}]]_{r}=(v_{d}-v_{c})[\frac{1}{r^{\kappa}}\,\frac{\partial}{\partial r}(r^{\kappa}v)-\frac{1}{r^{\kappa}}\,\frac{\partial u}{\partial \theta}]_{c}-(w_{d}-w_{c})(\frac{\partial u}{\partial z}-\frac{\partial w}{\partial r})_{c}, \tag{A6.1}$$

$$[[V_{d}-V_{c}]x[\nabla xV_{c}]]_{\theta}=(w_{d}-w_{c})[\frac{1}{r^{\kappa}}\,\frac{\partial w}{\partial \theta}-\frac{\partial v}{\partial z}]_{c}-(u_{d}-u_{c})[\frac{1}{r^{\kappa}}\,\frac{\partial}{\partial r}(r^{\kappa}v)-\frac{1}{r^{\kappa}}\,\frac{\partial u}{\partial \theta}]_{c} \tag{A6.2}$$

$$[[V_{d}-V_{c}]x[\nabla xV_{c}]]_{z}=(u_{d}-u_{c})(\frac{\partial u}{\partial z}-\frac{\partial w}{\partial r})_{c}-(v_{d}-v_{c})[\frac{1}{r^{\kappa}}\,\frac{\partial w}{\partial \theta}-\frac{\partial v}{\partial z}]_{c}, \tag{A6.3}$$

APPENDIX 7 Scalar Components of the Virtual Mass Force

$$[V_{d}\cdot\nabla\cdot(V_{c}-V_{d})]_{r}=u_{d}\,\frac{\partial}{\partial r}(u_{c}-u_{d})+v_{d}\,[\frac{1}{r^{\kappa}}\,\frac{\partial}{\partial \theta}(u_{c}-u_{d})-\kappa\frac{v_{c}-v_{d}}{r^{\kappa}}]+w_{d}\,\frac{\partial}{\partial z}(u_{c}-u_{d}), \tag{A7.1}$$

$$[V_{d}\cdot\nabla\cdot(V_{c}-V_{d})]_{\theta}=u_{d}\,\frac{\partial}{\partial r}(v_{c}-v_{d})+v_{d}\,[\frac{1}{r^{\kappa}}\,\frac{\partial}{\partial \theta}(v_{c}-v_{d})+\kappa\frac{u_{c}-u_{d}}{r^{\kappa}}]+w_{d}\,\frac{\partial}{\partial z}(v_{c}-v_{d}), \tag{A7.2}$$

$$[V_{d}\cdot\nabla\cdot(V_{c}-V_{d})]_{z}=u_{d}\,\frac{\partial}{\partial r}(w_{c}-w_{d})+v_{d}\,\frac{1}{r^{\kappa}}\,\frac{\partial}{\partial \theta}\,(w_{c}-w_{d})+w_{d}\,\frac{\partial}{\partial z}(w_{c}-w_{d}). \tag{A7.3}$$

APPENDIX 8 Specific Internal Energy Equation

As already explained in the previous Chapter the use of the specific entropies as components of the dependent variable vector, the entropy concept, gives the simplest form of the mathematical description of the flow. The use of any other state variables instead of the entropies makes the description more complicated. In case that the engineer has in his personal library approximations of the state variables and transport properties in terms e.g. of the specific internal energy, the entropy equation 2.4.1.17 should be rewritten in terms of the specific internal energy. Next we will show how to do that. With similar transformations one can rewrite the entropy equation in any other form e.g. in terms of the specific enthalpy.

Using Eqs. 2.4.1.1, 2, 10, 16 the nonaveraged Eq. 2.4.1.16 receives the following form

$$\frac{\partial}{\partial\tau}[(\sum_{i=1}^{i_{max}} \alpha_{il}\rho_{il}e_{il})\gamma_v]+\nabla.[(\sum_{i=1}^{i_{max}} \alpha_{il}\rho_{il}e_{il}V_{il})\gamma]+\sum_{i=1}^{i_{max}} p_{il}\,[\frac{\partial}{\partial\tau}(\alpha_{il}\gamma_v)+\nabla.(\alpha_{il}V_{il}\gamma)]$$

$$-\gamma_v[\sum_{i=1}^{i_{max}} \mu_{il}(e_{il}+\frac{p_{il}}{\rho_{il}})]-\nabla.[(\alpha_l\lambda_l^l\,\nabla T_l)\gamma]+\alpha_l\gamma.(\tau:\nabla V)_l=\gamma_v q_l. \tag{A8.1}$$

or

$$\frac{\partial}{\partial\tau}(\alpha_l\rho_l e_l\gamma_v)+\nabla.(\alpha_l\rho_l e_l V_l\gamma)+p\,[\frac{\partial}{\partial\tau}(\alpha_l\gamma_v)+\nabla.(\alpha_l V_l\gamma)]-\gamma_v(\sum_{i=1}^{i_{max}} \mu_{il}h_{il})$$

$$-\nabla.[\alpha_l\rho_l(c_p\frac{\nu_l^l}{Pr_l}\nabla T_l+\sum_{i=1}^{i_{max}} e_{il}D_{il}^l\nabla C_{il})\gamma]-\sum_{i=1}^{i_{max}} p_{il}\,\nabla.(\alpha_{il}D_{il}^l\frac{1}{C_{il}}\nabla C_{il}\gamma)$$

$$+\alpha_l\gamma.(\tau:\nabla V)_l=\gamma_v q_l. \tag{A8.2}$$

where

$$\alpha_l\rho_l e_l=\sum_{i=1}^{i_{max}} \alpha_{il}\rho_{il}e_{il}. \tag{A8.3}$$

In order to obtain the averaged form of the above equation we introduce Eq. 2.4.2.1 and average the so obtained equation (for simplicity we drop the averaging sign). The result is

$$\frac{\partial}{\partial\tau}(\alpha_l\rho_l e_l\gamma_v)+\nabla.(\alpha_l\rho_l e_l V_l\gamma)+p\,[\frac{\partial}{\partial\tau}(\alpha_l\gamma_v)+\nabla.(\alpha_l V_l\gamma)]-\gamma_v(\sum_{i=1}^{i_{max}} \mu_{il}h_{il})$$

$$-\nabla.[\alpha_l\rho_l(c_p \frac{\nu_l^l}{Pr_l}\nabla T_l + \sum_{i=1}^{i_{max}} e_{il} D_{il}^l \nabla C_{il})\gamma] - \sum_{i=1}^{i_{max}} p_{il}\, \nabla.(\alpha_{il} D_{il}^l \frac{1}{C_{il}} \nabla C_{il}\gamma)$$

$$+ \nabla.(\alpha_l\rho_l e_l V_l'\gamma) + p\, \nabla.(\alpha_l V_l'\gamma) = \gamma_v(q_l + q_l^t) + \alpha_l\rho_l(P_{kl} + \epsilon_l). \qquad (A8.4)$$

APPENDIX 9. Scalar Notation of the Conservative Form of the Momentum Equations Without Taking into Acount Turbulence Effects.

r direction:

$$\frac{\partial}{\partial \tau}(\alpha_l\rho_l u_l\gamma_v) + \frac{1}{r^\kappa}\frac{\partial}{\partial r}[r^\kappa\, \alpha_l\rho_l(u_l u_l - \nu_l \frac{\partial u_l}{\partial r})\gamma_r] + \frac{1}{r^\kappa}\frac{\partial}{\partial \theta}[\alpha_l\rho_l(v_l u_l - \nu_l \frac{1}{r^\kappa}\frac{\partial u_l}{\partial \theta})\gamma_\theta]$$

$$-\frac{\kappa}{r}\,\alpha_l\rho_l[v_l v_l - \frac{2}{r^\kappa}(\nu_l \frac{\partial v_l}{\partial \theta} + \nu_l u_l)]\gamma_\theta + \frac{\partial}{\partial z}[\alpha_l\rho_l(w_l u_l - \nu_l \frac{\partial u_l}{\partial z})\gamma_z]$$

$$+\alpha_l\gamma_r \frac{\partial p}{\partial r} + (\alpha_l\rho_l g_r + f_{ul})\gamma_v = \gamma_v[\mu_{Al}u_{Al} - \mu_{lA}u_{lA} + \sum_{m=1}^{l_{max}}(\mu_{ml}u_{ml} - \mu_{lm}u_l)] + f_{\nu ul}$$

$$(A9.1)$$

where

$$f_{\nu ul} = \frac{1}{r^\kappa}\frac{\partial}{\partial r}(r^\kappa\, \alpha_l\rho_l\nu_l \frac{\partial u_l}{\partial r}\gamma_r) + \frac{1}{r^\kappa}\frac{\partial}{\partial \theta}[\alpha_l\rho_l\nu_l r^\kappa \frac{\partial}{\partial r}(\frac{v_l}{r})\gamma_\theta] + \frac{\partial}{\partial z}(\alpha_l\rho_l\nu_l \frac{\partial w_l}{\partial r}\gamma_z)$$

$$-\frac{2}{3}\frac{1}{r^\kappa}\{\frac{\partial}{\partial r}[r^\kappa(\alpha_l\rho_l\nu_l\nabla.V_l)\gamma_r] - (\alpha_l\rho_l\nu_l\nabla.V_l)\gamma_\theta\}; \qquad (A9.2)$$

θ direction

$$\frac{\partial}{\partial \tau}(\alpha_l\rho_l v_l\gamma_v) + \frac{1}{r^\kappa}\frac{\partial}{\partial r}[r^\kappa\, \alpha_l\rho_l(u_l v_l - \nu_l \frac{\partial v_l}{\partial r})\gamma_r] + \frac{1}{r^\kappa}\frac{\partial}{\partial \theta}[\alpha_l\rho_l(v_l v_l - \nu_l \frac{1}{r^\kappa}\frac{\partial v_l}{\partial \theta}]\gamma_\theta]$$

$$+\kappa\frac{\alpha_l\rho_l}{r^\kappa}[v_l u_l - r^\kappa\nu_l \frac{\partial}{\partial r}(\frac{v_l}{r}) - \nu_l \frac{1}{r^\kappa}\frac{\partial u_l}{\partial \theta}]\gamma_\theta + \frac{\partial}{\partial z}[\alpha_l\rho_l(w_l v_l - \nu_l \frac{\partial v_l}{\partial z})\gamma_z]$$

$$+\alpha_l\gamma_\theta \frac{1}{r^\kappa}\frac{\partial p}{\partial \theta} + (\alpha_l\rho_l g_\theta + f_{vl})\gamma_v = \gamma_v[\mu_{Al}v_{Al} - \mu_{lA}v_{lA} + \sum_{m=1}^{l_{max}}(\mu_{ml}v_{ml} - \mu_{lm}v_l)] + f_{\nu vl}$$

$$(A9.3)$$

where

$$f_{\nu v l}=\frac{1}{r^{\kappa}}\frac{\partial}{\partial r}\left[\alpha_l\rho_l\left(\nu_l\frac{\partial u_l}{\partial\theta}-\nu_l v_l\right)\gamma_r\right]+\frac{1}{r^{\kappa}}\frac{\partial}{\partial\theta}\left[\alpha_l\rho_l\frac{1}{r^{\kappa}}\left(\nu_l\frac{\partial v_l}{\partial\theta}+2\nu_l u_l\right)\gamma_\theta\right]+\frac{\partial}{\partial z}\left(\alpha_l\rho_l\nu_l\frac{1}{r^{\kappa}}\frac{\partial w_l}{\partial\theta}\gamma_z\right)$$

$$-\frac{2}{3}\frac{1}{r^{\kappa}}\frac{\partial}{\partial\theta}\left[(\alpha_l\rho_l\nu_l\nabla.V_l)\gamma_\theta\right]; \qquad \text{(A9.4)}$$

z–direction

$$\frac{\partial}{\partial\tau}(\alpha_l\rho_l w_l\gamma_v)+\frac{1}{r^{\kappa}}\frac{\partial}{\partial r}\left[r^{\kappa}\alpha_l\rho_l\left(u_l w_l-\nu_l\frac{\partial w_l}{\partial r}\right)\gamma_r\right]+\frac{1}{r^{\kappa}}\frac{\partial}{\partial\theta}\left[\alpha_l\rho_l\left(v_l w_l-\frac{1}{r^{\kappa}}\nu_l\frac{\partial w_l}{\partial\theta}\right)\gamma_\theta\right]$$

$$+\frac{\partial}{\partial z}\left[\alpha_l\rho_l\left(w_l w_l-\nu_l\frac{\partial w_l}{\partial z}\right)\gamma_z\right]+\alpha_l\gamma_z\frac{\partial p}{\partial z}+(\alpha_l\rho_l g_z+f_{wl})\gamma_v=$$

$$\gamma_v\left[\mu_{Al}w_{Al}-\mu_{lA}w_{lA}+\sum_{m=1}^{l_{max}}(\mu_{ml}w_{ml}-\mu_{lm}w_l)\right]+f_{\nu wl} \qquad \text{(A9.5)}$$

where

$$f_{\nu w}=\frac{1}{r^{\kappa}}\frac{\partial}{\partial r}\left(r^{\kappa}\alpha_l\rho_l\nu_l\frac{\partial u_l}{\partial z}\gamma_r\right)+\frac{1}{r^{\kappa}}\frac{\partial}{\partial\theta}\left(\alpha_l\rho_l\nu_l\frac{\partial v_l}{\partial z}\gamma_\theta\right)+\frac{\partial}{\partial z}\left(\alpha_l\rho_l\nu_l\frac{\partial w_l}{\partial z}\gamma_z\right)-\frac{2}{3}\frac{\partial}{\partial z}\left[(\alpha_l\rho_l\nu_l\nabla.V_l)\gamma_z\right]$$

$$(\nu_l\nabla.V_l)=\nu_l\left[\frac{1}{r^{\kappa}}\frac{\partial}{\partial r}(r^{\kappa}u_l)+\frac{1}{r^{\kappa}}\frac{\partial v_l}{\partial\theta}+\frac{\partial w_l}{\partial z}\right]. \qquad \text{(A9.6)}$$

APPENDIX 10. Discretized Momentum Equations in r–direction.

$$\gamma_{vu}\alpha_{lua}\rho_{lua}\frac{u_l-u_{la}}{\Delta\tau}$$

$$+\frac{\dfrac{r_{i+1}^{\kappa}}{(r+\Delta r_h/2)^{\kappa}\Delta r_h}\left\{\min[0,(\alpha_l\rho_l u_l\gamma)_1]-(\alpha_l\rho_l\nu_l\gamma_1)_1\dfrac{1}{\Delta r_{i+1}}\right\}(u_{li+1}-u_l)}{bu_{l1}}$$

$$-\frac{\dfrac{r^{\kappa}}{(r+\Delta r_h/2)^{\kappa}\Delta r_h}\left\{\max[0,(\alpha_l\rho_l u_l\gamma)_2]+(\alpha_l\rho_l\nu_l\gamma)_2\dfrac{1}{\Delta r}\right\}(u_{li-1}-u_l)}{bu_{l2}}$$

$$+\underbrace{\frac{1}{(r+\Delta r_h/2)^{\kappa}\Delta\theta}\{\min[0,(\alpha_l\rho_l v_l\gamma)_3]-(\alpha_l\rho_l\nu_l\gamma)_3]\ \frac{1}{r_h^{\kappa}\Delta\theta_h}\}}_{bu_{13}}(u_{lj+1}-u_l)$$

$$-\underbrace{\frac{1}{(r+\Delta r_h/2)^{\kappa}\Delta\theta}\{\max[0,(\alpha_l\rho_l v_l\gamma)_4]+(\alpha_l\rho_l\nu_l\gamma)_4]\ \frac{1}{r_h^{\kappa}\Delta\theta_{h,j-1}}\}}_{bu_{14}}(u_{lj-1}-u_l)$$

$$+\underbrace{\frac{1}{\Delta z}\{\min[0,(\alpha_l\rho_l w_l\gamma)_5]-(\alpha_l\rho_l\nu_l\gamma)_5]\ \frac{1}{\Delta z_h}\}(u_{lk+1}-u_l)}_{bu_{l5}}$$

$$-\underbrace{\frac{1}{\Delta z}\{\max[0,(\alpha_l\rho_l w_l\gamma)_6]+(\alpha_l\rho_l\nu_l\gamma)_6]\ \frac{1}{\Delta z_{h,k-1}}\}}_{bu_{l6}}(u_{lk-1}-u_l)$$

$$-\frac{\sin(\Delta\theta/2)}{(r+\Delta r_h/2)^{\kappa}\Delta\theta}\{[(\alpha_l\rho_l v_l\gamma_\theta)_3 v_{l3}]+[(\alpha_l\rho_l v_l\gamma_\theta)_4 v_{l4}]$$

$$-\frac{2}{(r+\Delta r_h/2)^{\kappa}}\{(\alpha\rho\nu)_{l3}[(\frac{\partial v_l}{\partial\theta})_3+u_{l3}]\gamma_3+(\alpha\rho\nu)_{l4}[(\frac{\partial v_l}{\partial\theta})_4+u_{l4}]\gamma_4\ \}\}$$

$$+\frac{\gamma_{lua}}{\Delta r_h}(p_{i+1}-p)+\gamma_{vu}(\alpha_{lua}\rho_{ua}g_r+c_{lu}|u_l|u_l+f_{ul})=$$

$$\gamma_{vu}[\mu_{Alu}(u_{Al}-u_l)-\mu_{lAu}(u_{lA}-u_l)+\sum_{\substack{m=1\\ m\neq l}}^{l_{max}}\mu_{mlu}(u_m-u_l)]+\underset{\approx 0}{f_{\nu ul}} \tag{A10.1}$$

or

$$[\frac{\alpha_{lau}\rho_{lau}}{\Delta\tau}+a_{ll}^{*}-\sum_{\substack{m=1\\ m\neq l}}^{l_{max}}(a_{ml}-\mu_{mlu})]\,u_l+\sum_{\substack{m=1\\ m\neq l}}^{l_{max}}(a_{ml}-\mu_{mlu})\,u_m=$$

$$b_l+b_l^{*}-\alpha_{lua}\frac{1}{\Delta r_h}\frac{\gamma_r}{\gamma_{vu}}(p_{i+1}-p) \tag{A10.2}$$

where

$$a_{ll}^{*} = c_{lu}|u_l| + \mu_{Alu} - \mu_{lAu} - \frac{1}{\gamma_{vu}} \sum_{m=1}^{6} bu_{lm} \qquad (A9.3)$$

$$b_l^{*} = \mu_{Alu} u_{Al} - \mu_{lAu} u_{lA} - \frac{1}{\gamma_{vu}} (\overline{R}_{ul} + \sum_{m=1}^{6} bu_{lm} u_{lm}), \qquad (A10.4)$$

$$\overline{R}_{ul} = -\frac{\sin(\Delta\theta/2)}{(r+\Delta r_h/2)^{\kappa}\Delta\theta}\{[(\alpha_l\rho_l v_l \gamma_\theta)_3 v_{l3}] + [(\alpha_l\rho_l v_l \gamma_\theta)_4 v_{l4}]$$

$$- \frac{2}{(r+\Delta r_h/2)^{\kappa}}\{(\alpha\rho\nu)_{l3}[(\frac{\partial v_l}{\partial\theta})_3 + u_{l3}]\gamma_3 + (\alpha\rho\nu)_{l4}[(\frac{\partial v_l}{\partial\theta})_4 + u_{l4}]\gamma_4 \}\}.$$

$$(A10.5)$$

We derive the discretized working form of the momentum equations in the other two directions analogously to Eq. 4.3.6.1. The corresponding control volumes are shown in Figs. 6 and 7. The result is

$$[\frac{\alpha_{lav}\rho_{lav}}{\Delta\tau} + a_{ll}^{*} - \sum_{\substack{m=1\\ m\neq l}}^{l_{max}} (a_{ml} - \mu_{mlv})]\, v_l + \sum_{\substack{m=1\\ m\neq l}}^{l_{max}} (a_{ml} - \mu_{mlv})\, v_m =$$

$$b_l + b_l^{*} - \alpha_{lva} \frac{1}{r\Delta\theta_h} \frac{\gamma_\theta}{\gamma_{vv}} (p_{j+1} - p) \qquad (A10.6)$$

where

$$a_{ll}^{*} = c_{lv}|v_l| - \frac{1}{\gamma_{vu}} \sum_{m=1}^{6} bv_{lm} + \mu_{Alv} - \mu_{lAv} \qquad (A10.7)$$

$$b_l^{*} = \mu_{Alv} v_{Al} - \mu_{lAv} v_{lA} - \frac{1}{\gamma_{vv}} (\overline{R}_{vl} + \sum_{m=1}^{6} bv_{lm} v_{lm}). \qquad (A10.8)$$

or

$$v_l = dv_l - RV_l\,(p_{j+1} - p) \qquad (A10.9)$$

and

$$[\frac{\alpha_{law}\rho_{law}}{\Delta\tau} + a_{ll}^{*} - \sum_{\substack{m=1\\ m\neq l}}^{l_{max}} (a_{ml} - \mu_{mlw})]\, w_l + \sum_{\substack{m=1\\ m\neq l}}^{l_{max}} (a_{ml} - \mu_{mlw})\, w_m =$$

$$b_l + b_l^* - \alpha_{lwa} \frac{1}{\Delta z_h} \frac{\gamma_z}{\gamma_{vw}} (p_{k+1} - p) \qquad \text{(A10.10)}$$

where

$$a_{ll}^* = c_{lw} |w_l| - \frac{1}{\gamma_{vw}} \sum_{m=1}^{6} bw_{lm} + \mu_{Alw} - \mu_{lAw} \qquad \text{(A10.11)}$$

$$b_l^* = \mu_{Alw} w_{Al} - \mu_{lAw} w_{lA} - \frac{1}{\gamma_{vw}} (\overline{R}_{wl} + \sum_{m=1}^{6} bw_{lm} w_{lm}). \qquad \text{(A10.12)}$$

or

$$w_l = dw_l - RW_l (p_{k+1} - p). \qquad \text{(A10.13)}$$

NOMENCLATURE

Symbol	Dimension	Meaning
A	m^2	cross section
A,a	–	matrix, constant
a	m^2/s	thermal diffusivity
a	m/s	speed of sound
B,b	–	matrix, constant
C_{nl}	–	mass concentration of the inert component n in the velocity field l
C_{Ml}	–	mass concentration of the noninert component M in the velocity field l
C,c	–	vector, constant
c_p	J/(kgK)	specific heat at constant pressure
D,d	m	diameter
D^*	m^2/s	diffusivity
D^s	Km^2/s	diffusivity based on entropy driving force
d	–	total differential
$(\rho w)_{32}$	$kg/(m^2s)$	mass flow rate perpendicular to the interface – drop deposition
E	–	unit matrix
e	J/kg	specific internal energy
F	N	force
f	N/m^3	force per unit mixture volume
$=F,f(\ldots$	–	function of (...
f	1/s	frequency
G	$kg/(m^2s)$	mass flow rate
g	m/s^2	gravitational acceleration
H	J	enthalpy
h	J/kg	specific enthalpy
j	m/s	volume flux density
k	m	roughness
k	J/kg	specific kinetic energy of the turbulent pulsations
n	m^{-3}	number of nuclei per unit flow volume, number of particles per unit flow volume
$\dot{n}$	$1/(m^3s)$	change of the number of nucli or particles per unit time and unit volume of the mixture
P_k	J/kg	direct dissipation of kinetic energy and simultaneously direct production of turbulent kinetic energy per unit mass
p	Pa	pressure
$\dot{q}'''$	W/m^3	thermal power per unit flow volume
$\dot{q}''$	Wt/m^2	heat flux density
R	N/m^3	pressure drop per unit length due to friction

R	J/(kgK)	(with indeces) gas constant
r	m	radius
s	J/(kgK)	specific entropy
T	K	absolute temperature
t	C	temperature
U	–	dependent variable vector
u	m/s	radial velocity
V	m/s	velocity vector
v	m/s	azimuthal velocity
v	m^3/kg	specific volume
z	m	axial coordinates

Greek

α_l	m^3/m^3	volume fraction of field l in the flow mixture
α	$W/(m^2K)$	heat transfer coefficient
γ_v	–	volume porosity
$\gamma_{r,\theta,z}$	–	permeabilities in r,θ, and z directions
Δ	–	finite difference
Δu, Δv, Δw	m/s	diffusion velocities in r,θ, and z directions
δ	–	small deviation with respect to the average value
∂	–	partial differential
$(\rho w)_{23}$	$kg/(m^2s)$	entrainment mass flow rate perpendicular to the interface
ϵ	J/(kgs)	dissipated kinetic energy of turbulent pulsations per unit time
φ	rad	angle between upward vertical direction and V
ζ,λ_R	–	friction coefficient
η	kg/(ms)	dynamic viscosity
θ	rad	azimuthal coordinate
κ	–	isentropic exponent
λ	W/(mK)	thermal conductivity
μ	$kg/(m^3s)$	mass source term for velocity field l (mass introduced into the field l per unit time and unit mixture volume)
ν	m^2/s	kinematic viscosity
Π	m	perimeter
π	–	3.141592....
ρ	kg/m^3	density; without indeces: mixture density
Σ	–	sum
σ	N/m	surface tension
τ	s	time
τ	N/m^2	with indeces – tension

Dimensionles numbers

M	Mach number
Pr	Prandtl number
Sc	Schmidt number

Superscripts

"'	saturated solid
"	saturated steam
'	saturated liquid
'	for velocities: fluctuation
n	for the time τ
n+1	for the time $\tau+\Delta\tau$
t	turbulent
l	laminar

Subscripts

A	outside of the definition region
nl	inert component (either non condensing gas or solid particles) of the velocity field l
Ml	not inert component (e.g. water or water steam)
l	velocity field l
i,j,k	integer indeces for the three coordinates r, θ, z
w	wall
c	continuous
d	dispersed
h	hydraulic
heat	heated
1	gas, bubble
2	continuous liquid plus microscopic solid particles
3	dispersed liquid plus microscopic solid particles, drops

Summary of all thermodynamic and thermophysical properties needed for the description of multiphase flows consisting of water, steam, air and metallic materials being in liquid or in liquid–solid or in solid state.

Water–steam saturation line

T'	K	saturation temperature at system pressure.
v'	m^3/kg	water specific volume at the saturation line.
v"	m^3/kg	steam specific volume at the saturation line.
h'	J/kg	specific water enthalpy at the saturation line.
h"	J/kg	specific steam enthalpy at the saturation line.
h"–h'	J/kg	latent heat of vaporization.
s'	J/(kgK)	specific water entropy at the saturation line.
s"	J/(kgK)	specific steam entropy at the saturation line.
dT'/dp	K/Pa	derivative of the temperature with respect to pressure at the saturation line.
c'_p	J/(kgK)	water specific heat at constant pressure at the saturation line.
c''_p	J/(kgK)	steam specific heat at constant pressure at the saturation line.
η'	kg/(ms)	water dynamic viscosity at the saturation line.
η''	kg/(ms)	steam dynamic viscosity at the saturation line.
λ'	kg/(ms)	water thermal conductivity at the saturation line.
λ''	kg/(ms)	steam thermal conductivity at the saturation line.
σ'	N/m	surface tension water steam at the saturation line.

The above mentioned properties can be computed either as a function of temperature T' in K or as a function of pressure p' in Pa, respectively.

The thermodynamic and thermophysical properties of water are computed as functions of temperature in K and system pressure in Pa:

ρ_{1M}	kg/m^3	density.
h_{1M}	J/kg	specific enthalpy.
s_{1M}	J/(kgK)	specific entropy.
c_{p1M}	J/(kgK)	specific heat at constant pressure.
a_{1M}	m/s	velocity of sound.
η_{1M}	kg/(ms)	dynamic viscosity.
λ_{1M}	W/(mK)	thermal conductivity.
Pr_{1M}	–	Prandtl number.
$\left(\frac{\partial h_{1M}}{\partial p}\right)_{T_1}$	(J/kg)/Pa	specific enthalpy derivative with respect to pressure at constant temperature.

$\left(\frac{\partial \rho_{1M}}{\partial T_1}\right)_p$	kg/(m^{3}K)	density derivative with respect to the temperature at constant pressure.
$\left(\frac{\partial \rho_{1M}}{\partial p}\right)_{T_1}$	(kg/m^3)/Pa	density derivative with respect to the pressure at constant temperature.
σ_{1M}	N/m	surface tension metallic phase/gas.

The thermodynamic and thermophysical properties of air are computed as a function of temperature T_1 in K and partial pressure p_{1n} in Pa:

ρ_{1n}	kg/m^3	density.
h_{1n}	J/kg	specific enthalpy.
s_{1n}	J/(kgK)	specific entropy.
c_{p1n}	J/(kgK)	specific heat at constant pressure.
a_{1n}	m/s	velocity of sound.
η_{1n}	kg/(ms)	dynamic viscosity.
λ_{1n}	W/(mK)	thermal conductivity.
Pr_{1n}	–	Prandtl number.

The thermodynamic and thermophysical properties of steam are computed as functions of temperature T in K and of the partial pressure P_{1M} in Pa:

ρ_{1M}	kg/m^3	density.
h_{1M}	J/kg	specific enthalpy.
s_{1M}	J/(kgK)	specific entropy.
c_{p1M}	J/(kgK)	specific heat at constant pressure.
a_{1M}	m/s	velocity of sound.
η_{1M}	kg/(ms)	dynamic viscosity.
λ_{1M}	W/(mK)	thermal conductivity.
Pr_{1M}	–	Prandtl number.
$\left(\frac{\partial h_{1M}}{\partial p}\right)_{T_1}$	(J/kg)/Pa	specific enthalpy derivative with respect to pressure at constant temperature.
$\left(\frac{\partial \rho_{1M}}{\partial T_1}\right)_{p_{1M}}$	kg/(m^{3}K)	density derivative with respect to the temperature at constant pressure.

$(\frac{\partial \rho_{lM}}{\partial p_{lM}})_{T_l}$	$(kg/m^3)/Pa$	density derivative with respect to the pressure at constant temperature.

The properties of a binary mixture consisting of inert (solid particles) and not inert (water) components are computed as functions of the field temperature T_l in K, system pressure p in Pa, and inert mass concentration C_{ln} (where l=2,3):

s_l	J/(kgK)	specific entropy.
h_{lM}	J/kg	specific water enthalpy.
ρ_l	kg/m^3	density.
a_l	m/s	velocity of sound.
$(\frac{\partial \rho_l}{\partial s_l})_{p,C_{ln}}$	$(kg/m^3)/(J/kgK)$	density derivative with respect to the specific entropy at constant pressure and inert mass concentrations.
$(\frac{\partial \rho_l}{\partial C_{ln}})_{p,s_l}$	(kg/m^3)	density derivative with respect to the inert mass concentration at constant pressure and specific entropy.
$(\frac{\partial T_l}{\partial s_l})_{p,C_{ln}}$	K/[J/(kgK)]	temperature derivative with respect to the specific entropy at constant pressure and inert mass concentration.
$(\frac{\partial T_l}{\partial p})_{s_l,C_{ln}}$	K/Pa	temperature derivative with respect to the pressure at constant specific entropy and inert mass concentrations.
$(\frac{\partial T_l}{\partial C_{ln}})_{p,s_l}$	K	temperature derivative with respect to the inert mass concentration at constant pressure and specific entropy.
c_{pl}	J/(kgK)	specific heat at constant pressure.
η_l	kg/(ms)	dynamic viscosity.
λ_l	W/(mK)	thermal conductivity.
Pr_l	–	Prandtl number.
σ_l	N/m	surface tension metallic phase/gas.
s_{ln}	J/(kgK)	specific entropy of the inert component.
s_{lM}	J/(kgK)	specific entropy of the water component.
h_{ln}	J/kg	specific enthalpy of the inert component.

The properties of a binary gas mixture consisting of inert component (air) and not inert component (steam) are computed as functions of the gas temperature T_1 in K, of the system pressure p in Pa and of the inert mass concentration C_{1n}:

s_1	J/(kgK)	specific entropy.
h_{1M}	J/kg	specific steam enthalpy.
ρ_1	kg/m^3	density.
a_1	m/s	velocity of sound.
$(\frac{\partial\rho_1}{\partial s_1})_{p,C_{1n}}$	(kg/m^3)/(J/kgK)	density derivative with respect to the specific entropy at constant pressure and inert mass concentration.
$(\frac{\partial\rho_1}{\partial C_{1n}})_{p,s_1}$	(kg/m^3)	density derivative with respect to the inert mass concentration at constant pressure and specific entropy.
$(\frac{\partial T_1}{\partial s_1})_{p,C_{1n}}$	K/[J/(kgK)]	temperature derivative with respect to the specific entropy at constant pressure and inert mass concentration.
$(\frac{\partial T_1}{\partial p})_{s_1,C_{1n}}$	K/Pa	temperature derivative with respect to the pressure at constant specific entropy and inert mass concentrations.
$(\frac{\partial T_1}{\partial C_{1n}})_{p,s_1}$	K	temperature derivative with respect to the inert mass concentration at constant pressure and specific entropy.
c_{p1}	J/(kgK)	specific heat at constant pressure.
η_1	kg/(ms)	dynamic viscosity.
λ_1	W/(mK)	thermal conductivity.
Pr_1	–	Prandtl number.
D_{1n}	m^2/s	diffusion constant of air in steam.
p_{1n}	Pa	partial pressure of the inert component.
s_{1n}	J/(kgK)	specific entropy of the inert component.
s_{1M}	J/(kgK)	specific entropy of the steam component.
h_{1n}	J/kg	specific enthalpy of the inert component.

The quantities describing the solid–liquid transition are computed as functions of the temperature in K:

T''_{3n}	K	liquidus temperature.
ρ'''_{3n}	kg/m^3	saturated solid phase density.
ρ''_{3n}	kg/m^3	saturated liquid density.
$d\rho'''_{3n}/dT_3$	kg/(m^{3}K)	density derivative with respect to temperature at the two phase/solid transition line.

$d\rho''_{3n}/dT_3$	kg/(m^{3}K)	density derivative with respect to temperature at the liquid/two phase transition line.
h'''_{3n}	J/kg	saturated solid phase specific enthalpy.
h''_{3n}	K/kg	saturated liquid phase specific enthalpy.
$h''_{3n}-h'''_{3n}$	J/kg	latent heat of solidification.
s'''_{3n}	J/(kgK)	saturated solid phase specific entropy.
s''_{3n}	J/(kgK)	saturated liquid phase specific entropy.
$s''_{3n}-s'''_{3n}$	J/(kgK)	latent specific solidification entropy.
c'''_{p3n}	J/(kgK)	specific heat at constant pressure of the saturated solid phase.
c''_{p3n}	J/(kgK)	specific heat at constant pressure of the saturated liquid phase.
η'''_{3n}	kg/(ms)	saturated solid phase dynamic density.
η''_{3n}	kg/(ms)	saturated liquid phase dynamic viscosity.
λ'''_{3n}	W/(mK)	saturated solid phase thermal conductivity.
λ''_{3n}	W/(mK)	saturated liquid phase thermal conductivity.
σ''_{3n}	N/m	surface tension liquid metal/gas.

For description of the thermophysical properties of solid and liquid materials the following approximations are necessary:

T_{3n}	K	temperature of the liquid metal as a function of specific entropy in J/(kgK).
$\sigma_{3n,solid}$	N/m	surface tension of the liquid metal as a function of temperature in K.
$\eta_{3n,solid}$	kg/(ms)	solid phase dynamic viscosity as a function of temperature in K.
$h_{3n,solid}$	J/kg	specific enthalpy of the solid phase as a function of temperature in K.
$h_{3n,liquid}$	J/kg	specific liquid metal enthalpy as a function of temperature in K.
$c_{p3n,solid}$	J/(kgK)	specific heat at constant pressure for solid phase as a function of temperature in K.
$c_{p3n,liquid}$	J/(kgK)	specific heat at constant pressure for liquid metal as a function of temperature in K.

$s_{3n,solid}$	J/(kgK)	specific solid phase entropy as a function of temperature in K.
$s_{3n,liquid}$	J/(kgK)	specific liquid metal entropy as a function of the temperature in K.
$\rho_{3n,solid}$	kg/m^3	solid phase density as a function of temperature in K.
$\frac{d\rho_{3n,solid}}{dT_3}$	kg/(m^{3}K)	solid density derivatives with respect to the temperature as a function of temperature in K.
$\rho_{3n,liquid}$	kg/m^3	liquid metal density as a function of temperature in K.
$\frac{d\rho_{3n,liquid}}{dT_3}$	kg/(m^{3}K)	liquid metal density derivatives with respect to the temperature as a function of temperature in K.
$\lambda_{3n,solid}$	W/(mK)	solid phase thermal conductivity as a function of temperature in K.
$\lambda_{3n,liquid}$	W/(mK)	liquid metal thermal conductivity as a function of temperature.

Having the entropy one checks in which state the metallic, velocity field is and computes properties either for liquid state or for two–phase liquid–solid equilibrium state or for solid state. The following properties as functions of temperature in K and/or of the specific entropy in J/(kgK) are the result:

ρ_{3n}	kg/m^3	density.
h_{3n}	J/kg	specific enthalpy.
c_{p3n}	J/(kgK)	specific heat at constant pressure.
a_{3n}	m/s	velocity of sound.
η_{3n}	kg/(ms)	dynamic viscosity.
λ_{3n}	W/(mK)	thermal conductivity.
Pr_{3n}	–	Prandtl number.
$(\frac{\partial h_{3n}}{\partial p})_{T_3}$	(J/kg)/Pa	specific enthalpy derivative with respect to pressure at constant temperature.
$(\frac{\partial \rho_{3n}}{\partial T_3})_p$	kg/(m^{3}K)	density derivative with respect to the temperature at constant pressure.

$(\frac{\partial \rho_{3n}}{\partial p})_{T_3}$	$(kg/m^3)/Pa$	density derivative with respect to the pressure at constant temperature.
σ_{3n}	N/m	surface tension metallic phase/gas.

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FIGURES

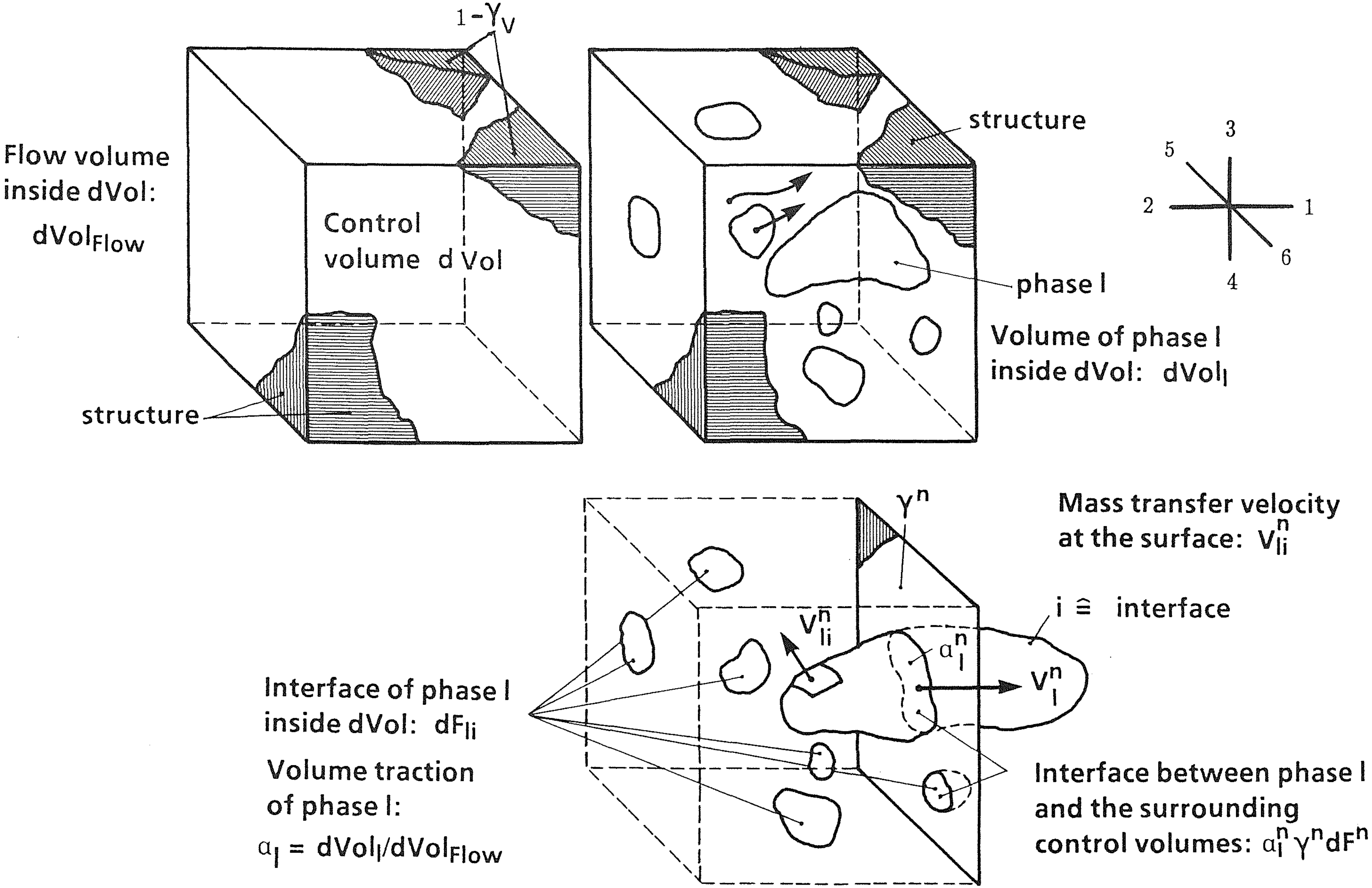

FIGURE 1. Control volume for derivation of the mass conservation equation – volume occupied partially by structure and two different phases.

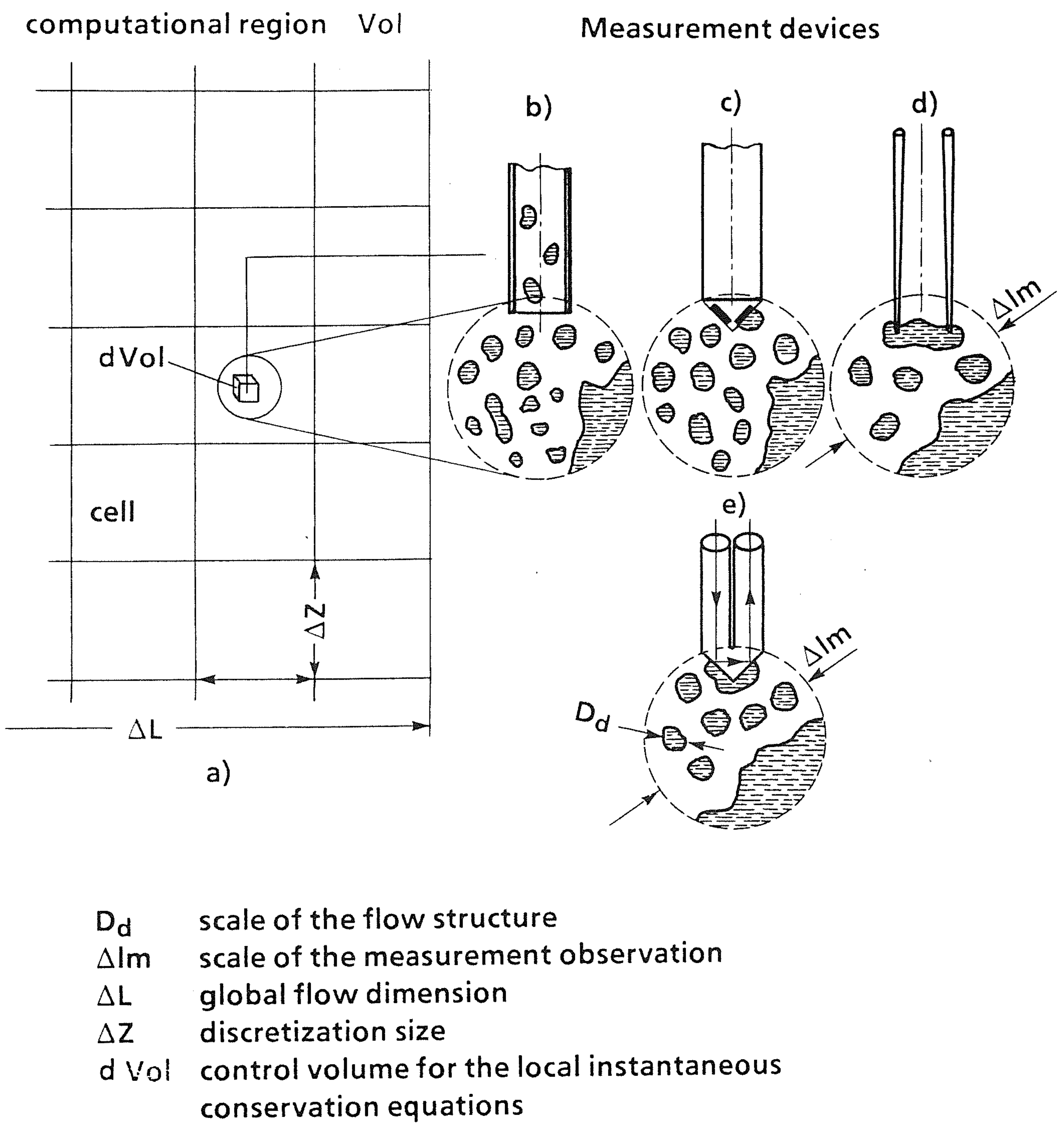

FIGURE 2. Control volume for derivation of the mass conservation equation – to the scale of the observable control volume by means of different measurement devices.

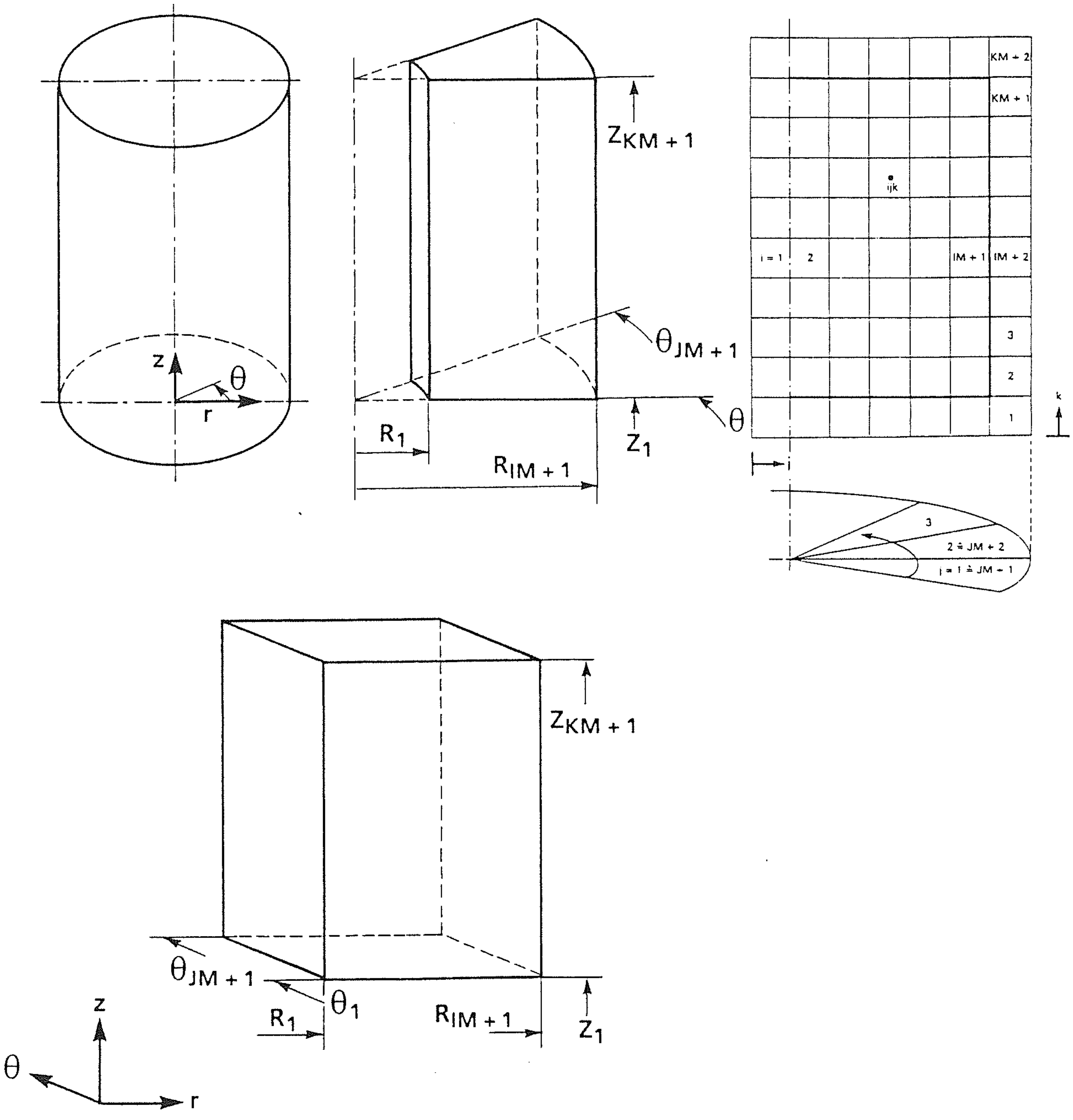

FIGURE 3. Three–dimensional mesh construction.

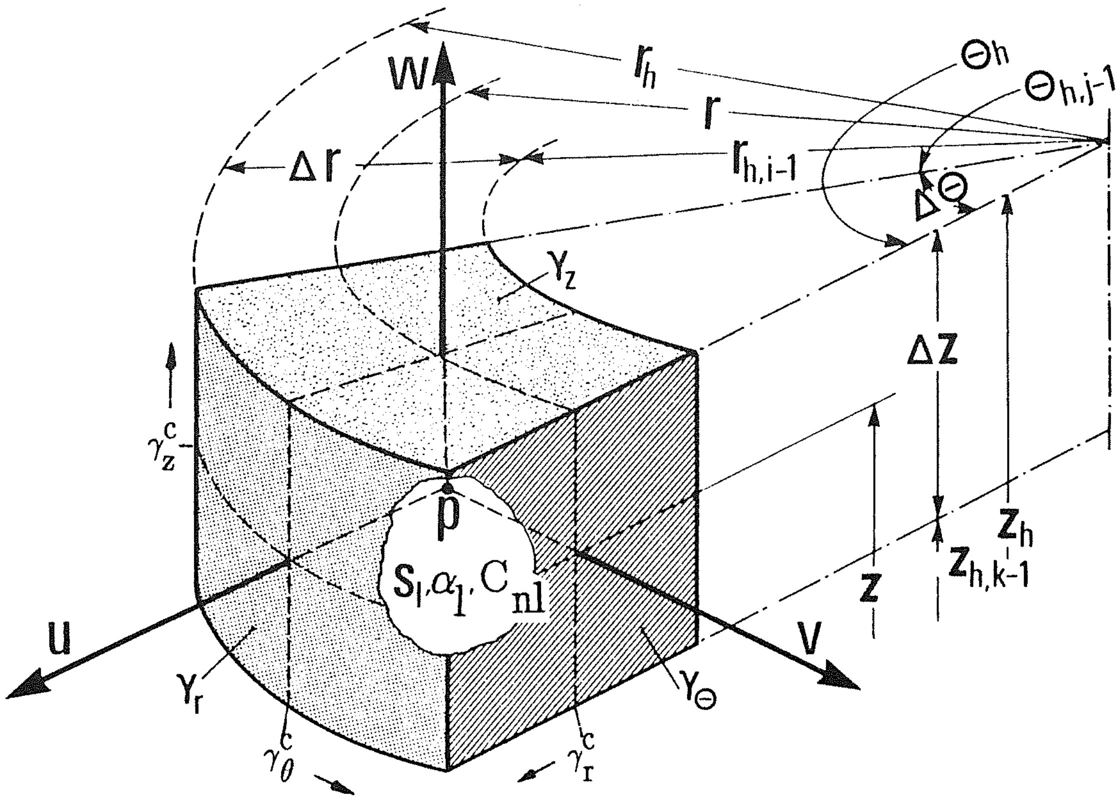

FIGURE 4. Definition of the geometrical parameters and the location of the dependent variables.

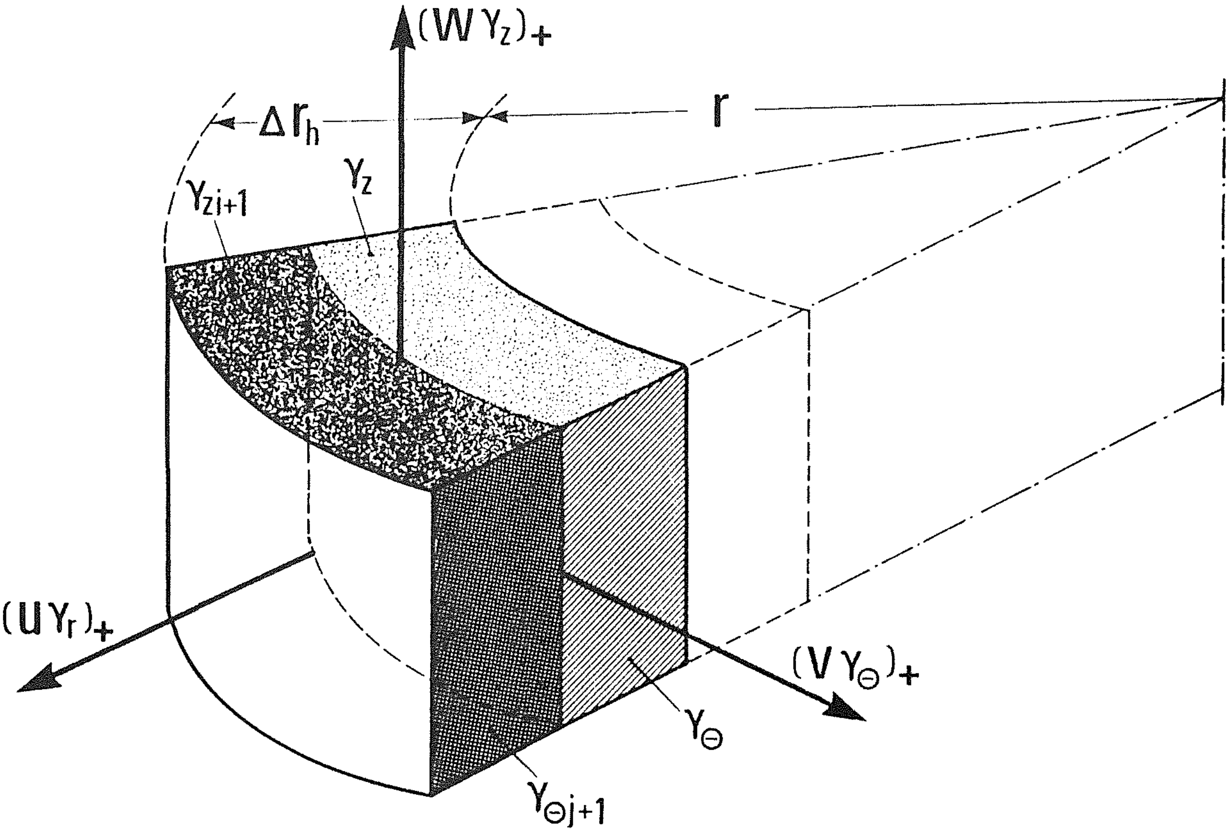

FIGURE 5. Three – dimensional mesh cell for discretization of the momentum equations for the r direction.

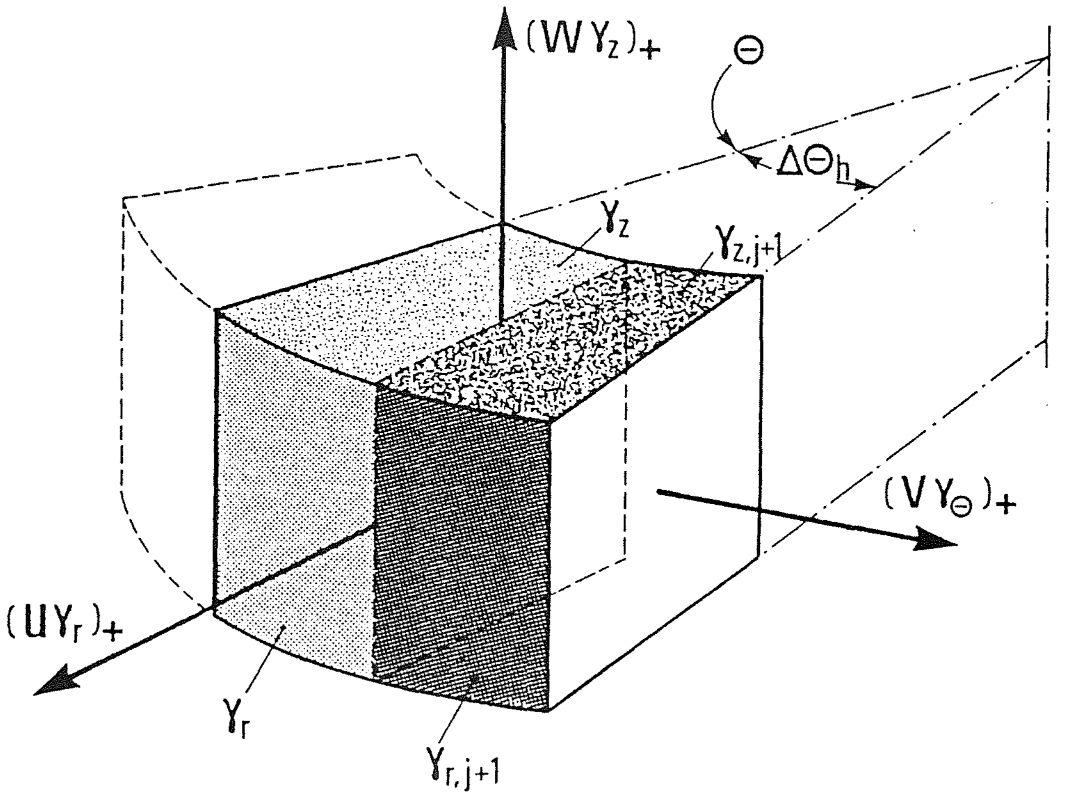

FIGURE 6. Three – dimensional mesh cell for discretization of the momentum equations for the θ direction.

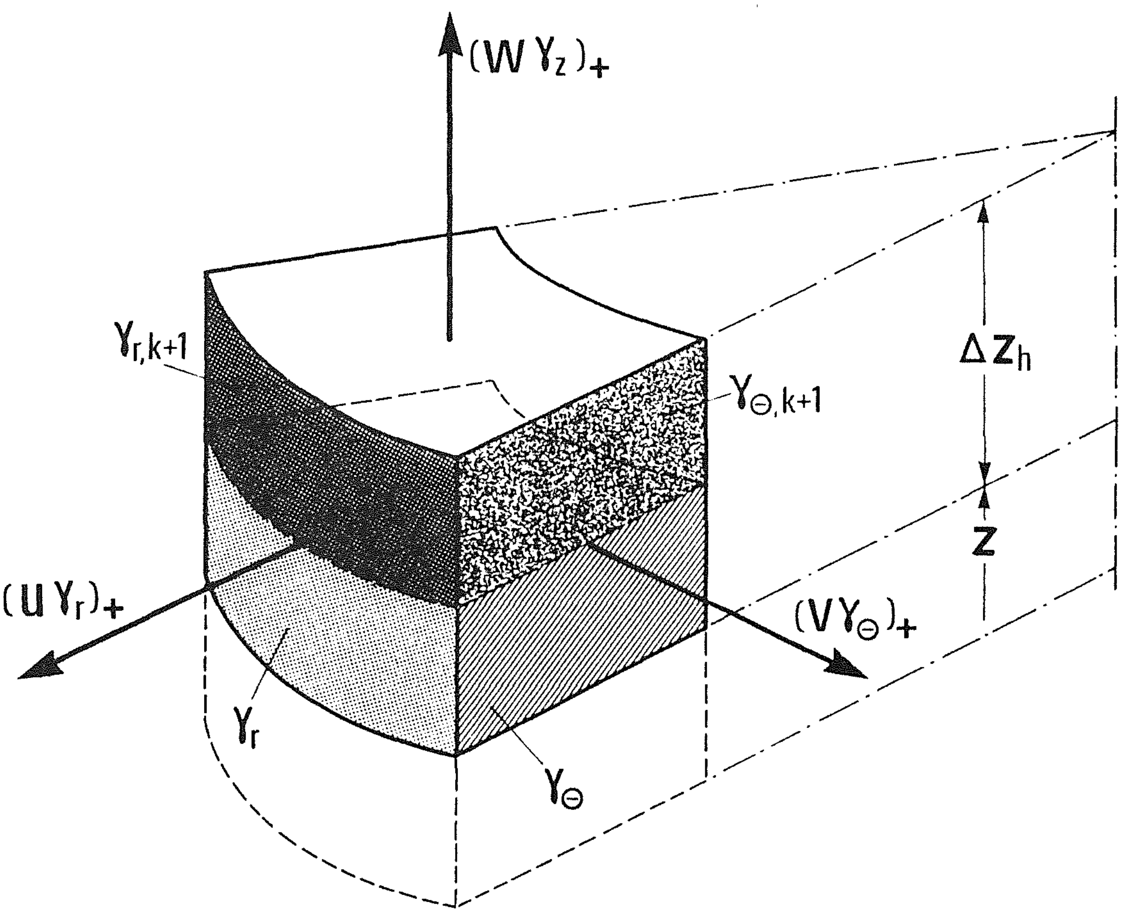

FIGURE 7. Three – dimensional mesh cell for discretization of the momentum equations for the z direction.