
Computational Fluid Dynamics in Screw Machines

2.1 Introduction

As computer technology and its associated computational methods advance, the use of 3-D Computational Fluid Dynamics (CFD) to design and analyse positive displacement machinery working processes is gradually becoming more practicable. In general, the CFD modelling process can be split into four phases.

The first phase is concerned with defining the problem that has to be solved. Both the ease of solution and implementation of results into the design process are heavily dependent on this critical starting step. Two different approaches are available for screw machines. The first is to select one interlobe on the main rotor and the corresponding interlobe on the gate rotor in order to make a computational domain. This is probably the easiest to implement but takes no account of important phenomena such as interlobe leakage, blow-hole losses, oil injection and oil distribution. Another approach assumes that the whole domain of a screw machine is analysed. This includes the suction chamber and its port, the compression or expansion chamber with its moving rotor boundaries and the discharge system of the machine. By this means, the leakage paths and any additional inlet or outlet ports are included in the domain to be analysed. Realism in representing the machine working process gives a large advantage to this approach. The design procedure and the CFD numerical analysis can then be easily connected and interchanged and the calculation of the operational parameters of such machines is thereby facilitated. Unfortunately, such a complex geometry cannot be represented by a small number of computational points.

In the second phase, a mathematical model that is capable of describing the problem has to be selected. There are again two types of situation. The first is where an adequate mathematical description exists and can be used, e.g. heat conduction, elastic stress analysis and laminar fluid flow. The second is where such a description either does not exist or is impracticable to use, e.g. non-linear stress analysis and turbulent fluid flow. In the case of positive displacement machines, it is unlikely that any analytical solutions exist. This is because highly compressible flow appears inside both domains with turbulent flow regimes and domains with low Reynolds numbers. There is additional non-linearity introduced by two-phase flow, particle flow, moving and stretching domains and sliding boundaries. Due to

all these, the mathematical model implemented here needs to cope with a variety of different requirements. It is based on the general laws of mass, momentum, energy and space conservation. The resulting system of governing equations is not closed because it contains more unknowns than resulting equations. It is closed by constitutive relations, which give information about the response of a particular continuum material to external influences. The whole concept of mathematical modelling is based on a phenomenological approach which employs the principle of a continuum as the physical background. It can be applied only when an elementary part of material or the smallest characteristic length of the flow, which has to be analysed, is much bigger than the mean free molecular path. Fortunately, this condition is fulfilled for the majority of fluids and practically for all solid structures.

The mathematical description of problems in continuum mechanics is very rarely amenable in a closed-form of analytical solution and an iterative numerical procedure is thus the only alternative that can be applied to solve models in positive displacement machines. Numerical methods transform the differential equations of the mathematical model into a system of algebraic equations. The third phase is therefore to select the discretisation method. To do that a number of approximations are made: the continuum is replaced by a set of computational points with finite distances between them in space and time, while the continuous functions which represent the exact solution of the mathematical model are approximated by polynomials, typically of a second order. Because of the complexity of positive displacement machines, the standard approach to spatial discretisation is not applicable and a special grid generation method has to be developed and applied to them. The equations are discretised by the finite volume method, which appears to have a more conservative form of governing laws than any other numerical method. The result of discretisation is a system of algebraic equations the size of which depends on the number of numerical cells.

The resulting set of algebraic equations is then solved by approximate iterative methods. Iterations are necessary due to the non-linearity of the mathematical model. Even for linear problems, an iterative solution method is usually more efficient than a direct one. In addition, iterative solution methods are less sensitive to round-off errors due to the finite accuracy of the computer arithmetic.

2.2 Continuum Model applied to Processes in Screw Machines

A mathematical model of the transport processes, which exist within both twin screw and other types of positive displacement machine, is presented here. It includes the mass, momentum and energy conservation equations in integral form, a space conservation law, which has to be satisfied for problems with a moving mesh, constitutive relations required for the problem closure, a model of dispersed flow, models of turbulence in fluid flow and boundary conditions.

All the equations are presented in a symbolic coordinate-free notation which directly conveys the physical meaning of particular terms without unnecessary ref-

erence to any coordinate system. However, numerical solution of these equations requires a coordinate system and vectors and tensors have to be specified in terms of their components.

2.2.1 Governing Equations

Fluid contained within a screw compressor can be gas, vapour or a wet mixture of liquid and vapour. In some cases, it can be pure liquid. Its density varies with both pressure and temperature. The compressor flow is governed by equations based on the general laws of continuity, momentum and energy conservation. The most general approach is to write these equations in integral form and apply them to an arbitrary part of the fluid or solid continuum of volume V , which is bounded by a moving surface S , as shown in Figure 2-1.

Reynolds' transport theorem can be expressed as:

$$\frac{d}{dt} \int_{V_{CM}} \rho \phi dV = \frac{d}{dt} \int_{V_{CV}} \rho \phi dV + \int_S \rho \phi (\mathbf{v} - \mathbf{v}_s) \cdot d\mathbf{s} \quad (2.1)$$

where, V_{CM} is the volume of the control mass, V_{CV} is the control volume enclosed by the surface S . Vector $d\mathbf{s}$ stands for the outward pointing surface vector, defined by its unit vector \mathbf{n} and surface area dS as $d\mathbf{s} = \mathbf{n} dS$. In equation (2.1), ϕ represents any intensive property based on mass, momentum, energy, concentration or other parameter.

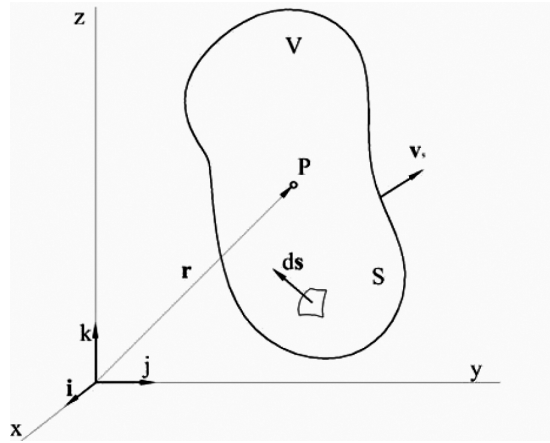


Figure 2-1 Control volume of part of the continuum

Vector \mathbf{v}_s is the velocity with which the surface of the control volume moves. If the control volume is fixed, then its surface velocity $\mathbf{v}_s = 0$. Equation (2.1) then makes the rate of change of the amount of property in the control mass equal to the sum of the rate of change of that property within the control volume and its net

flux through the control volume boundary due to relative fluid motion. If the control volume moves with the same velocity as the boundary of the control mass, then the boundary velocity is equal to the velocity of the control mass, $\mathbf{v}=\mathbf{v}_s$. For convenience, the control volume is denoted as V and its surface as S .

If the variable ϕ in equation (2.1) has the value of 1, then the equation represents that of continuity:

$$\frac{d}{dt} \int_V \rho dV + \int_S \rho(\mathbf{v} - \mathbf{v}_s) \cdot d\mathbf{s} = 0, \quad (2.2)$$

If the conserved property is velocity, i.e. $\phi=\mathbf{v}$, then equation (2.1) becomes that of the conservation of momentum:

$$\frac{d}{dt} \int_V \rho \mathbf{v} dV + \int_S \rho \mathbf{v}(\mathbf{v} - \mathbf{v}_s) \cdot d\mathbf{s} = \sum \mathbf{f} \quad (2.3)$$

where the right hand side of the equation represents the sum of surface and body forces which act on the matter in the control volume. Since the body forces acting on the whole matter trapped in the control volume are independent of the shape of the boundary surface, they represent a vector field and can be integrated over the control volume. However, surface forces such as pressure forces, normal and shear stress forces or surface tension forces, depend on the surface on which they act, and they represent momentum fluxes across the surface. More details of this can be found in *Ferziger and Peric* (1995). In order to close the system of equations, these fluxes must be written in terms of properties whose conservation is governed by the equation in question. In equation (2.3) the conserved property is the velocity \mathbf{v} . For Newtonian fluids, a constitutive relation between stress \mathbf{T} and strain \mathbf{D} is Stokes' law. Hookes' law gives a constitutive relation for thermo-elastic solids. The momentum equation (2.3) then becomes:

$$\frac{d}{dt} \int_V \rho \mathbf{v} dV + \int_S \rho \mathbf{v}(\mathbf{v} - \mathbf{v}_s) \cdot d\mathbf{s} = \int_S \mathbf{T} \cdot d\mathbf{s} + \int_V \mathbf{f}_b dV \quad (2.4)$$

where \mathbf{T} is the stress tensor and \mathbf{f}_b is the resultant body force.

If the conserved property ϕ in equation (2.1) is scalar, then the equation can be written in the following form:

$$\frac{d}{dt} \int_V \rho \phi dV + \int_S \rho \phi(\mathbf{v} - \mathbf{v}_s) \cdot d\mathbf{s} = \sum \mathbf{f}_\phi, \quad (2.5)$$

where the term on the right hand side is the sum of all the modes of transport of the property ϕ , other than convection, which is already on the left side of this equation, and any sources or sinks of that property. This sum generally consists of

two terms; the diffusive transport and the sink or source of the conserved property. The diffusive transport is:

$$f_{\phi}^d = \int_S \Gamma \text{grad} \phi \cdot d\mathbf{s} = \int_S \mathbf{q}_{\phi} \cdot d\mathbf{s} . \quad (2.6)$$

Γ is the diffusivity of ϕ . Equation (2.5) in that case becomes a general conservation equation:

$$\frac{d}{dt} \int_V \rho \phi dV + \int_S \rho \phi (\mathbf{v} - \mathbf{v}_s) \cdot d\mathbf{s} = \int_S \mathbf{q}_{\phi} \cdot d\mathbf{s} + \int_V S_{\phi} dV \quad (2.7)$$

where S_{ϕ} is the source or sink of property ϕ per unit mass. Equation (2.7) appears to be a generic equation valid for all intensive properties of matter.

From equation (2.7) one can get the energy equation, in the form of enthalpy, directly as:

$$\begin{aligned} \frac{d}{dt} \int_V \rho h dV + \int_S \rho h (\mathbf{v} - \mathbf{v}_s) \cdot d\mathbf{s} = & \int_S \mathbf{q}_h \cdot d\mathbf{s} + \int_V s_h dV + \\ & \int_V (\mathbf{v} \cdot \text{grad} p + \mathbf{S} : \text{grad} \mathbf{v}) dV - \int_S p \mathbf{v}_s \cdot d\mathbf{s} + \frac{d}{dt} \int_V p dV \end{aligned} \quad (2.8)$$

\mathbf{S} is the viscous part of the stress tensor:

$$\mathbf{S} = \mathbf{T} + p \mathbf{I} \quad (2.9)$$

\mathbf{I} is a unit tensor.

If applied to the concentration scalar $c_i = m_i/m$, where m_i denotes the mass of the dispersed fluid in the working fluid and m defines the overall mass, equation (2.7) becomes:

$$\frac{d}{dt} \int_V \rho c_i dV + \int_S \rho c_i (\mathbf{v} - \mathbf{v}_s) \cdot d\mathbf{s} = \int_S \mathbf{q}_{c_i} \cdot d\mathbf{s} + \int_V S_{c_i} dV , \quad (2.10)$$

where \mathbf{q}_{c_i} is the diffusion flux and S_{c_i} is the source or sink of the dispersed phase.

If the conserved property in equation (2.7) is defined as $\phi = 1/\rho$ then this equation becomes the space conservation law which must be satisfied in all cases even if the domain boundaries move:

$$\frac{d}{dt} \int_V dV - \int_S \mathbf{v}_s \cdot d\mathbf{s} = 0 . \quad (2.11)$$

This equation links the rate of change of volume V and surface the velocity \mathbf{v}_s .

Equations (2.2), (2.4), (2.8), (2.10) and (2.11) constitute a mathematical model which is valid for the majority of fluids and solids in engineering practice. For the numerical modelling of a screw machine, the first three of these equations should be solved for the working gas or vapour, which is a background fluid. Equation (2.10) is solved for the disperse phase, which is either oil or other fluid injected into the working chamber and dispersed into the background fluid, while the equation of space must be satisfied for any case, because the compression or expansion in a positive displacement machine is caused entirely by the movement of the boundary. In two-phase flow, the liquid phase of the working fluid can also be considered as the dispersed phase. This approach assumes that the dispersed phase is a passive ‘species’ in the background fluid. It allows separate calculation for these two phases. The influence of the dispersed phase on the main flow and vice versa is through the source terms in the governing equations. Such a method does not require the additional calculation of mixture properties such as density and viscosity. This is convenient and physically sound in the case of an oil-injected compressor where the two phases are fluids of a different type. Although these two flows are usually calculated from the unique density and viscosity of the vapour-liquid mixture, it is more convenient to take account of the values of the vapour and liquid properties separately with concentration as the blending factor between them.

2.2.2 Constitutive Relations

The numerical method contains information about material properties that have to be incorporated into the model. These are used to express the stress tensor \mathbf{T} , heat flux \mathbf{q}_h and diffusion flux \mathbf{q}_{ci} . Relatively simple assumptions can be made to define values for these in many engineering circumstances. The stress tensor, which represents the viscous rate of transport of momentum and closes equation (2.4), can be defined for Newtonian fluids by Stokes law as:

$$\mathbf{T} = 2\mu\dot{\mathbf{D}} - \frac{2}{3}\mu\text{div } \mathbf{v}\mathbf{I} - p\mathbf{I}, \quad (2.12)$$

where the rate of strain is defined as:

$$\dot{\mathbf{D}} = \frac{1}{2} \left[\text{grad } \mathbf{v} + (\text{grad } \mathbf{v})^T \right]. \quad (2.13)$$

Superscript T represents the transposed tensor. Stokes law gives the relation between the stress and the rate of deformation for Newtonian fluids.

Solid material can be treated as thermo-elastic. For such solids, the constitutive relation that closes equation (2.4) is Hooke’s law. It defines the relation between the stress and strain in solids as:

$$\mathbf{T} = 2\eta\mathbf{D} - \lambda \operatorname{div} \mathbf{u} \mathbf{I} + (3\lambda + 2\eta)\alpha_i \Delta T \mathbf{I}, \quad (2.14)$$

where the strain tensor is:

$$\mathbf{D} = \frac{1}{2} \left[\operatorname{grad} \mathbf{u} + (\operatorname{grad} \mathbf{u})^T \right]. \quad (2.15)$$

Equations (2.12) and (2.14) have the same form. This allows them to be incorporated into a mathematical model and solved by the same method. By this means, the simultaneous calculation of fluid flow and deformation in solids permits the analysis of fluid-solid interaction.

The viscous part of the stress tensor, which appears in equation (2.8), is now fully defined by equations (2.9), (2.12) and (2.13).

The heat flux through the surface boundary \mathbf{q}_h is defined through Fourier's law as the product of the thermal conductivity κ and the temperature gradient.

$$\mathbf{q}_h = \kappa \operatorname{grad} T. \quad (2.16)$$

The mass flux of the dispersed phase, relative to the mean flow is defined by equation (2.10), by the use of Fick's law:

$$\mathbf{q}_{c_i} = \rho D_i \operatorname{grad} c_i, \quad (2.17)$$

where D_i is the mass diffusivity of the dispersed phase. In the case of only one fluid dispersed in the main flow, which is the most common case in oil injected screw compressors, equation (2.17) satisfies the overall mass concentration equation:

$$\mathbf{q}_{c_i} = \rho c_i (\mathbf{v}_{c_i} - \mathbf{v}_m). \quad (2.18)$$

The velocity of the dispersed phase is \mathbf{v}_{c_i} , while the mass averaged velocity of the mixture is $\mathbf{v}_m = \sum_{i=0}^N c_i \mathbf{v}_{c_i}$. Equation (2.18) is satisfied if the fluid is dispersed. Otherwise, it is valid if each fluid satisfies its own equation. On the other hand, Fick's law satisfies equation (2.18) only if $\sum_{i=0}^N c_i \mathbf{q}_{c_i} = 0$. This happens only if the diffusion coefficients of all the dispersed fluids have the same value.

Even if all the variables, which define the material properties, are known, the system of equations is still not closed because the pressure p exists in both, the energy equation (2.8) and in the stress tensor (2.12) which forms part of the momentum equation (2.10). An equation of state, which balances the mass equation with thermodynamic properties, usually pressure and temperature, is then required to close the system. This is normally of the form:

$$\rho = \rho(p, T), \quad e = e(\rho, T) \quad (2.19)$$

Equations of state are directly applicable to all engineering fluids and solids, both ideal and real. Common examples are incompressible fluids and solids where $\rho = \text{const}$, or ideal gases where $\rho = p/RT$. However, real fluids are not rare in screw machinery. In that case, the density of the real gas or mixture can be calculated based on a user specified procedure and later introduced to the model. These equations must have the form of equation (2.19).

2.2.3 Multiphase Flow

In an oil-flooded screw compressor, the dispersed phase in the working fluid is comprised of both the liquid part of the working fluid and the oil. Both components give flow through the machine a multiphase character. There are two different approaches to multiphase flows. One of them is the Eulerian approach where each of two or more phases is contained in its own domain, strictly separated in space from any other but connected with them through a boundary interface. An example of this is an oil tank in which the level of oil is above space occupied by water. If the Eulerian approach is assumed, then a sharp interface exists between the oil and the water and separate numerical meshes can be generated. Both, the oil and the water have to satisfy the governing equations described in 2.2.1.

This is not applicable to two-phase flow within a screw machine. Here, the so-called Eulerian-Lagrangian approach is more appropriate, in which both phases occupy a common working domain without a strict interface between them. In such a case, the background fluid must satisfy the governing equations of mass, energy and momentum, while the dispersed phase should satisfy the governing equation of concentration. Such an approach allows for the dispersed phase to be either a passive or an active component. The dispersed phase in the form of oil or other injected liquid has an important role in the screw compressor working cycle. It is there to cool the fluid, seal the clearance gaps and lubricate the compressor moving parts. The influence of the dispersed phase on the background fluid and vice versa must be incorporated in the governing equations. This is done through source terms in the mass, momentum and energy equations.

The Energy Source

The energy balance of a dispersed phase trapped in the control volume can be written in the following form:

$$\frac{d(m_i h_i)}{dt} = m_i \frac{dh_i}{dt} + h_{iL} \frac{dm_i}{dt} = \dot{Q}_{con} + \dot{Q}_{mass} \quad (2.20)$$

The first term on the right hand side of this equation represents the convective heat flux between the dispersed phase and the background fluid while the second term

represents the heat transfer due to mass interchange between the phases. The last one is significant only for two-phase flow of the same fluid in the working chamber. In the case of an oil-flooded compressor, the convection term has a significant role. In equation (2.20) h_i is the specific enthalpy per unit mass while h_{iL} defines the specific enthalpy of vaporisation. It represents the difference between the specific enthalpies of the liquid and vapour phases, i.e. the dispersed and continuous phases. If the specific heat of oil is constant, then equation (2.20) becomes:

$$\frac{d(m_i T_i)}{dt} = m_o C_{p_o} \frac{dT_o}{dt} + h_L \frac{dm_L}{dt} = \dot{Q}_{con} + \dot{Q}_{mass}, \quad (2.21)$$

There are two approaches to allow for convective heat transport between the dispersed phase and the background fluid.

The first approach assumes that the dispersed phase is completely dissolved in the background fluid. That means that the droplet size of the dispersed phase is very small, ie. $d_o \rightarrow 0$. In that case, an ideal process of heat transfer can be assumed where the temperature of the dispersed phase is assumed to be equal to the temperature of the background fluid $T=T_o$. Heat exchange between the phases is then calculated from the temperature difference of the continuous phase, at two consecutive instants of time, multiplied by the mass and specific heat of the dispersed phase as:

$$\dot{Q}_{con} = m_o C_{p_o} \frac{dT}{dt} \approx m_o C_{p_o} \frac{T^k - T^{k-1}}{\delta t}, \quad (2.22)$$

where T^k is the temperature in the current time step and T^{k-1} is the temperature from the previous time step or iteration. δt is the time step. If the time step is small then this equation has the exact differential form of convective heat transfer. The assumption of an infinitesimally small droplet size is not completely correct but analysis of the influence of oil on screw compressor process performance by *Stosic et al* (1992) showed that a change in droplet size from 0 to 10 μm , does not affect the oil and consequently the gas temperature very much. Therefore, it is accurate enough to calculate the heat exchanged between the continuous and dispersed phases by means of equation (2.22).

When necessary, another approach can be used to calculate the convective heat transfer term in equation (2.21). It should be applied whenever the temperatures of the continuous and dispersed phases cannot be considered to be equal. It is then assumed that the dispersed phase, contained in the control volume, consists of spherical droplets with a Sauter mean diameter defined as:

$$d_o = 0.0092 \left(\frac{\rho_o \sigma_o}{|\mathbf{v}|} \right) \left(1 + \frac{1}{c_o} \right)^{0.7} \quad (2.23)$$

where σ_o is the surface tension and $|\mathbf{v}|$ is the absolute value of the fluid velocity. The convective heat flux then becomes:

$$\dot{Q}_{con} = \pi d_o \kappa \text{Nu} (T - T_o), \quad (2.24)$$

where, T and T_o are temperatures of the continuous and dispersed phases respectively and the Nusselt number is given by:

$$\text{Nu} = 2 + 0.6 \text{Re}^{0.5} \text{Pr}^{0.33}. \quad (2.25)$$

In the previous equation the Prandtl number is defined as:

$$\text{Pr} = \frac{\mu C_p}{\kappa} \quad (2.26)$$

Reynolds number is:

$$\text{Re} = \frac{\rho |\mathbf{v}_o - \mathbf{v}| d_o}{\mu}, \quad (2.27)$$

The velocity of the dispersed phase is $|\mathbf{v}_o|$. There are again two possible approaches. The first is to assume the velocity of the dispersed phase to be the same as the velocity of the continuous phase. In this case $\mathbf{v} = \mathbf{v}_o$. This can be assumed if the size of the droplet defined by equation (2.23) is small, e.g. less than 20 μm . If this is not the case, a different approach has to be applied and the velocity vector of the dispersed phase has to be calculated by another procedure. Whatever the velocity, the temperature of the dispersed phase is derived from the balance of two equations that define heat transfer namely: (2.22), which represents the amount of heat taken in by the dispersed phase, and (2.24) which defines amount of heat given out by the continuous phase. This can be written as:

$$m_o C_{p_o} \frac{T_o^k - T_o^{k-1}}{\delta t} = \pi d_o \kappa \text{Nu} (T - T_o^k), \quad (2.28)$$

where T_o^k and T_o^{k-1} are temperatures of the dispersed phase in the two consecutive time steps.

When equation (2.25) is applied, the temperature of the dispersed phase becomes:

$$T_o = T_o^k = \frac{T + k_t T_o^{k-1}}{1 + k_t}, \quad (2.29)$$

where the time constant k_t is defined as:

$$k_t = \frac{m_o C_{p_o}}{\pi d_o \text{Nu } \kappa \delta t} \quad (2.30)$$

In all the previous equations, the mass of the dispersed phase in the control volume is calculated from the mass concentration c_o defined from equation (2.10) as:

$$m_o = \rho_o V_o = \frac{\rho_o \rho V c_o}{\rho(1 - c_o) + \rho_o c_o} \quad (2.31)$$

where ρ_o and ρ are the densities of the dispersed and the continuous phases respectively. Both densities are calculated from the equation of state (2.19).

The last term in equation (2.21) represents heat transfer due to mass transfer between the phases. It is significant when a real fluid evaporates or condenses in the machine. It can be expressed as:

$$\dot{Q}_{mass} = h_L \frac{dm_L}{dt} \approx h_L \frac{\Delta m_L}{\delta t} = h_L \frac{m_L - m_L^s}{\delta t} = h_L \dot{m}_L, \quad (2.32)$$

where Δm_L is the mass exchanged between the liquid dispersed phase and the continuous phase. It is defined as the difference between the mass of the continuous phase in the control volume, calculated from the mass balance equation (2.2), and the mass of the continuous phase, calculated by the equation of state (2.19), at the pressure obtained from the governing equations and the saturation temperature at the same pressure.

The latent heat of evaporation h_L is the difference between the specific enthalpy of the liquid h_l and the specific enthalpy of the vapour h_v at saturation pressure p , which is calculated from the model:

$$h_L = h_v - h_l \quad (2.33)$$

Since these two specific enthalpies at present are not known they should be calculated together with other properties of the real fluid.

The heat fluxes calculated from equations (2.24) and (2.32) represent the source terms in the energy equation (2.8).

The Mass Source

The mass of the dispersed phase changes in two-phase flow because of evaporation or condensation in the control volume. The amount of mass exchanged between the two phases is defined as:

$$\dot{m}_L = \frac{dm_L}{dt} \approx \frac{\Delta m_L}{\delta t} = \frac{m_L - m_L^s}{\delta t}. \quad (2.34)$$

In practice, if the control volume is assumed constant during one time step, the pressure and temperature are calculated from the governing equations together with the mass of the continuous phase. The mass concentration of the dispersed phase is calculated from equation (2.10). This procedure defines the mass of the dispersed phase m_o through equation (2.31). If two-phase flow exists in the control volume, the temperature of the mixture is the saturation temperature for the calculated pressure. If the temperature calculated by the model does not satisfy this condition, mass must be exchanged between the dispersed and continuous phases to establish equilibrium. The exchanged mass transfers the heat of evaporation between the phases until equilibrium is established. The heat of evaporation is calculated from the balance equation of the heat exchanged between the phases and the heat required to adjust the temperature of the mixture to the saturation temperature for the pressure calculated in the control volume:

$$\Delta m_L \cdot h_L = m \cdot C_{pm} \cdot (T - T_{sat}) \quad (2.35)$$

This mass becomes either a source or a sink in the mass equation for the continuous phase. Also, it is subtracted from the concentration of the dispersed phase through the source term in equation (2.10).

The Momentum Source

The equation of motion for an individual droplet of the dispersed phase in a positive displacement machine is given in the form of an ordinary differential equation based on Newton's second law:

$$\frac{d(m_o \mathbf{v}_o)}{dt} = \mathbf{f}_{drag} + \mathbf{f}_{pres} + \mathbf{f}_{body} + \mathbf{f}_{am}, \quad (2.36)$$

where, often, the pressure forces, \mathbf{f}_{pres} , body forces, \mathbf{f}_{body} , and apparent mass forces, \mathbf{f}_{am} , can be neglected. The interphase drag force \mathbf{f}_{drag} is:

$$\mathbf{f}_{drag} = -\frac{1}{2} \rho A_o C_{drag} |\mathbf{v}_o - \mathbf{v}| (\mathbf{v}_o - \mathbf{v}), \quad (2.37)$$

where $A_o = d_o^2 \pi / 4$ is the surface of the dispersed phase particle with Sauter mean diameter d_o , \mathbf{v}_o is the velocity of the dispersed phase in the control volume and C_{drag} is the drag coefficient which, in case of a Newtonian fluid, depends only on the Reynolds number defined by equation (2.27). When applicable, equation (2.36) is used to calculate the velocity of the dispersed phase while equation (2.27)

gives a source term for the momentum equation. If one assumes ideal heat transfer with a particle of size 0, then the drag force is also 0.

2.2.4 Equation of State of Real Fluids

Refrigerating and air conditioning and process compressors, as well as process gas compressors operate with real fluids i.e. where the assumption of ideal gas relationships is too gross. In such a case, complex functions are required to describe the fluid property changes. Commercial software packages are available today for the calculation of real fluids. Most of these packages are impractical for use in CFD because of the large number of calculations required to obtain the required thermodynamic properties. However, often users develop property software for their own requirements which gives good agreement over the required range of operating conditions.

In the case of two-phase flow, the required thermodynamic properties are: saturation temperature, density of the mixture, specific heat of the mixture, latent heat of evaporation and C_ρ . The latter is a constant that appears in the mass flux correction in the coupling procedure of the mass equation and equation of state. It defines the rate of change of density with change in pressure to correct the pressure-velocity coupling procedure. It is expressed as:

$$C_\rho = \left(\frac{\partial \rho}{\partial p} \right)_T, \quad (2.38)$$

for constant temperature in one iteration. In the case of an ideal gas, the value of this constant is derived directly from the equation of state $\frac{p}{\rho} = RT$ as:

$$C_\rho = \left(\frac{\partial \rho}{\partial p} \right)_T = \frac{\rho}{p} = \frac{1}{RT}. \quad (2.39)$$

However, for a real fluid, the equation of state is expressed as:

$$\frac{p}{\rho} = z RT = z(p, T) RT, \quad (2.40)$$

where z is the compressibility factor. This is generally a non-linear function of pressure and temperature. There are approximations derived for this factor and it is assumed here to be a linear function of the working pressure:

$$z = p B_1 + B_2, \quad (2.41)$$

where B_1 and B_2 are constants with different values for each fluid. For the ideal gas $B_1=0$ and $B_2=1$. The compressibility factor is approximated such that coefficients B_1 and B_2 are calculated from measured thermodynamic properties of saturated vapour at pressures of 1 and 20 bar. Screw machines usually operate within this range of working pressures regardless of their application and this approximation does not involve a large error in the estimation of thermodynamic properties. It leads to a maximum error of approximately 2% at 10 bar. This is sufficiently accurate, but outside this range different coefficients need to be used.

If the compressibility factor at the working pressure and temperature is known, then the density of the vapour or gas is derived from:

$$\rho_v = \frac{p}{zRT}, \quad (2.42)$$

It can be assumed that liquids in screw machines used for lubrication and generated as a result of the condensation process, are incompressible at the machine pressures. This means that the density of the liquid is constant:

$$\rho_l = \text{const}, \quad (2.43)$$

The density of a liquid-vapour mixture in the saturated domain can be written as:

$$\rho = \frac{1}{\frac{1-c_2}{\rho_v} + \frac{c_2}{\rho_l}} = \frac{p}{(1-c_2)zRT + \frac{c_2}{\rho_l}p}, \quad (2.44)$$

To obtain an equation for C_p , the temperature is regarded as constant within the iteration. The first derivative of equation (2.44) gives:

$$\left(\frac{d\rho}{dp} \right)_T = \frac{1 - (1-c_2)\rho RT \frac{dz}{dp} - \frac{c_2}{\rho_l}\rho}{(1-c_2)zRT + \frac{c_2}{\rho_l}p}. \quad (2.45)$$

The derivative in the second term on the right side represents the change of compressibility factor with pressure. It follows from equation (2.41) that this derivative is constant and has the value B_1 . Introducing that feature into the previous equation, the coefficient C_p can finally be obtained as:

$$C_\rho = \left(\frac{d\rho}{dp} \right)_T = \frac{1 - (1 - c_2) \rho RT B_1 - \frac{c_2}{\rho_l} \rho}{(1 - c_2) z RT + \frac{c_2}{\rho_l} p}. \quad (2.46)$$

If as a consequence of the pressure and temperature in the control volume, the working fluid is liquid, which gives $c_2 = 1$, the coefficient C_ρ reads zero and its value is not a function of pressure. If only vapour or real gas occupy the working chamber, $c_2 = 0$ and equation (2.46) becomes:

$$C_\rho = \left(\frac{d\rho}{dp} \right)_T = \frac{1}{zRT} - \frac{\rho_v B_1}{z}. \quad (2.47)$$

If the fluid is ideal, then B_1 becomes zero and z tends to one. In that case equation (2.46) becomes the same as equation (2.39). However, if the fluid is real, B_1 becomes slightly negative and z tends to values less than 1. This means that the second term becomes positive and it contributes to the value of the first term. The value of that term increases with the change of the 'fluid reality', which is expressed through constants B_1 and B_2 in (2.41). This term becomes significant in comparison with the first term if the fluid is real. In the case of ammonia, for example, at a pressure of 5 bar the first term has a value of $6.7 \cdot 10^{-6}$ while the value of the second term is $2.9 \cdot 10^{-2}$. The coefficient C_ρ derived from equation (2.47) is later used for the calculation of pressure in the pressure-velocity-density coupling procedure.

Other thermodynamic properties are not directly derived from the equation of state but, as a consequence of the fluid behaviour, these are calculated from thermodynamic properties of both the liquid and vapour phases.

The saturation temperature is calculated from a modified version of Antoine's equation, which is in its original form expressed as:

$$\log p = A_1 - \frac{A_2}{t + A_3} \quad (2.48)$$

which is an explicit expression for saturation pressure as a function of temperature, *Walas* (1984). Constants A_1 , A_2 and A_3 vary for different fluids and they are obtained from experimental results. The value of the coefficient A_3 is usually small and in many cases can be neglected. In that case, the equation explicitly gives saturation temperature in terms of pressure as:

$$T_{sat} = \frac{A_2}{A_1 - \log p} - A_3 \quad (2.49)$$

The saturation temperature calculated from the previous equation is used in equation (2.35) to estimate the mass exchanged during evaporation/condensation. That equation gives the mass which transfers the latent heat of evaporation from one phase to the other. The latent heat of evaporation is calculated for the saturation pressure by means of the Clapeyron equation. This is expressed as:

$$h_L = T_{sat} v_{lv} \left(\frac{dp}{dT} \right)_{sat}, \quad (2.50)$$

where v_{lv} is the difference between the vapour and liquid specific volumes. Typically, more about equation (2.50) can be found in *Cengel and Boles* (1989).

The specific heat at constant pressure is a fluid property needed to calculate the specific enthalpy of the mixture. The specific heat of the mixture C_{pm} is the weighted sum of the specific heats of vapour C_{pv} and liquid C_{pl} for constant pressure, ie:

$$C_{pm} = (1 - c_2) C_{pv} + c_2 C_{pl} \quad (2.51)$$

The specific heat of vapour can be calculated from the following equation:

$$C_{pv} = D_0 + D_1 T + D_2 T^2 + D_3 T^3 \quad (2.52)$$

where D_0 , D_1 , D_2 and D_3 are constants which vary for different fluids. Their values can be found in *Sonntag and Borgnakke* (2001). If the specific heat of liquid at constant pressure is assumed constant, which is reasonably accurate over a limited temperature range, then equation (2.51) gives the specific heat of the mixture. Even if the concentration of the liquid phase in the working chamber is equal to zero, this equation can be used to express the specific heat of the working fluid, which in this case is vapour.

By use of the equations derived in this Section, the properties of real fluids, which are liquid, vapour or their mixture, are completely described. The procedure is fast and efficient for calculation in the numerical CFD solver, because all equations are analytical and the variables are derived explicitly from the pressure, the value of which is obtained from the mass-velocity-pressure coupling procedure. The procedure is equally applicable to ideal gases, and incompressible fluids. The coefficient C_p calculated from the equation (2.46) is used in the next iteration as a source term.

2.2.5 Turbulent Flow

Turbulent flows are well described by the governing differential equations presented in section 2.2. However, their direct numerical simulation requires a mesh with spacing smaller than the length scale of the smallest turbulent eddies, at

which the energy is transformed to heat, and time steps smaller than the smallest time scale of the turbulent fluctuations. Some calculations show that the average length scale of the smallest eddies in positive displacement machines is of the order of $10\mu m$ while their time scale is of the order of a couple of milliseconds. This requires computer resources, which are not yet available.

Alternatives are either large eddy simulation, in which only the largest unsteady motions are resolved and the rest is modelled, or a solution to the Reynolds averaged Navier-Stokes equations where all turbulent effects on the mean flow are modelled as functions of mean fluid flow quantities.

The Reynolds averaged Navier-Stokes equations (RANS) are obtained by using a statistical description of the turbulent motion formulated in terms of averaged flow quantities. Many such models of turbulence are developed to date, which are suitable for different fluid flow situations. Only two of them are described in some details in Appendix A. These are the Zero-Equation model and the Standard $k-\varepsilon$ two-equation model. More details on turbulence phenomena can be found for example in *Wilcox* (1993).

2.2.6 Pressure Calculation

The pressure in the source term of the fluid momentum equation is unknown because it does not appear explicitly in the continuity equation. This constraint is satisfied only if the pressure field is adjusted to the resulting fluid flow. The method of calculation of the pressure and pressure gradient fields consists now of three steps. The first one is to obtain the velocity field from the momentum equation regardless of whether the continuity equation is satisfied or not. The second is a predictor stage in which a pressure correction is calculated to satisfy the continuity equation and the third one is a corrector stage in which new values of the velocity, pressure and density fields are calculated. The method is known as a SIMPLE algorithm and is described in Appendix C.

2.2.7 Boundary Conditions

Special treatment of boundaries is introduced due to the compressor communicating with its surroundings through small receivers at suction and discharge and also through oil injection. The common practice is to keep the pressure in these receivers constant. Therefore, an appropriate amount of mass and energy is added or subtracted from these receivers.

Wall Boundaries

There are two types of walls applied to a screw compressor; moving walls, if they bound the domain on the compressor rotors, and stationary walls in other places. Boundary conditions on these walls are explicitly given for all equations in the

numerical model. In the case of turbulent flow, dependent variables vary steeply near the solid boundaries and a method, which can model near wall effects, is used. If the flow is laminar, then the dependent variable is either known on the boundary, or its flux is given on the boundary. The walls are treated as ‘no-slip walls’, which is the case when viscous fluid sticks to the boundary wall.

Boundary conditions for the momentum equation are given through the known velocities on the wall. For the rotor walls, the velocities are calculated from the given rotational speed n of the male rotor as:

$$\begin{aligned}\omega_1 &= \frac{2n\pi}{60}; & \mathbf{v}_{1i} &= \mathbf{r}_{1i} \omega_1 \\ \omega_2 &= -\omega_1 \frac{z_1}{z_2}; & \mathbf{v}_{2i} &= \mathbf{r}_{2i} \omega_2\end{aligned}\tag{2.53}$$

Subscript 1 indicates the male rotor while the value 2 is related to the female rotor. z_1 and z_2 are the number of lobes on the rotors, \mathbf{r}_{1i} and \mathbf{r}_{2i} are radius vectors of the boundary points on the male and female rotors respectively in an absolute coordinate system. ω_1 and ω_2 are the angular velocities on the male and female rotors respectively. For all stationary walls, the wall velocity is equal to zero.

More details of the equations, which incorporate wall boundaries to the mathematical model of the screw compressor process, are given in B.

Constant Pressure in the Inlet, Outlet and Oil Receivers

Even if the compressor cycle can be considered steady, this is true only if it is averaged in time over a period in which a compressor completes a number of cycles. However, within one cycle, the compressor system is always in a state of transition. Such a transition is caused by rotation of the rotors, which moves the corresponding part of the numerical mesh. That movement is defined by the angular velocity ω_r . Movement of the computational domain causes change in its volume, which further causes pressure change within it. The pressure difference between the cells causes fluid to flow through the machine. Contrary to the rotor domains, other parts of the compressor such as the inlet and outlet ports and receivers maintain a constant volume. The fluid flow induced between the rotors inevitably leads to change of the pressure in the parts which keep a constant volume. In a real compressor, such a situation causes additional fluid to flow into or out of the chambers, keeping the pressure constant. This process is simulated in the numerical procedure.

The first possibility is to apply standard inlet and outlet boundaries. However, in that case, either the inlet velocity or the mass flux should be prescribed in advance, which is extremely difficult. The compressor flow depends on the rotor speed and varies considerably during the cycle. Additionally, reverse flow can exist at the outlet boundary if it is not far enough from the discharge port. That situa-

tion is not allowed with the standard boundary conditions. Therefore, these boundary conditions are not adequate for a screw compressor.

The other possibility is to apply pressure boundaries at the inlet and outlet. In the standard pressure boundary condition a prescribed pressure on the boundary is combined with the following boundary condition:

$$\left(\frac{\partial \mathbf{v}}{\partial n} \right)_B = 0 \quad (2.54)$$

to obtain boundary velocities $\mathbf{v}_B(\mathbf{r}_b, t)$. Other treatments are necessary in the case of supersonic and subsonic flows. If the outlet flow is supersonic, then both the pressure and the velocity should be obtained by extrapolating from the upstream region. It is obvious that the pressure boundary conditions are similar to the inlet or outlet boundaries, firstly because they couple pressure and velocity directly and secondly because for all equations, apart from the momentum equation, the boundary properties are calculated from the velocity. This procedure may cause instability in the compressor cycle especially when the flow changes its direction at the boundary.

In opposition to both types of boundary condition mentioned above, application of the boundary domain, in which an amount of mass is added or subtracted to maintain constant pressure, is natural and gives a stable and relatively fast solution.

Starting from the equation of state for a real fluid (2.40) for constant instant temperature and density of fluid in a receiver of volume V , or in an individual numerical cell of volume V_i , the following equation can be derived:

$$\dot{V}_{add} = \frac{\partial V_i}{\partial t} = \frac{V_i}{p_i} \frac{\partial p_i}{\partial t} \quad (2.55)$$

It gives the relation between the volume change and the pressure change. The value of V_i is the volume flow that corresponds to the change in pressure ∂p_i during time ∂t . As the density is assumed constant, then the mass flux, which corresponds to the pressure change, is:

$$\dot{m}_{add} = \rho_i \frac{V_i}{p_i} \frac{\partial p_i}{\partial t} \quad (2.56)$$

This is the amount of mass, which must be added or subtracted to a receiver of constant volume V or to an individual numerical cell placed in the considered receiver to maintain constant pressure.

The amount of mass calculated from (2.56) represents a mass source in the pressure correction procedure explained in Section 2.2.6. It will maintain constant

pressure in the considered cell and the momentum equation correction would result in a new velocity in the cell.

The energy equation is corrected in order to keep the system in balance. It is done through the volume source in the governing equation of energy:

$$\dot{q}_{add} = m_i C_{pi} \frac{\partial T_i}{\partial t} = m_i C_{pi} \frac{T_i - T_r}{\partial t}. \quad (2.57)$$

In the last term of equation (0.57) T_i is the temperature calculated in the cell, T_r is the specified temperature which has to be maintained and ∂t is the time step.

When an amount of mass of dispersed phase is added to the selected set of cells, the equation for species also has to be updated. The concentration of the dispersed phase can be known, or prescribed, in some domains while in others it has to be estimated. For example, the concentration of oil in the oil injection port always has a value which is close to 1. Similarly, the concentration of liquid in the inlet port of a two-phase expander is defined by the pressure and quality of the mixture. However, there are some compressor domains where the value of concentration is not known but the pressure has to be maintained constant. In that case, the value of concentration must be extrapolated from the neighbouring domain.

When the concentration is known, then its value should be kept as close as possible to the prescribed value. The mass of the dispersed phase carried by the continuous phase is calculated by equation (2.31) in which the concentration c_o is substituted by the prescribed value c_p . The last term in the transport equation for the concentration of the dispersed phase (2.10), is the volume source term, which is expressed as:

$$\int_V S_{c_i} dV = S_{c_i} V_i = \rho \frac{\partial c_i}{\partial t} V_i = \dot{m}_i. \quad (2.58)$$

This volume source, when integrated over the cell volume, is the amount of mass of the dispersed phase added to or subtracted from the mass of the numerical cell. If the concentration of the dispersed phase has to be maintained constant, a correction to the equation of species has to be added through the volume source. The source term in equation (2.10) is the mass flux of the dispersed phase. Its calculation is based on the desired concentration of the dispersed phase. Equation (2.31) is used for that and c_o is replaced by the desired concentration in the cell. In such a situation, the volume source in the oil concentration equation becomes:

$$S_{c_o} = \int_V S_{c_o} dV = m_{oadd} = \frac{\rho_o \rho_m V c_{ocons}}{\rho_m (1 - c_{ocons}) + \rho_o c_{ocons}} \quad (2.59)$$

In the case of two-phase flow with evaporation or condensation, the equation for the concentration of the liquid phase of the working fluid has to be updated through its volume source term. This term is calculated from equation (2.34) as:

$$S_{c_l} = \int_V S_{c_l} dV = -\dot{m}_L \approx -\frac{\Delta m_L}{\delta t} \quad (2.60)$$

Other equations, like these for the turbulence model, do not need to be updated for this case.

2.3 Finite Volume Discretisation

2.3.1 Introduction

The finite volume method is employed to solve fluid flow equations. It can also be applied to solid body stress analysis, independently or when coupled with fluid flow. The method is fully implicit and can accommodate both structured and unstructured moving grids with cells of arbitrary topology. Although the procedure is described here for fluid flow in screw compressors, it is general and can be used for any physical problem which is described by the given equation set.

A segregated approach is used to solve the resulting set of coupled non-linear system of algebraic equations. The equations are solved by an iterative conjugate gradient solver which retains the sparsity of a coefficient matrix, thus achieving the efficient use of computer resources.

If an appropriate constitutive relation is applied to each conservation law, namely mass, momentum and energy balance, a closed set of M equations is obtained for each numerical cell in a particular time step. The number of equations M depends on the problem that has to be solved. 7 equations are required for a screw compressor, including two-phase flow with oil injection. All the conservation equations can be conveniently written in the form of the following generic transport equation:

$$\frac{d}{dt} \int_V \rho \phi dV + \int_S \rho \phi (\mathbf{v} - \mathbf{v}_s) \cdot d\mathbf{s} = \int_S \Gamma_\phi \text{grad } \phi \cdot d\mathbf{s} + \int_S \mathbf{q}_{\phi S} \cdot d\mathbf{s} + \int_V q_{\phi V} \cdot dV \quad (2.61)$$

The continuity equation is combined with the momentum equation to obtain an equation for pressure or pressure correction. The meaning of symbols used in this equation is given in the nomenclature. The diffusive flux and sources are given in

Table 2-1 for each property ϕ .

Table 2-1 Terms in the generic transport equation (2.61)

Equation	ϕ	Γ_ϕ	$\mathbf{q}_{\phi S}$	$q_{\phi V}$
Continuity	1	0	0	0
Fluid Momentum	v_i	μ_{eff}	$\left[\mu_{\text{eff}} (\text{grad } \mathbf{v})^T - \left(\frac{2}{3} \mu_{\text{eff}} \text{div } \mathbf{v} + p \right) \mathbf{I} \right] \cdot \mathbf{i}_i$	$f_{b,i}$
Solid Momentum	$\frac{\partial u_i}{\partial t}$	η	$\left[\eta (\text{grad } \mathbf{u})^T + (\lambda \text{div } \mathbf{u} - 3K\alpha\Delta T) \mathbf{I} \right] \cdot \mathbf{i}_i$	$f_{b,i}$
Energy	e	$\frac{k}{\partial e / \partial T} + \frac{\mu_t}{\sigma_T}$	$-\frac{k}{\partial e / \partial T} \frac{\partial e}{\partial p} \cdot \text{grad } p$	$\mathbf{T} : \text{grad } \mathbf{v} + h$
Concentration	c_i	$\rho D_{i,\text{eff}}$	0	s_{ci}
Space	$\frac{1}{\rho}$	0	0	0
Turbulent kinetic energy	k	$\mu + \frac{\mu_t}{\sigma_k}$	0	$P - \rho \varepsilon$
Dissipation	ε	$\mu + \frac{\mu_t}{\sigma_\varepsilon}$	0	$C_1 P \frac{\varepsilon}{k} - C_2 \rho \frac{\varepsilon^2}{k} - C_3 \rho \varepsilon \text{div } \mathbf{v}$

The ability of expressing all transport equations in the form of a prototype equation (2.61) facilitates the discretisation procedure, which together with the appropriate initial and boundary conditions, forms the mathematical model of continuum mechanics problems.

The Finite Volume Method (FVM) is used to discretise the governing equations. All dependent variables are stored in a collocated variable arrangement, which requires only one set of control volumes to be generated. This enables eventual implementation of the multigrid method and local grid refinement.

Equation (2.61) can be written for a control volume in a Cartesian coordinate frame, as presented in Figure 2-2. This equation is still general and exact:

$$\frac{d}{dt} \int_V \rho \phi dV + \sum_{j=1}^{n_f} \int_{S_j} \rho \phi (\mathbf{v} - \mathbf{v}_s) \cdot d\mathbf{s} = \sum_{j=1}^{n_f} \int_{S_j} \Gamma_\phi \text{grad } \phi \cdot d\mathbf{s} + \left(\sum_{j=1}^{n_f} \int_{S_j} \mathbf{q}_{\phi S} \cdot d\mathbf{s} + \int_V q_{\phi V} \cdot dV \right) \quad (2.62)$$

It consists of four terms which describe the effects of rate of change with time, convection, diffusion and source respectively. For each cell, all quantities are then written in the form of equation (2.62) and set up as a system of $n*m$ partial differential equations. Each cell acts as a control volume, the total number of which is n , while the number of unknowns for each cell is m . These are all transferred to a system of $n*m$ algebraic equations in order to be solved numerically.

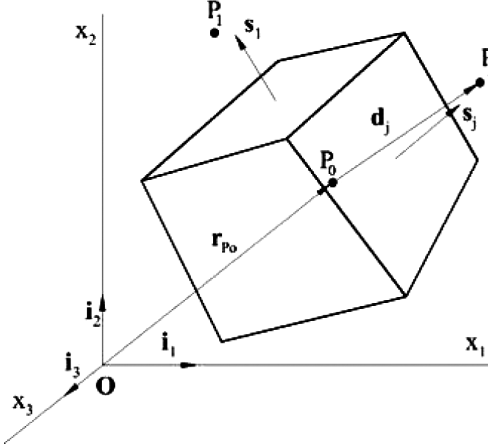


Figure 2-2 Notation applied to a hexahedral control volume

Therefore, the surface and volume integrals, appearing in the equations are replaced by quadrature approximations, the spatial derivatives are replaced by an interpolation function and the time integration scheme is selected and after that the control volume surface velocities \mathbf{v}_s are determined.

2.3.2 Space Discretisation

In this work, space is discretised by an unstructured mesh with polyhedral control volumes with an arbitrary number of faces. However, hexahedra are used wherever possible, which facilitates the local grid refinement. In some cases this may be essential for accuracy. The spatial discretisation of a screw compressor working domain is presented in a separate chapter.

2.3.3 Time Discretisation

The time interval of interest is divided into an arbitrary number of subinterval time steps, which are not necessarily of the same duration. However, the procedure used for mesh movement requires the time steps in the simulation procedure of the screw compressor working cycle to be constant. It is aimed that all variables at the start and end of a calculation cycle are equal. The calculation cycle is represented by rotation of the male rotor either for a full revolution or only for one lobe rotation. The constant time step, however, is not given arbitrarily. It depends on the chosen number of rotational steps within the tooth span angle on the male rotor and the speed of rotation n . The angular speed of the male rotor is:

$$\omega_1 = 2\pi \frac{n}{60} \quad [\text{rad} / \text{s}]. \quad (2.63)$$

If the compressor rotates at constant speed, the unit angle is:

$$\delta\varphi = \frac{\varphi}{n_{ang}} \quad (2.64)$$

where φ is the interlobe angle of the male rotor and n_{ang} is number of divisions of that angle for the rotation of one full interlobe. The time step is then defined as

$$\delta t = \frac{\delta\varphi}{\omega_1} \quad (2.65)$$

Although the time step in the majority of calculations of screw compressor performance is constant, if a transient state has to be calculated, the time step changes during marching in time. This is especially the case for compressor start up and shut down procedures. In these cases, the time step within two consequent rotations of the compressor rotors depends on the first time derivative of the compressor speed. Again, it is necessary to calculate the angular velocity for each time step and consequently to update the time step.

2.3.4 Discretisation of Equations

Discretisation Principles

The result of discretisation of the prototype equation (2.62) is a system of algebraic equations. Surface and volume integrals are replaced by quadrature approximations, spatial derivatives are replaced by some interpolation function and either a two-times-level or a three-times-level integration scheme in time is selected. These procedures are explained in detail in Appendix C.

Boundary and Initial Conditions

The boundary conditions on the cell faces which coincide with the solution domain boundary are applied prior to solution of the algebraic equations. All compressor solid parts are no-slip walls with either, a known temperature or a temperature approximated, in advance, through a known procedure. Therefore a cell face flux ϕ_j^* represents the boundary flux ϕ_B for all equations in the boundary cells. In such a case, the mass flux in the momentum equation at the boundary is zero, the heat flux through the boundary for the energy equation is calculated from the wall temperature and the thermal conductivity in the near wall region, while the concentration flux is zero. Diffusive fluxes are also replaced with their boundary values.

Screw compressor flow simulation is transient, which requires initial conditions to be prescribed for the dependent variables in each control volume. A close match of these is important for quick solution convergence.

The initial values of the velocities in the momentum equation are set to zero in all cells within the working chamber. The initial pressures prescribed for the cells in the inlet and outlet receiver are the inlet and outlet pressure. For all other cells the initial values are calculated by linear interpolation between these values with respect to the relative distance in the z direction as:

$$p_i^0 = p_{inl}^0 + \frac{z_i}{L} (p_{out}^0 - p_{inl}^0). \quad (2.66)$$

z_i is the cell centre distance starting from the coordinate origin, while L is the overall compressor length. This simple method to prescribe initial values often gives a consistent final solution within 4 to 5 compressor cycles. The initial temperature is calculated in the same manner as the pressure by linear interpolation between prescribed inlet and outlet temperatures. The density is then calculated according to equation (2.44). Concentration is also interpolated between the prescribed values at the inlet ρ_{inl}^0 and outlet ρ_{out}^0 of the compressor similarly to the other variables. The initial values of kinetic energy and its dissipation rate are set as zero throughout the domain.

If implicit time integration is employed, these prescribed values at time t_0 are sufficient for the calculation. If, however, the three time level implicit scheme is used, values at the time $t_{-1} = t_0 - \delta t_0$ must be given. They are set at the same value as those at time t_0 .

Derived System of Algebraic Equations

If discretisation methods and boundary conditions are implemented in the prototype equation (2.62) for all control volumes then the derived algebraic equation has the same form for all variables:

$$a_{\phi 0} \phi_{P_0} - \sum_{j=1}^{n_i} a_{\phi j} \phi_{P_j} = b_{\phi} \quad (2.67)$$

where index 0 determines the control volume in which the variable is calculated and index j defines the neighbouring cells. Symbol n_i represents a number of internal cell faces between the calculating cell and its neighbouring cells. The right hand side contains all terms for which the variables are known from either the previous iteration or the time step. All the coefficients, central $a_{\phi 0}$, neighbouring $a_{\phi j}$ and right hand side b_{ϕ} , are treated explicitly using a deferred correction approach to increase computational efficiency.

$$\begin{aligned}
a_{\phi j} &= \Gamma_{\phi j} \frac{\mathbf{s}_j \cdot \mathbf{s}_j}{\mathbf{d}_j \cdot \mathbf{s}_j} - \min(\dot{m}_j, 0), \\
a_{\phi 0} &= \sum_{j=1}^{n_f} a_{\phi j} + \frac{(\rho V)_{P_0}^{m-1}}{\delta t_m}, \\
b_{\phi} &= \sum_{j=1}^{n_f} \Gamma_{\phi j} \left((\text{grad } \phi)_j \cdot \mathbf{s}_j - \overline{\text{grad } \phi} \cdot \mathbf{d}_j \frac{\mathbf{s}_j \cdot \mathbf{s}_j}{\mathbf{d}_j \cdot \mathbf{s}_j} \right) - \\
&\quad \sum_{j=1}^{n_f} \frac{\gamma_{\phi}}{2} \dot{m}_j \left((\mathbf{r}_j - \mathbf{r}_{P_0}) \cdot (\text{grad } \phi)_{P_0} + (\mathbf{r}_j - \mathbf{r}_{P_0}) \cdot (\text{grad } \phi)_{P_j} + (\phi_{P_j} - \phi_{P_0}) \frac{\dot{m}_j}{\text{abs}(\dot{m}_j)} \right) + \\
&\quad Q_{\phi S} + Q_{\phi V} + \sum_{B=1}^{n_B} a_{\phi B} \phi_B + \frac{(\rho V \phi)_{P_0}^{m-1}}{\delta t_m}.
\end{aligned} \tag{2.68}$$

\mathbf{d}_j is a distance vector. It is effective if the mesh is non-orthogonal and it is then used to correct the cell face value. It is defined as the normal distance between the line connecting two neighbouring cell points and the cell face centre. n_B is the number of boundary faces surrounding the cell P_0 . The coefficient $a_{\phi B}$ for the centre point at the boundary cell face is calculated similarly to the neighbouring coefficient $a_{\phi j}$, assuming the distance between the boundary point and the centre of the cell.

2.4 Solution of a Coupled System of Nonlinear Equations

Equations in the form of (2.67) are obtained for each dependent variable like velocity, pressure, temperature and concentration at all points of the computational domain. As a consequence of convective transport and because of other flow characteristics, the equations are non-linear and coupled. In order to be solved, they are linearized and decoupled. The segregate iterative algorithm is adopted.

Coefficients $a_{\phi j}$ and source terms b_{ϕ} are known in advance from the previous iteration or time step. As a result, a system of linear algebraic equations is obtained for each dependent variable. This can be written in matrix notation as:

$$A_{\phi} \boldsymbol{\phi} = \mathbf{b}_{\phi} \tag{2.69}$$

Here A_{ϕ} is an $N \times N$ matrix, the vector $\boldsymbol{\phi}$ contains values of the dependent variables ϕ at N nodal points in the CV centres and \mathbf{b}_{ϕ} is the source vector. The resulting matrix A_{ϕ} obtained by the discretisation method is sparse, with the number of non-zero elements in each row equal to the number of nearest neighbours plus one, $n_i + 1$. The matrix is symmetric only for the momentum equation of an elastic solid body and the pressure correction for incompressible fluids. The matrix is diagonally dominant $A_{\phi 0} \geq \sum_{j=1}^{n_i} a_{\phi j}$. This allows solution of the equation system

(2.69) by a number of iterative methods resulting in reasonable computer memory requirements. The conjugate gradient method (CG) is used when the matrix is symmetric and the preconditioned conjugate gradient stable method (CGSTAB) is used when the matrix is asymmetric.

Equation (2.69) is then solved in sequence for each dependent variable. There is no need to solve it to a tight tolerance since its coefficients and sources are only approximate based on the values of the dependent variables from the previous iteration or time step. These iterations are called inner iterations.

The sequence is then repeated in the outer iterations by updating the coefficient matrix and the source terms until the solution converges.

$$\mathbf{r}_\phi = A_\phi \phi - \mathbf{b}_\phi \quad (2.70)$$

The convergence criterion is usually achieved when the residuals of (2.70) are reduced by three to four orders of magnitude.

2.5 Calculation of Screw Compressor Integral Parameters

Once a solution is obtained in the form of the velocity and pressure fields within the compressor, integral parameters which quantify the screw compressor working cycle, are calculated.

Integral parameters are used to evaluate and compare the processes in screw machines and to serve as input parameters for the design of these machines. They are divided into two groups; those based on the compressor delivery, which is the volume flow calculated at the suction conditions, and those based on the compressor power input. Other integral parameters are calculated from the previous two. These are specific power, volumetric and adiabatic efficiencies, load on the compressor rotors and bearings, torque on the male and female rotors and oil flow. Apart from these, the indicator diagram can be calculated from the pressure distribution within the compressor working cycle.

The volume flow is calculated at the inlet and at the outlet of the screw compressor by the use of the Gauss divergence theorem to calculate flow from the velocity in each particular cell in a cross section and then to integrate all of them over the complete cross section, or by integration of the mass sources along the inlet and outlet receivers.

The Gauss divergence theorem:

$$\int_s \mathbf{v} \cdot d\mathbf{s} = \int_V \text{div} \mathbf{v} dV \quad (2.71)$$

This equation is integrated over a layer of cells in the cross section of the inlet or outlet port to get:

$$\dot{V}_f^{(t)} = \sum_{i=1}^I v_f S_{fi} \quad (i = 1, 2, \dots, I) \quad (2.72)$$

where index f represents the direction of flow. S and v are the cell surface area and the velocity component in the direction of fluid flow. Equation (2.72) is calculated for each time step in the compressor working cycle and integrated over the complete cycle to estimate the volumetric flow at that cross section pressure and temperature:

$$\dot{V} = 60 \cdot \sum_{t=t_{start}}^{t_{end}} \dot{V}^{(t)} \quad [m^3/\min] \quad (2.73)$$

The volume flow obtained from this equation can be compared with the volume flow calculated from the mass added to or subtracted from the inlet and outlet receivers. These two should be the same for each time step as well as for the complete compressor cycle.

The mean density values for equal cell volumes are calculated for each time step together with the main flow:

$$\bar{\rho}^{(t)} = \frac{\sum_{i=1}^I \rho_i}{I} \quad (2.74)$$

If the mean density is multiplied by the corresponding volume flow it gives the mass flow in its integral form as:

$$\dot{m} = \sum_{t=t_{start}}^{t_{end}} \dot{V}^{(t)} \cdot \bar{\rho}^{(t)} \quad (2.75)$$

The compressor mass flow is calculated separately for the inlet and outlet chambers and these values must be identical for steady flow conditions. If they differ, then the procedure has not converged.

Another group of variables is based on the value of pressure in the working chamber.

A cell on the rotor boundary is shown in Figure 2-3. The pressure in the cell generates the force on the boundary surface. That force is calculated as the product of the pressure in the rotor boundary cell and the boundary cell surface area. This force can be also divided in three components acting in the x , y and z directions of the absolute coordinate system. When calculated, these three components are:

$$F_x = p_b A_{xb}; \quad F_y = p_b A_{yb}; \quad F_z = p_b A_{zb}, \quad (2.76)$$

where p_b is the pressure in the boundary cell and A_{xb} , A_{yb} and A_{zb} are projections of the boundary cell surface in the main directions of the absolute coordinate system.

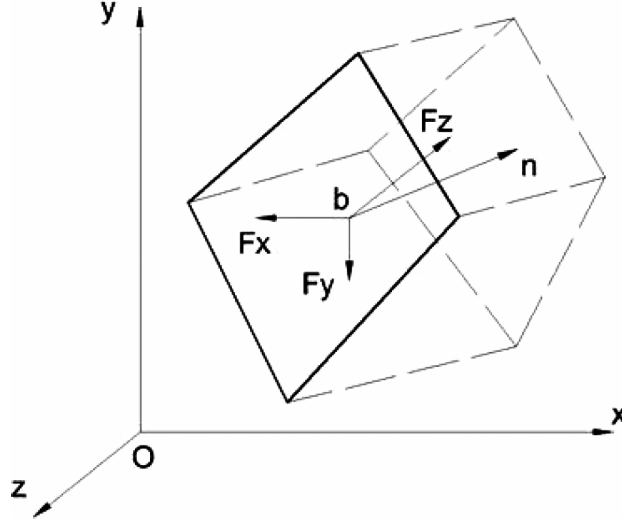


Figure 2-3 Pressure forces on the boundary surface

A free body diagram, with all pressure forces acting on a cell face and the restraint forces, is shown in Figure 2-4.

The balance for both, male and female rotor is expressed by the same set of equations:

$$\begin{aligned}
 \Sigma F_x=0: & \quad F_{xD}(i) + F_{xS}(i) - F_x(i) = 0 \\
 \Sigma F_y=0: & \quad F_{yD}(i) + F_{yS}(i) - F_y(i) = 0 \\
 \Sigma F_z=0: & \quad F_a(i) - F_z(i) = 0 \\
 \Sigma M_x=0: & \quad -F_{yD}(i)l + F_y(i)z(i) - F_z(i)y(i) = 0 \\
 \Sigma M_y=0: & \quad F_{xD}(i)l - F_x(i)z(i) + F_z(i)[x(i) - a] = 0 \\
 \Sigma M_z=0: & \quad T + F_x(i)y(i) - F_y(i)[x(i) - a] = 0
 \end{aligned} \tag{2.77}$$

In these equations l is the rotor length. This set of equations applies both to the male rotor, where $a=0$ and to the female rotor where a is equal to the distance between the centre lines of the rotor axes.

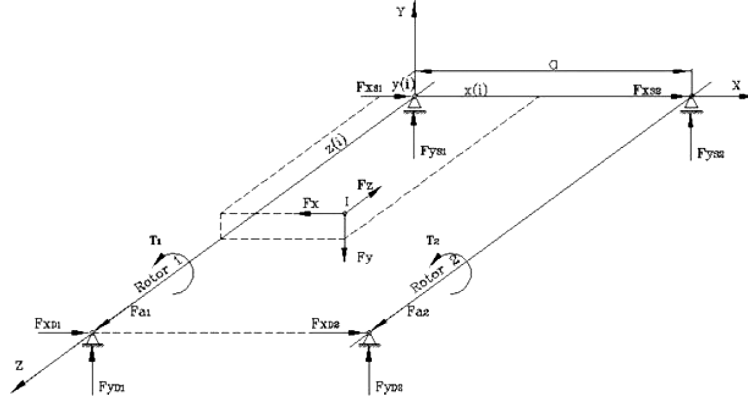


Figure 2-4 Restraint forces and torques on rotors

The torque and restraint forces on the suction and discharge bearings are calculated from these equations as:

$$\begin{aligned}
 F_{xs}(i) &= \frac{F_y(i)z(i) - F_z(i)y(i)}{l} & F_{xd}(i) &= F_x(i) - F_{xs}(i) \\
 F_{ys}(i) &= \frac{F_x(i)z(i) - F_z(i)[x(i) - a]}{l} & F_{yd}(i) &= F_x(i) - F_{xs}(i) \\
 F_{rs}(i) &= \sqrt{F_{xs}^2(i) + F_{ys}^2(i)} & F_{rd}(i) &= \sqrt{F_{xd}^2(i) + F_{yd}^2(i)} \\
 T(i) &= F_x(i)y(i) - F_y(i)[x(i) - a] & F_a(i) &= F_z(i)
 \end{aligned} \tag{2.78}$$

All the forces in equation (2.78) are support forces caused by the pressure loads in one boundary cell i . To obtain the integral radial and axial forces and the torque they are integrated over the whole boundary and for both rotors:

$$\begin{aligned}
 F_{rs} &= \sum_{i=1}^l F_{rs}(i), [N] & F_{rd} &= \sum_{i=1}^l F_{rd}(i), [N] \\
 F_a &= \sum_{i=1}^l F_a(i), [N] & T &= \sum_{i=1}^l T(i), [Nm]
 \end{aligned} \tag{2.79}$$

Once calculated, the torque is used to estimate the power transmitted to the rotor shaft:

$$P = 2\pi(n_m T_m + n_f T_f), [W] \tag{2.80}$$

where n is the speed of the male rotor while T_M and T_F are the torque on the male and female rotors respectively. Specific power is defined as:

$$P_{spec} = \frac{P}{\dot{V}} \cdot 1000 \quad , \left[\frac{kW}{m^3 \text{ min}} \right] \quad (2.81)$$

And finally, the values η_v and η_i , the volumetric and adiabatic efficiencies respectively are:

$$\eta_v = \frac{\dot{V}}{V_d} \quad \eta_i = \frac{P_{ad}}{P} \quad (2.82)$$

where V_d is the theoretical displacement and P_{ad} is the adiabatic power input.

Since the pressure across the working chamber does not vary too much within one time step, it is sufficiently accurate to average the pressure values arithmetically in each working chamber in order to plot a pressure versus shaft angle, (p- α) diagram.

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