

Introduction to Fluid Dynamics

2.1 Basic Concepts

The behaviour of metals during filling and solidification can be described by applying the laws of fluid dynamics. In the liquid state, metals behave largely like common liquids such as water or liquefied natural gas. Molecules in liquids do not form a rigid crystalloid structure and, therefore, can move easily relative to each other. This behaviour distinguishes fluids in general from solid materials. At the same time, these molecules are packed sufficiently close to each other to experience strong forces of mutual attraction that make it hard to pull a piece of liquid apart. For the same reason, it is also hard to compress a liquid to a smaller volume. Therefore, liquids, unlike gases, can be treated as essentially *incompressible* materials, a property that greatly simplifies the governing equations.²

Fluid flow behaviour is characterized by density, pressure, temperature and velocity. Density, ρ , is the amount of mass, represented by molecules, in a unit volume of fluid. The incompressibility property implies that density stays constant during flow. In other words, no matter how a fluid is stretched, sheared or pressed, the number of molecules in a fixed volume stays more or less constant, even though some molecules may have moved out of it and others have entered it in their place.

2.1.1 Pressure

The resistance of fluid to compression is characterized by *pressure*. Huge pressures must be applied to compress a fluid by as little as 1% of its original volume. In

² In this chapter, when referring to metals we will use the terms *liquid* and *fluid*. Although the term *fluid* generally includes both incompressible liquids and compressible gases, we will primarily mean the former unless specifically clarified otherwise.

most situations, even in high-pressure die casting, the pressures are not sufficient to change the fluid volume noticeably.

Pressure is one of the main parameters that control the flow of fluid. It is related to the rate at which molecules transfer the momentum of their random microscopic motion to their neighbours through collisions. Since this random motion occurs in all directions, pressure at a point in the fluid also acts in all directions. But when molecules in one part of the fluid transfer more momentum to the molecules in an adjacent region than they receive in return, a macroscopic force arises between these fluid regions. This force can be described as the *pressure gradient*, which is the difference in pressures at two locations in the fluid, divided by the distance between those points. When pressure P is a function of the three-dimensional coordinates x , y and z , then at every point in the fluid, the pressure gradient is a vector, defined as

$$\nabla P = \left(\frac{\partial P}{\partial x}, \frac{\partial P}{\partial y}, \frac{\partial P}{\partial z} \right). \quad (2.1)$$

In the absence of other forces, flow is initiated in the direction of the pressure variation from high values to low, that is, in the direction opposite to the direction of the pressure gradient, as shown in Figure 2.1.

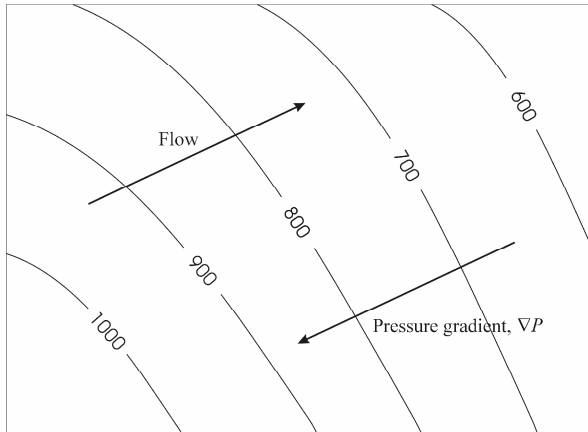


Figure 2.1. Iso-lines of pressure (isobars) showing the distribution of pressure and the direction of the pressure gradient

2.1.2 Viscosity

As with any moving objects, the motion of most fluids experiences additional forces due to *friction*. Frictional forces also arise from the collisions of molecules in a moving fluid with molecules in the slower adjacent fluid regions. These collisions result in a net transfer of momentum from the faster flow regions to the

slower ones, giving rise to frictional force. This force acts in the direction opposite the faster flow, dissipating its energy and generating heat, similar to the effect of taxes on the flow of capital. For example, if two streams of fluid are moving at different speeds parallel and next to each another, the faster moving stream will gradually slow down and the slower one will accelerate. As a result, the boundary between the two layers will widen with time leading to the development of the *viscous boundary layer*, the region where flow transitions from the velocity in one fluid layer to the velocity in the other. It is noteworthy that, as the two fluid layers exchange momentum, the overall kinetic energy in the flow decreases.

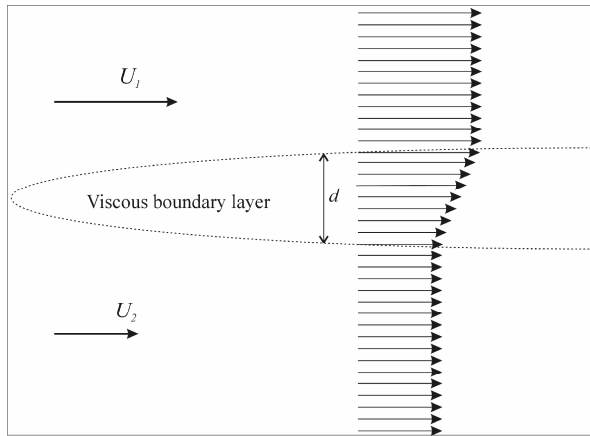


Figure 2.2. Viscous frictional force acting between two streams of fluid

The frictional properties of a fluid are conveniently described with a single variable called the *dynamic viscosity coefficient* μ , and these forces are called *viscous* forces or stresses. Fluids with larger dynamic viscosity coefficients generate higher viscous forces than less viscous fluids in the same flow conditions. Additionally, larger differences in velocities result in a higher rate of transfer of the momentum from the faster moving fluid to the slower and hence in more viscous friction. Finally, the distance between two fluid regions also plays a role: the closer they are, the faster the transfer of momentum occurs. According to these observations, the viscous frictional force F_{fr} acting between the two streams of fluid in Figure 2.2 can be estimated as

$$F_{fr} = A\mu \frac{U_1 - U_2}{d} . \quad (2.2)$$

where A is the contact area between the streams, U_1 and U_2 the average velocities in the two streams and d the distance between them. In this form, F_{fr} is the force acting on the fluid moving with the velocity U_2 . For the fluid stream with the velocity U_1 the sign of the force is the opposite. In a differential form, the right-hand side of Equation 2.2 can be expressed for a unit contact area as

$$\frac{F_{fr}}{A} = \mu \frac{\partial U}{\partial z} . \quad (2.3)$$

where z is the coordinate axis normal to the direction of flow. The expression on the right-hand side of Equation 2.3 is called *shear stress*.

Note that viscous stresses are reduced to zero in a uniform flow since the right-hand side of Equation 2.3 vanishes when there is no velocity variation. However, it is hard to achieve uniform flow in practical situations where a fluid is typically confined by the walls of the channel or the container. Fluid molecules collide with these walls and bounce back. The surface of a typical material has roughness that far exceeds the size of a fluid molecule. Even a super finished metal surface at best has a roughness in excess of tens of nanometres. This is still more than a hundred times bigger than a fluid molecule. Other cutting and finishing techniques produce roughness in the range from 100 to 50,000 nm (0.1 to 50 μm). So for a fluid molecule hitting a wall, its surface looks like the Black Forest to a football. After several collisions, it is very likely to lose all information about where it was coming from before it hit the surface. The usually irregular shape of the molecules and atoms only accelerates the “loss of memory.” When a fluid molecule returns into the flow after interacting with the wall, its original momentum component normal to the wall may be retained, but the direction of the tangential component is completely random. In macroscopic terms this behaviour is expressed in the form of the *no-slip* boundary condition. It means that the fluid velocity component tangential to the surface of a wall boundary is equal to zero.

The no-slip boundary condition means that friction, or viscous shear stress, is always present in a flow near walls. In addition to the pressure gradient, it is one of the main factors controlling flow. It leads to the development of viscous boundary layers, in which flow transitions from zero velocity at the surface to the flow in the bulk. Moreover, the relatively large size of the surface roughness may produce more flow loss than can be suggested just by its interaction with the individual fluid molecules. Large clusters of these molecules can be deflected, redirected and trapped by the small bumps and pits on the surface that make up the surface roughness. This may contribute to the development of *turbulence* in the flow. Turbulence can be described as a form of flow instability, when random oscillatory motion develops in the otherwise ordered mean fluid flow. This random motion occurs on much larger time and length scales than the molecular motion, but its effect is similar. It accelerates the transfer of momentum between different parts of the fluid and, therefore, results in more friction.

2.1.3 Temperature and Enthalpy

The thermal state of a fluid is usually represented by *temperature*, T , which is a measure of and proportional to the kinetic energy of the chaotic motion of its molecules. Fluid specific thermal energy, I , is proportional to the temperature

$$I = C_V T , \quad (2.4)$$

with the coefficient of proportionality C_v , called the *specific heat at constant volume*. It is equal to the amount of heat that is needed to raise the temperature of a unit mass of fluid by 1° . The subscript 'V' means that the volume of fluid would be kept constant during such a procedure. This clarification is necessary for a compressible gas, which, if allowed to expand upon heating, would require more energy to raise its temperature. For incompressible fluids, this distinction is not very important. As a result, the value of the specific heat at constant volume is very close to that of the *specific heat at constant pressure*, C_p . For obvious reasons, it is easier to measure C_p for metals by simply keeping the specimen at atmospheric pressure during measurement, whereas for a gas placed in a fixed container, it is easier to measure C_v .

C_p is used to calculate another useful quantity called *enthalpy*, E ,

$$E = C_p T + L(1 - f_s). \quad (2.5)$$

The second term on the right-hand side accounts for the release of thermal energy during solidification. Fluid molecules in the liquid phase have more freedom to move than in the solid state where they are locked in a crystalloid structure. As the metal cools and passes from the liquid state to the solid, the excess energy is released in the form of *latent heat*. The *solid fraction*, f_s , is the mass fraction of the solidified phase in a given amount of metal. Upon cooling, its value changes from 0.0 in the pure liquid to 1.0 in the pure solid phase allowing for the latent heat release in Equation 2.5.

One of the mechanisms for the exchange of thermal energy within fluids is *thermal conduction*. As molecules collide with each other, they transfer momentum, which is responsible for pressure and viscous forces, and also the kinetic energy of their chaotic motion. Consequently, any temperature variations in a thermally insulated volume of fluid would disappear over time, resulting in a uniform temperature distribution. The rate of heat exchange by conduction is described by the *thermal conduction coefficient*, k . The heat flux q between two regions of fluid at temperatures T_1 and T_2 separated by the distance d is then calculated as

$$q = k \frac{T_2 - T_1}{d}, \quad (2.6)$$

or in differential form,

$$q = k \frac{\partial T}{\partial x}. \quad (2.7)$$

Equation 2.7 is the *Fourier law* stating that the heat flux by thermal conduction is linearly proportional to the temperature gradient [Holman, 1976]. Note that the form of Equation 2.7 is similar to that of Equation 2.3 for the viscous dissipation of momentum.

2.2 Equations of Motion

Pressure gradients and viscous stresses are the main *internal* forces present in fluids. *External* forces can include gravity and electro-magnetic forces. According to Newton's second law, the sum of all these forces results in a net acceleration of the fluid, which is inversely proportional to its mass, or density. This can be expressed in the form of the Navier-Stokes equations, which for an incompressible viscous fluid can be written in the following form [Batchelor, 1967]

$$\begin{aligned}\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} + w \frac{\partial u}{\partial z} &= -\frac{1}{\rho} \frac{\partial P}{\partial x} + \frac{\mu}{\rho} \cdot \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} \right) + G_x \\ \frac{\partial v}{\partial t} + u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} + w \frac{\partial v}{\partial z} &= -\frac{1}{\rho} \frac{\partial P}{\partial y} + \frac{\mu}{\rho} \cdot \left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} + \frac{\partial^2 v}{\partial z^2} \right) + G_y \\ \frac{\partial w}{\partial t} + u \frac{\partial w}{\partial x} + v \frac{\partial w}{\partial y} + w \frac{\partial w}{\partial z} &= -\frac{1}{\rho} \frac{\partial P}{\partial z} + \frac{\mu}{\rho} \cdot \left(\frac{\partial^2 w}{\partial x^2} + \frac{\partial^2 w}{\partial y^2} + \frac{\partial^2 w}{\partial z^2} \right) + G_z.\end{aligned}\quad (2.8)$$

Here u , v and w are the three components of the fluid velocity vector \mathbf{U} at any point in the flow, and $\mathbf{G} = (G_x, G_y, G_z)$ is the external force, which we will assume here consists only of gravity.

The left-hand side of Equation 2.8 represents the components of fluid acceleration, the components of the pressure gradient, viscous stresses and gravity are summed up on the right-hand side. These forces are divided by fluid density ρ , therefore, the same forces would produce a higher acceleration for a lighter fluid. The ratio of the dynamic viscosity coefficient and density is often called the *kinematic* viscosity coefficient $\nu = \mu/\rho$.

Mass conservation is another important law governing the motion of fluids. It states that mass cannot be created or lost and is expressed through the *continuity equation*. For incompressible fluids, this equation reduces to the condition of zero divergence of the velocity vector

$$\text{div}\mathbf{U} = \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} = 0. \quad (2.9)$$

and simply means that for any amount of fluid entering a given volume from one side, exactly the same amount must leave on the other side.

When heat transfer and solidification are of interest, then additional equations are needed to track the evolution of temperature and the solid fraction. This is done in the *energy conservation* equation, which, similar to the mass conservation one, says that energy is not lost or created. As for the equation of motion, the energy transport equation is simplified by the assumption of incompressibility. Written in terms of enthalpy, defined in Equation 2.5, it has the following form:

$$\frac{\partial E}{\partial t} + u \frac{\partial E}{\partial x} + v \frac{\partial E}{\partial y} + w \frac{\partial E}{\partial z} = \frac{k}{\rho} \left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2} \right). \quad (2.10)$$

The left-hand side of Equation 2.10 constitutes the rate of change of enthalpy, and the right-hand side describes thermal conduction. An appropriate relationship between solid fraction and temperature must also be devised to complete the model.

Equations 2.8 – 2.10 constitute the basic set of equations describing the evolution of an incompressible fluid such as metal. It can be applied to a wide range of flow problems, from ocean currents to MEMS, from external to internal flows, steady-state or transient. Metal casting, of course, is one of the areas where the rules of fluid dynamics can be used. When turbulence is present, conventional turbulence models seek to enhance viscous mixing and dissipation in the flow by evaluating the *turbulent* dynamic viscosity coefficient and using it in Equation 2.8 in place of the molecular value [Batchelor, 1967].

The left-hand sides of Equations 2.8 and 2.10 have similar forms and describe the *transport* of the quantities shown in the partial derivatives (u , v , w in Equation 2.8, and E in Equation 2.10). The leading term is called the *temporal* derivative. It is the rate of change of a quantity at a given point in the flow. For instance, $\partial E / \partial t$ could be evaluated by inserting a thermocouple into the flow and then using its readings and Equation 2.5.

The rest of the terms on the left-hand sides of these equations are *convective* terms. They are responsible for carrying fluid quantities with the flow and are characteristic of *continuum* mechanics when a particle of fluid moves, another particle comes in its place bringing with it its unique properties such as temperature and velocity.

Diffusion is another means of transport in fluids. The diffusion of thermal energy is described by the thermal conduction terms on the right-hand side of Equation 2.10. The diffusion of momentum is represented by the terms in parentheses on the right-hand side of Equation 2.8.

In incompressible fluids, as well as in solids, pressure can actually be negative because the intermolecular forces in these materials include the forces of attraction that are responsible for keeping the molecules close together.

Pressure in Equation 2.8 can be relative, or *gauge* pressure. For example, it can be set relative to one atmosphere, in which case the normal pressure will be equal to zero. This is possible for incompressible materials because pressure in the equations of motion is present only in the gradient operand, therefore, adding or subtracting a constant does not change the flow dynamics.

2.3 Boundary Conditions

Equations 2.8 – 2.10 are usually solved in a finite domain that has external and internal boundaries. Therefore, proper descriptions of these boundaries, or *boundary conditions*, are needed to find the flow solution. In addition to material properties, boundary conditions distinguish low-pressure from high-pressure die

casting or lost foam casting from gravity pour. Boundary conditions, therefore, play an important role in determining the solution, and it is worth saying a few words about them here.

2.3.1 Velocity Boundary Conditions at Walls

There are two flow boundary conditions at the walls bounding the flow. Since fluid cannot penetrate solid obstacles, the component of the velocity normal to the wall must be equal to zero:

$$\mathbf{U} \cdot \mathbf{n} = u \cdot n_x + v \cdot n_y + w \cdot n_z = 0, \quad (2.11)$$

where $\mathbf{n}(n_x, n_y, n_z)$ is the unit length vector normal to the wall surface.

The second boundary condition enforces the no-slip condition, that is, the velocity component tangential to the wall must also be equal to zero:

$$\mathbf{U}_\tau = 0. \quad (2.12)$$

Combined together, Equations 2.11 and 2.12 simply state that flow velocity at the wall is equal to zero. It is useful, however, to define the two conditions separately since Equation 2.12 is not necessary when an inviscid flow approximation is used (*i.e.*, when viscous stresses are small and can be neglected in Equation 2.8).

2.3.2 Thermal Boundary Conditions at Walls

A boundary condition at walls is also needed for Equation 2.10 for enthalpy. This is typically done by defining a heat flux, q , at the interface between fluid (metal) and wall (mould) as follows:

$$q = h \cdot (T_{\text{fluid}} - T_{\text{wall}}) \quad (2.13)$$

with the *heat transfer coefficient*, h , representing the thermal properties of the interface itself. Factors like surface roughness, coating or lubrication affect the value of h .

The wall boundary condition given by Equation 2.13 can be replaced by the one that directly specifies the heat flux, possibly as a function of time,

$$q = q_0(t). \quad (2.14)$$

Equation 2.14 is useful when modeling exothermic sleeves or water-cooled mould surfaces.

2.3.3 Free Surface Boundary Conditions

Free surface is a special type of boundary; it moves with the liquid. The influence of air on flow can usually be ignored because air is much lighter than most liquids, especially metals. The fact that free surface is a boundary between a liquid and the ambient air is expressed in the so-called *kinematic* boundary condition, stating that the velocity of the free surface, \mathbf{U}_b , is equal to the velocity of the liquid:

$$\mathbf{U}_b = \mathbf{U}(t, x, y, z). \quad (2.15)$$

This obvious condition is nevertheless necessary to include free surface properly in the flow model. Equation 2.15 ensures that liquid and free surface do not get separated.

The lightness of the ambient air in comparison with liquid gives rise to the *dynamic* boundary conditions at a free surface. The first one states that fluid pressure at a free surface, P_0 , is equal to the air pressure, P_a .

$$P_0 = P_a. \quad (2.16)$$

Moreover, if we ignore the variation of pressure in the air due to gravity, then P_a is constant along a contiguous section of the free surface. This does not necessarily mean that it is constant in time, however. For example, during filling, the air may not be able to escape quickly enough, causing the air pressure in the cavity to increase, thus making P_a a function of time. Moreover, multiple air pockets will generally have as many different pressures, each serving as the boundary condition for the segment of metal surface bounding the respective air pocket.

Surface tension forces at a free surface can also be taken into account. A liquid molecule located at the free surface interacts with the liquid molecules on one side of the interface and with the adjacent air molecules on the other side. The asymmetry of the inter molecular forces gives rise to a macroscopic force, which is proportional to the curvature of the interface. This force is typically expressed in terms of the *surface tension pressure*, P_s , which is a product of the *surface tension coefficient*, σ , and the interface curvature, κ ,³

$$P_s = \sigma\kappa = \sigma(\nabla \mathbf{n}), \quad (2.17)$$

where $\nabla \cdot \mathbf{n} = \partial n_x / \partial x + \partial n_y / \partial y + \partial n_z / \partial z$ is the divergence of the unit outward normal vector of the surface (Figure 2.3). Liquid metals have the highest surface tension coefficients among liquids, with mercury leading the pack. Additionally, the buildup of a surface film due to the oxidation of metal in contact with air adds to the molecular forces at a free surface [Campbell, 1991].

³ The surface tension coefficient is not so much a property of the fluid as of the interface between two media, such as aluminium and air.

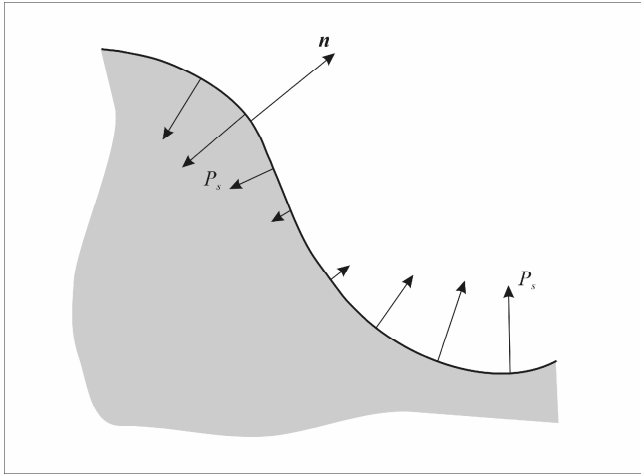


Figure 2.3. Surface tension pressure acting on an element of free surface

Surface tension is an important force when the free surface curvature is large as, for example, in small droplets in an *atomized* flow common in high-pressure die casting. Equation 2.16 then needs to be modified to include the surface tension force.

$$P_0 = P_a + P_s. \quad (2.18)$$

The second dynamic boundary condition at a free surface is derived from the assertion that viscous friction between fluid and air is negligibly small or, using Equation 2.3,

$$\frac{\partial \mathbf{U}}{\partial n} = 0. \quad (2.19)$$

where the derivative of the fluid velocity near a free surface is taken in the direction normal to the surface.

Thermal boundary conditions at the free surface during casting are often assumed to be adiabatic, *i.e.*, for simplicity heat losses to the air are neglected in comparison with the heat fluxes inside metal and at mould walls. However, more realistic relationships, similar to that given by Equation 2.13, can also be used. For example, radiative heat losses, q_R , which maybe important for high temperature alloys, can be computed as

$$q_R = \varepsilon \cdot \zeta \cdot (T_{\text{fluid}}^4 - T_{\text{air}}^4), \quad (2.20)$$

where ε is the emissivity of the surface ($\varepsilon < 1$), $\zeta = 5.5604 \cdot 10^{-8} \text{ kg s}^{-3} \text{ K}^{-4}$ the Stefan-Boltzmann constant, and temperature is expressed in the absolute units of degrees

Kelvin, K. Due to the power of four on the right-hand side of Equation 2.20, the radiative heat flux grows quickly with an increase in surface temperature. For example, the pouring temperature of steels, 1700 – 1800 K, is around twice that of a die-cast aluminium alloy and, therefore, with similar emissivity coefficients, the radiative heat loss from the surface of the steel is about sixteen times larger.

2.4 Useful Dimensionless Numbers

Equations 2.8 – 2.10, together with the appropriate boundary conditions, describe a very wide range of flows. It is often useful to estimate the relative importance of various terms in these equations and thus determine the most significant aspects of the physical behaviour of the fluid in a given situation. This, in turn, may enable simplification of the equations before one proceeds with the solution. As a minimum, it would be useful to understand what type of flow to expect.

A set of dimensionless numbers, each representing an estimate of the ratio of a pair of forces, can be conveniently employed for that purpose. These numbers are derived from the *dimensionless* form of the equations of motion. This form, in turn, is obtained by scaling the equations by the characteristic values of length and velocity. As their name suggests, for a given flow each dimensionless number has the same value, irrespective of the units system employed to evaluate it.

2.4.1 Definitions

The commonly used dimensionless numbers are

$$\text{Reynolds number: } Re = \frac{\rho U d}{\mu} = \frac{\text{fluid inertia}}{\text{viscous forces}}. \quad (2.21)$$

$$\text{Weber number: } We = \frac{\rho U^2 l}{\sigma} = \frac{\text{fluid inertia}}{\text{surface tension}}. \quad (2.22)$$

$$\text{Bond number: } Bo = \frac{\rho G l^2}{\sigma} = \frac{\text{gravity}}{\text{surface tension}}. \quad (2.23)$$

$$\text{Froude number: } Fr = \frac{U}{\sqrt{Gh}} = \frac{\text{fluid inertia}}{\text{gravity}}. \quad (2.24)$$

Here U is the characteristic velocity, d , l and h denote the appropriate characteristic lengths and G is gravity.

2.4.2 The Reynolds Number

For the Reynolds number U is the average variation of the velocity in the flow between its minimum and maximum values, and d is the distance over which this variation occurs. According to Equation 2.12, in a typical filling, U can be defined as the difference between the velocity at the walls, which is zero, and in the bulk of the flow, or as the average metal velocity. Then d becomes half of the minimum wall thickness or half of the channel width.

The Reynolds number is one of the most important parameters characterizing fluid flow. When its value is small, $Re < 1$, then flow is dominated by viscous forces. For very small values of Re , the convective terms in Equation 2.8 can be neglected in comparison with viscous dissipation of the momentum, reducing it to the so-called *creeping*, or *Stokes*, flow approximation.

As is shown in the next section, the Reynolds number in metal flow in most castings is much greater than one, indicating that, at least during filling, viscosity plays a secondary role to fluid inertia. With the increase in the speed of the flow, it transitions from laminar to turbulent due to the development of flow instabilities initiated by spatial variations in fluid velocity. The transition begins at $Re \approx 2000$ and turns into a fully turbulent flow when Re exceeds 10,000. Only in extremely carefully controlled flow experiments can the laminar regime be extended to Re up to 20,000. Fully developed turbulence enhances the dissipation of fluid momentum, in addition and significantly beyond the dissipation due to the molecular viscosity, even though a large value of the Reynolds number may suggest that viscous forces are not important in the flow.

2.4.3 The Weber Number

In Equation 2.22 for the Weber number, U characterizes the average variation in fluid velocity near a free surface. To be more precise, it is the velocity component normal to the free surface that is of the interest here. Due to the no-slip boundary condition at walls and Equation 2.15, we can say the U is the average velocity of the free surface. As with the Reynolds number, the distance l then becomes the minimum width of the flow channel.

During filling, internal fluid forces can cause distortion of the metal surface, sometimes called *surface turbulence* [Campbell, 1991], that would lead to folding of the surface, additional oxidation and other undesirable effects. The process can be visualized by imagining a submerged jet of metal directed at an area of the free surface. Its energy will create a bulge on the initially undisturbed surface. The Weber number can be used to determine if the surface tension forces can prevent the rupture of the surface film and restore its shape. The velocity U and distance l in Equation 2.22 in this case relate to the jet velocity and size of the bulge, respectively. If $We < 1$, then we can hope that the energy of the flow will be contained within the confines of the existing free surface. If $We > 1$, as is the case

in most filling scenarios, then the folding and entrainment of the surface oxide film and possibly air cannot be avoided.

It has also been observed experimentally that a free surface breaks up into small droplets when the Weber number exceeds the *critical* value of around 60 [Manzello and Yang 2003].

2.4.4 The Bond Number

The Bond number is another measure of the relative importance of surface tension. This time it is compared to gravity, which is useful to determine if a free surface will stay flat or bulge. The natural tendency of the surface tension forces is to bend the initially horizontal free surface to reach a constant curvature at its every point, and in the absence of other forces it will do just that. Gravity in this case acts in the opposite direction trying to flatten it. When gravity is strong and the surface's horizontal extent l is large, that is $Bo > 1$, a free surface is likely to stay flat and undisturbed by the surface tension forces as in a glass of water or a metal pouring cup.

If the size of the container is gradually reduced, then at some point the value of the Bond number will drop below unity and the shape of the free surface will be determined more by the surface tension than by gravity. This can be observed inside a half-filled (transparent) drinking straw or when placing a small droplet of water on a dry surface.

2.4.5 The Froude Number

The Froude number is often employed to estimate the importance of such as surface waves in open-channel flows, like rivers and canals. It is also useful to look at the waves in the horizontal runners in gravity pour castings and shot sleeves in high-pressure die casting. In all these cases, the waves are driven by gravity.

The variable h in Equation 2.24 is the average depth of the fluid. When Fr is much smaller than one, $Fr \ll 1$, surface waves are much faster than the main flow, U . Such flow is called *sub-critical*. In the time it takes for the fluid to move the length of the container, the waves will pass in both directions multiple times, dissipate their energy and, therefore, can be deemed unimportant for the overall configuration of the flow.

In the case of large values of the Froude number, $Fr > 1$, the flow is faster than the surface waves, or *super critical*. Any such waves are quickly swept away by the flow toward the boundaries of the flow domain. The fact that these waves can move in only one direction may result in their accumulation at the downstream walls. This, in turn, produces a buildup of fluid near the walls and eventually develops into a *hydraulic jump*, a narrow area in the flow in which the fluid transitions from the high velocity upstream to the low velocity downstream of the jump. The transition of the flow from one side of a hydraulic jump to the other is also characterized by an abrupt change in pressure, fluid depth and, of course, turbulence. The latter often results in excessive entrainment of air into the bulk of the fluid at the transition point, which is highly undesirable during mould filling.

2.5 The Bernoulli Equation

Once of the most commonly used solutions of the general fluid motion equations is the Bernoulli equation. It can be derived from Equations 2.8 and 2.9 when the flow is steady and inviscid, and can be expressed in the following form

$$P + \frac{1}{2} \rho U^2 + \rho gh = C, \quad (2.25)$$

where g is the magnitude of the gravity vector and h is the height above a reference point. C is an arbitrary parameter that is constant along any streamline. It can be evaluated by using pressure and velocity at a single point along the streamline

$$P + \frac{1}{2} \rho U^2 + \rho gh = P_1 + \frac{1}{2} \rho U_1^2 + \rho gh_1. \quad (2.26)$$

Stagnation, Dynamic and Total Pressure

If the variation in fluid elevation h is small or gravity forces are negligible compared to pressure and inertia, like in high pressure die casting or in air, then Equation 2.26 can be reduced to

$$P + \frac{1}{2} \rho U^2 = P_1 + \frac{1}{2} \rho U_1^2. \quad (2.27)$$

As fluid accelerates along a streamline, pressure drops so that the sum on the left-hand side of Equation 2.27 stays constant. The maximum value of pressure occurs at the point where velocity is zero, or at the *stagnation* point. This pressure is called *stagnation* pressure. The term $1/2 \rho U^2$ is the *dynamic* pressure, as opposed to the *static* pressure represented by P . The sum of static and dynamic pressures in Equation 2.27 is termed the *total* pressure.

The Bernoulli equation in the form of Equation 2.27 led to the development of the theory of the airfoil [Abbott, 1959]. The difference between the static pressures on the lower and upper surfaces of an airplane wing creates the lift necessary to keep the plane in the air.

2.6 Compressible Flow

Strictly speaking, all fluids are somewhat compressible. In other words, if external pressure is applied to a fluid volume, the latter will decrease in size. Among other things, compressibility of materials enables the propagation of acoustic waves. For most liquids, however, this change is negligible, even if the pressure is large.

Fluids for which the compressibility effect is significant are called *gases*. The average distance between molecules in a gas is large, much larger than the size of

the molecules themselves. This allows them to move freely in space, interacting with other molecules mostly through collisions. Unlike liquids, gases occupy all available space bound by solid or liquid surfaces as, for example, propane in a steel tank or an air bubble inside liquid metal.

2.6.1 Equation of State

If a gas is not too dense and sufficiently hot, then two things can be said about its molecules. First, they interact with each other mostly through collisions, with only two molecules participating in any collision. Second, the kinetic energy of the molecules comes primarily from their translational motion. That is, molecules of a gas can be closely approximated by small, elastic, identical spherical balls moving around and colliding with each other in a chaotic manner. Such a fluid is called an *ideal* or *perfect* gas [Sedov, 1972].

The variables that define a thermodynamic state of a gas are pressure, density and temperature. For an ideal gas, they are related to each other through *the equation of state*:

$$P = R\rho T, \quad (2.28)$$

where $R=8.3144 \text{ J mol}^{-1} \text{ K}^{-1}$ is the universal gas constant. One important result of this equation is that the thermodynamic state of an ideal gas is defined by just two parameters: density and temperature, pressure and temperature or pressure and density.

Equation 2.28 is a very common equation of state that has been successfully applied to many real gases. In general, molecules in a real gas are far from spherical, or elastic, or even of the same size. Therefore, their rotational and oscillatory motions contribute to the total kinetic energy and are also exchanged during collisions. Moreover, if the gas is dense and cold, interactions between a pair of molecules cannot be described as simple collisions. In this case, the exchange of energy and momentum between molecules occurs over longer distances and times and with multiple molecules interacting at the same time. All these factors result in the behaviour that deviates from Equation 2.28. However, it is only significant at near cryogenic temperatures or very high pressures. For most gases, they are negligible in a wide range of temperatures and pressures. Air is an example of a compressible multi component real gas that can be described by Equation 2.28 with good accuracy.

When modelling gas flow, the *absolute* values of pressure and temperature must be used. Degrees Kelvin or Rankine should be used for temperature. Unlike incompressible fluids, gauge pressure is not used for gases because pressure is present in the equation of state. The use of the absolute scale for these parameters is important for Equation 2.28 to be valid. A pressure of one atmosphere is $1.013 \cdot 10^6 \text{ dyne/cm}^2$ in CGS units or $1.013 \cdot 10^5 \text{ N/m}^2$ in SI units. Pressure, temperature and density for gases are *always positive*.

2.6.2 Equations of Motion

In general, the density of a gas can vary in time and space. The continuity equation that we wrote for incompressible fluids, Equation 2.9, is not valid in this case. It must be replaced by the full transport equation for density

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u}{\partial x} + \frac{\partial \rho v}{\partial y} + \frac{\partial \rho w}{\partial z} = 0. \quad (2.29)$$

The full form of the specific thermal energy transport equation for gases.

$$\begin{aligned} \frac{\partial(\rho I)}{\partial t} + u \frac{\partial(\rho I)}{\partial x} + v \frac{\partial(\rho I)}{\partial y} + w \frac{\partial(\rho I)}{\partial z} = \\ k \left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2} \right) + P \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} \right). \end{aligned} \quad (2.30)$$

The last term on the right-hand side is the work term associated with the compression and expansion of the gas. It is equal to zero for incompressible fluids.

Equation 2.30 manifests *the first law of thermodynamics* described in Section 2.6.3 below.

Solution of the flow equations for liquids, Equations 2.8 and 2.9, is not coupled to the energy equation since neither density nor pressure depend directly on temperature, so that, generally, the solution of the energy transport equation, Equation 2.10, for liquids is optional.

This is no longer true for gases. Both pressure and density depend on temperature through the equation of state. Therefore, the thermal energy transport equation above must always be included in the solution for gas flow.

Compared to the momentum equations for incompressible fluids, Equation 2.8, the viscous terms in the momentum equations for gases include extra terms associated with compression:

$$\begin{aligned}
& \frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} + w \frac{\partial u}{\partial z} = \\
& - \frac{1}{\rho} \frac{\partial P}{\partial x} + \frac{\mu}{\rho} \cdot \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} \right) + \frac{\mu}{\rho} \cdot \frac{\partial}{\partial x} \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} \right) + G_x \\
& \frac{\partial v}{\partial t} + u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} + w \frac{\partial v}{\partial z} = \\
& - \frac{1}{\rho} \frac{\partial P}{\partial y} + \frac{\mu}{\rho} \cdot \left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} + \frac{\partial^2 v}{\partial z^2} \right) + \frac{\mu}{\rho} \cdot \frac{\partial}{\partial y} \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} \right) + G_y \\
& \frac{\partial w}{\partial t} + u \frac{\partial w}{\partial x} + v \frac{\partial w}{\partial y} + w \frac{\partial w}{\partial z} = \\
& - \frac{1}{\rho} \frac{\partial P}{\partial z} + \frac{\mu}{\rho} \cdot \left(\frac{\partial^2 w}{\partial x^2} + \frac{\partial^2 w}{\partial y^2} + \frac{\partial^2 w}{\partial z^2} \right) + \frac{\mu}{\rho} \cdot \frac{\partial}{\partial z} \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} \right) + G_z.
\end{aligned} \tag{2.31}$$

The second term in parentheses on the right-hand side contains velocity divergence and represents the viscous force associated with the compression and expansion of the gas. According to Equation 2.8, it is equal to zero for incompressible fluids.

2.6.3 Specific Heats

As mentioned in Section 2.1.3, specific heats at constant volume, C_v , and at constant pressure, C_p , differ significantly from each other for a gas. Because, when held at constant pressure, the gas expands upon heating. A part of the thermal energy goes into the work against the external pressure, leaving less energy for the actual heating of the gas. Consequently, more thermal energy is required to raise the gas temperature by 1° than when the gas volume is kept constant, and, therefore, C_p is larger than C_v .

The difference between C_p and C_v is constant and identical for all ideal gases. It can be calculated from Equation 2.28 and the first law of thermodynamics. The latter states that the change in the total thermal energy of a gas, MdI , is equal to the amount of heat added to it, q , minus the amount of work done by the gas, W ,

$$MdI = q - W, \tag{2.32}$$

where M is the total mass of the gas (see Figure 2.4).

The work done by an expanding or contracting gas is the product of the gas pressure and the change in its volume

$$W = PdV. \tag{2.33}$$

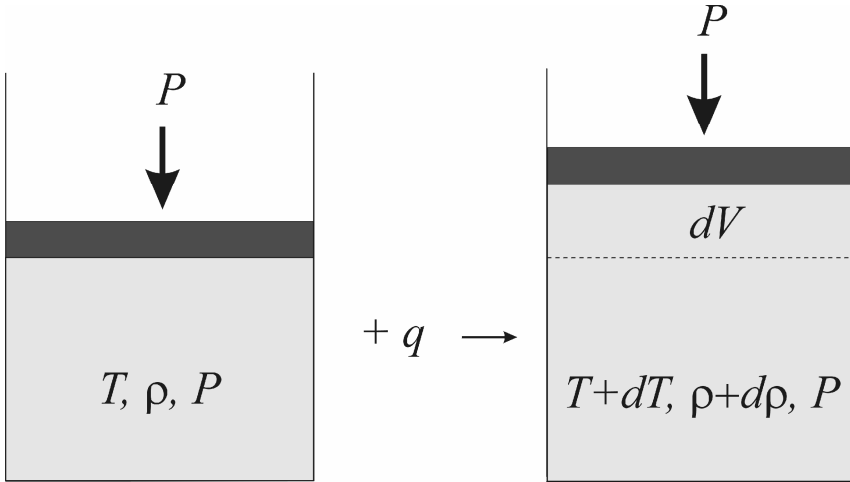


Figure 2.4. Heating of a gas volume at constant pressure P , during which its temperature and density change and the gas expands by volume dV , producing work PdV

Since

$$V = \frac{M}{\rho}, \quad (2.34)$$

then for the change in volume,

$$\frac{dV}{V} = -\frac{d\rho}{\rho}. \quad (2.35)$$

From Equation 2.28, it follows that when a gas is heated at a constant pressure, the corresponding changes in its density and temperature are related to each other:

$$Td\rho + \rho dT = 0, \quad (2.36)$$

and the heat flux in Equation 2.32 is by definition,

$$q = MC_p dT. \quad (2.37)$$

while from Equation 2.4,

$$dI = C_v dT. \quad (2.38)$$

Now combining Equations 2.32 – 2.38 yields

$$C_p - C_v = R \quad (2.39)$$

Equation 2.39 states that the difference between the specific heats is the same for all gases that fit the ideal gas model.

2.6.4 Adiabatic Processes

An adiabatic process is a process during which no heat is added or subtracted from the system, *i.e.*, $q = 0$ in Equation 2.32. Using Equations 2.32, 2.35 – 2.39, it can be derived that in such a process the change in pressure is related to the change in density according to

$$\frac{dP}{P} = \frac{C_p}{C_v} \frac{d\rho}{\rho}. \quad (2.40)$$

After combining Equations 2.35 and 2.40, the equation of state, expressed in terms of volume and pressure, can be written in the following form

$$P = P_0 \left(\frac{V}{V_0} \right)^{-\gamma}, \quad \gamma = \frac{C_p}{C_v}, \quad (2.41)$$

with pressure P_0 and volume V_0 expressing the state of the gas at a certain point in time. Note that, according to Equation 2.39, $\gamma > 1$ for ideal gases.

According to Equation 2.41, the thermodynamic state of gas during an adiabatic process is defined by only *one* parameter. This parameter can be either volume (or density), or pressure, or temperature. Given the simplicity of the equation of state, the adiabatic gas model is a useful approximation to gas flows where heat fluxes are small compared to other factors affecting the energy. This is often true when the process takes a relatively short time, for example, in supersonic flows. A Bernoulli-type solution can also be derived for processes governed by Equation 2.41 (see Section 2.6.7 below).

2.6.5 Speed of Sound

In an acoustic, or sound wave, the material undergoes small, localized compressions and expansions. These changes in density result in corresponding changes in pressure and temperature. In turn, the variations in pressure create a force that causes these perturbations to propagate through the medium, that is, to actually behave like a wave. The rate at which acoustic waves propagate is called the *speed of sound* and is a property of the material.

Note that, even though the sound speed in most solid and fluid materials is relatively large (of the order of several hundred metres per second), the actual displacement of the medium in an acoustic wave is small because of the small amplitude of the fluctuations in it. In other words, there is no transport of mass, energy and momentum associated with acoustic waves.

Heat transfer due to conduction in a sound wave is also negligible because temperature gradients are small and also because the rate of heat transfer due to conduction is usually small compared to the speed of sound. This means that the propagation of sound waves is an adiabatic process.

For small velocities in a sound wave, the viscous effects on its propagation are also negligible.

The speed of sound, a , can be easily derived from Equations of motion 2.29 and 2.31 in the following way. Let's assume for simplicity that the gas is initially at rest, in with a uniform pressure, temperature and density and that a single acoustic wave propagates in the x direction. As the wave moves, it introduces perturbations in the gas. Since all flow perturbations in such a wave are small, we will ignore all terms in these equations that are second order and higher with respect to these parameters.

A change of density $d\rho$ produced by the passing wave results in a corresponding change in pressure dP , which in turn causes a change in the velocity du . The latter two are related to each other through the momentum Equation 2.31

$$du = -\frac{dt}{\rho} \frac{dP}{dx}, \quad (2.42)$$

where dx is the distance travelled by the wave in the time dt , that is,

$$a = \frac{dx}{dt}. \quad (2.43)$$

According to the mass conservation Equation 2.29, du and $d\rho$ are also interrelated

$$d\rho = -dt\rho \frac{du}{dx}. \quad (2.44)$$

Now substituting Equation 2.44 in Equation 2.42 yields

$$a^2 = \frac{dP}{d\rho}, \quad (2.45)$$

where the derivative on the right-hand side is taken with the condition of adiabaticity. With the help of Equations 2.28, 2.34 and 2.41, this derivative can be evaluated as

$$a = \sqrt{\frac{\gamma P}{\rho}} = \sqrt{\gamma RT}. \quad (2.46)$$

Equation 2.46 shows that in an ideal gas the speed of sound is a function *solely* of temperature. At higher temperatures, the molecules are more energetic and, therefore, are more capable of transmitting local changes in pressure and density to the adjacent gas volume in the end, resulting in an increase in the speed of sound.

2.6.6 Mach Number

Sound waves provide the means of transmitting information about flow conditions in different parts of the gas. When the speed of the flow exceeds the speed of sound, that is, the flow travels faster than information about it, then *shock waves* can arise.

Typically, a shock wave separates two regions of the gas with principally different flow conditions. On the upstream side, the flow is supersonic, and on the downstream side, it becomes subsonic. The transition occurs on a very small length scale which can be estimated as the distance travelled by a gas molecule between two successive collisions with other molecules. That is to say that the thickness of a shock wave can be as small as 0.03 micron.

The flow of gas is characterized by the *Mach number* which is the ratio between the flow speed and the speed of sound

$$M = \frac{U}{a} . \quad (2.47)$$

Obviously, $M > 1$ in a supersonic flow and is less than one in the subsonic. When the Mach number is less than about 0.1, the compressibility effects can usually be neglected. It is possible then to model the gas as an incompressible liquid.

Shock waves may occur when a supersonic flow meets with geometric obstructions, such as a flying airplane, or near sudden changes in the flow path, such as at an orifice or at the entrance to a vent.

2.6.7 The Bernoulli Equation for Gases

The equations of motion 2.29 and 2.31 can be integrated for an adiabatic process to yield a solution similar to the Bernoulli equation for the incompressible fluids, Equation 2.25. Gravity is usually omitted for gases because its effect is small compared to pressure forces. The result is

$$\left(\frac{\gamma}{\gamma - 1} \right) \left(\frac{P}{\rho} \right) + \frac{1}{2} U^2 = C . \quad (2.48)$$

With the help of Equations 2.28 and 2.41, Equation 2.48 can be rendered in several other useful forms, for example,

$$\left(\frac{\gamma}{\gamma-1}\right)\left(\frac{P_0}{\rho_0}\right)\left(\frac{P}{P_0}\right)^{\frac{\gamma-1}{\gamma}} + \frac{1}{2}U^2 = C, \quad (2.49)$$

and

$$C_p T + \frac{1}{2}U^2 = C. \quad (2.50)$$

where the constant C is the same for all three equations. It can be determined by calculating the left-hand side at some point along the streamline. For example, it can be defined by the flow parameters at the *stagnation point*, that is, where $U=0$:

$$C = \left(\frac{\gamma}{\gamma-1}\right)\frac{P_0}{\rho_0} = C_p T_0, \quad (2.51)$$

where the subscript '0' indicates the values of the respective parameters at the stagnation point. P_0 and T_0 are also called the *total* pressure and temperature, respectively.

Maximum Speed

The Bernoulli equation can be used to calculate the maximum speed, U_{\max} , that can be achieved in a steady-state adiabatic gas flow. Since $\gamma > 1$, then, according to Equation 2.49, the maximum speed is obtained at a point where pressure is equal to zero, or

$$U_{\max} = \sqrt{\frac{2\gamma}{\gamma-1} \frac{P_0}{\rho_0}} = \sqrt{2C_p T_0}. \quad (2.51)$$

Note that the maximum velocity is only a function of the gas stagnation temperature.

Flow with close to adiabatic and steady-state conditions can be obtained by letting a gas escape from a large container (or cavity) through a small hole. If the container is sufficiently large compared to the hole, then we can assume that the conditions inside are close to stagnation. The maximum velocity can then be achieved by placing the container in vacuum. For air at room temperature of 300 Kelvin and $C_p = 1000$ J/Kg K, the maximum velocity comes to about 775 m/sec.

2.7 Computational Fluid Dynamics

In this and other sections, we have presented full systems of equations of motion for fluids, together with an array of approximate approaches to solving them. These approximations have the benefit of offering analytical dependencies for various flow parameters in simple situations and are useful tools in a design process. At the same time, they provide only limited information and often cannot be successfully applied to general, transient three-dimensional flows with turbulence, heat transfer and phase change. In this case, numerical methods must be employed to solve the fluid flow equations. The science (and often art) of developing numerical approximations to the differential and integral equations of fluid motion is called *computational fluid dynamics* [Roache, 1985].

Fluid motion is described with non linear, transient, coupled, second-order differential equations. A numerical solution of these equations involves approximating its various terms with algebraic expressions. The resulting equations are then solved to yield an *approximate solution* to the original problem. The process is called *simulation*.

2.7.1 Computational Mesh

Typically, a numerical model starts with a *computational mesh*, or *grid*. It consists of a number of interconnected elements of various shapes, *e.g.*, tetrahedrals or bricks. These elements subdivide the physical space into small volumes where at least one *node* is associated with each such volume. The nodes are used to store values of the unknowns, such as pressure, temperature and velocity. The mesh is effectively the numerical space that replaces the original physical one. It provides the means for defining the flow parameters at discrete locations, setting boundary conditions and, of course, for developing numerical approximations of the fluid motion equations.

The mesh *discretizes* the physical space. Each fluid parameter is represented in a mesh by an array of values at discrete points. Since the actual physical parameters vary continuously in space, a mesh with fine spacing between nodes provides a better representation of reality than a coarse one. We arrive then at a fundamental property of a numerical approximation: any valid numerical approximation approaches the original equations as the grid spacing is reduced to zero. If an approximation does not satisfy this condition, then it is incorrect.

Reducing the grid spacing, or *refining the mesh*, for the same physical space results in more elements and nodes and, therefore, increases the size of the numerical model. But apart from the physical reality of fluid flow and heat transfer, there is also the reality of design cycles, computer hardware and deadlines, which combine in forcing the simulation engineers to choose a reasonable size for the mesh. Reaching a compromise between satisfying these constraints and obtaining accurate solutions is a balancing act that is no lesser an art than the CFD model development itself.

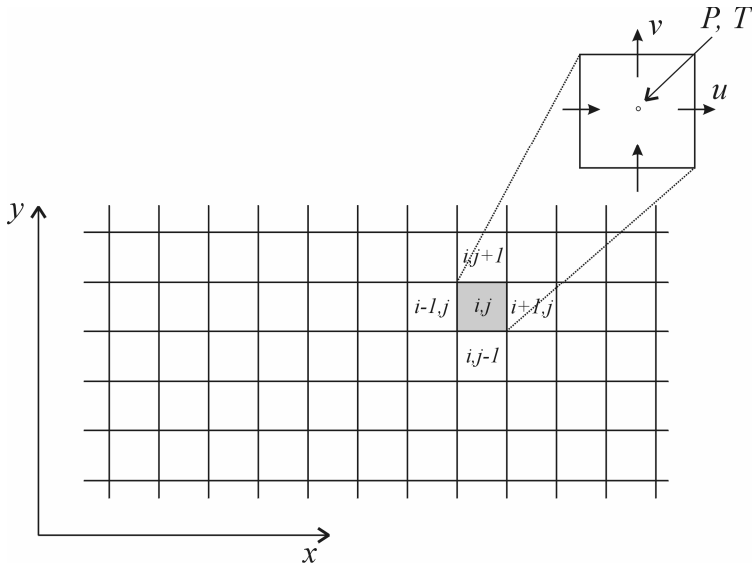


Figure 2.5. Regular two-dimensional staggered computational mesh. The cell indexing i and j are shown for a two-dimensional case

The regular two-dimensional grid shown in Figure 2.5 is called *staggered*. All scalar quantities, such as pressure and temperature, are calculated and stored at the centre of each rectangular cell, and velocity vectors are assigned to the respective faces of the cell for better stability of the numerical algorithm. The full velocity vector can be reconstructed at the centre of the cell by simply averaging its components from the four faces. Each element of such grid has five nodes one for the scalar quantities and four for the respective velocity components. Each cell shares velocity nodes with its immediate neighbours.

Grids like that one shown in Figure 2.5 are very easy to generate and store because of their regular, or *structured*, nature. A non uniform grid spacing adds flexibility when meshing complex flow domains. The computational cells are numbered in a consecutive manner using three indices: i in the x direction, j in the y direction and k in the z direction. This way each cell in a three-dimensional mesh can be identified by a unique address (i, j, k) , similar to coordinates of a point in the physical space.

Structured rectangular grids carry additional benefits of the relative ease of the development of numerical methods, transparency of the latter with respect to their relationship to the original physical problem and, finally, accuracy and stability of the numerical solutions. The oldest numerical algorithms based on the *finite difference* and *finite volume* approaches have been developed on such meshes and are still widely in use.

2.7.2 Numerical Approximations

The finite difference (FD) method is based on the properties of the Taylor expansion and on the straightforward application of the definition of derivatives. It

is the oldest of the methods applied to obtain numerical solutions to differential equations and the first application is considered to have been developed by Euler in 1768.

The idea of the finite difference method is quite simple. For a function $u(x)$, the derivative at a point x can be approximated as

$$\frac{\partial u}{\partial x} \approx \frac{u(x + \Delta x) - u(x)}{\Delta x}. \quad (2.51)$$

The spatial increment Δx can be now selected as the distance between two adjacent mesh nodes, $u(x + \Delta x)$ and $u(x)$ are the values of the function at these nodes. Then Equation 2.51 can be rewritten in the form that is more common in CFD:

$$\frac{\partial u}{\partial x} \approx \frac{u(x_i) - u(x_{i-1})}{x_i - x_{i-1}} = \frac{u_i - u_{i-1}}{x_i - x_{i-1}}. \quad (2.52)$$

Here we use a subscript i to indicate the location on the x axis where the values of u and x are taken. Thus we obtain an approximation of the derivative of the function $u(x)$ on a structured computational grid. From the definition of derivative, the accuracy of the approximation given by Equation 2.52 improves with smaller grid spacing.

A similar approach is taken to approximate all first and second-order spatial derivatives in the fluid equations of motion, Equations 2.8 – 2.10 for incompressible fluids and Equations 2.29 – 2.31 for gases. The approximation of the second-order derivatives, which are present in the diffusive terms, typically requires at least three nodes. A *time step*, Δt , is used to divide time into discrete increments so that the temporal derivatives can also be approximated:

$$\frac{\partial u}{\partial t} \approx \frac{u(t + \Delta t) - u(t)}{\Delta t} = \frac{u_i^{n+1} - u_i^n}{t^{n+1} - t^n}, \quad (2.53)$$

where superscript n refers to the order of the time points at which the values are taken.

Once all derivatives are replaced with their respective finite difference approximations, the differential equations are replaced by a set of algebraic equations. As with the original equations of motion, proper boundary conditions must also be defined for the finite difference equations. These, for example, include the no-slip and heat transfer conditions at the interface between the fluid and the surrounding walls.

The unknowns in that system of algebraic equations are the values of the flow parameters velocity, pressure and temperature at the mesh nodes. For a unique solution of this system to exist, the number of algebraic equations must match the number of nodes. Therefore, the size of a numerical model increases with the increase in mesh resolution. For example, for a three-dimensional mesh with a

hundred nodes in each coordinate direction, a million equations must be solved. Moreover, the solution must be found at each incremental time point t^n , starting at the beginning, $t = 0$, and finishing at a predefined moment $t^N = T$, multiplying accordingly the number of operations required to find the complete solution.

The actual procedure for the solution of each equation in the numerical model is usually quite simple. It is the huge number of the elementary operations that is so daunting for a human brain and where the electronic brain power is really needed.

CFD simulations in this book use a combination of the finite difference and finite volume approaches to the solution of the fluid flow equations on computational grids similar to that shown in Figure 2.5. Unlike the finite difference method, the *finite volume* (FV) method uses the integral form of conservation laws. For every elementary control volume, fluxes of the conserved quantity (e.g., mass) are calculated at its boundaries. The net flux then translates into the change in that quantity inside the control volume. One of the strengths of the finite volume method is its *conservation* property adherence to the physical conservations laws that naturally arises from the method's definition. For structured rectangular meshes, the look of the formal expressions for the control volume approximations is often indistinguishable from those of the finite difference method.

2.7.3 Representation of Geometry

As mentioned above, finite difference methodology has been in use for many decades. In modern times, it is difficult to accurately describe the complex geometry within the framework of the traditional finite difference method. A rectangular cells is either fully open or fully blocked by the mould resulting in a familiar stair-step representation of the curved surfaces. Such a limitation makes the definition of accurate boundary conditions problematic. For example, the zigzag shape of the interface introduces unphysical additional flow losses due to friction. Also the surface area of a zigzag surface is larger than that of the original smooth surface, and the difference does not improve with mesh refinement.

An innovative technique called Fractional Area Volume Obstacle Representation (FAVORTM) has been developed to remedy this problem [Hirt, 1985]. In this method, a geometric surface can cut through a rectangular mesh cell dividing it into blocked and open portions, as shown in Figure 2.6. The ratio of the open volume in a cell to its total volume is called the *fractional volume*. The intersections of the surface with the faces of the cell (six in three dimensions) are computed and stored as *fractional areas*, which are the ratios of the open area to the total area at respective cell faces. Similarly to the velocity vectors, the fractional areas are computed and stored at the staggered, cell-face locations. The complete geometry in every computational cell is thus converted into fractional volumes and areas. With adequate mesh resolution, the reconstruction of the original geometry from those fractional quantities is possible with a high degree of reliability.

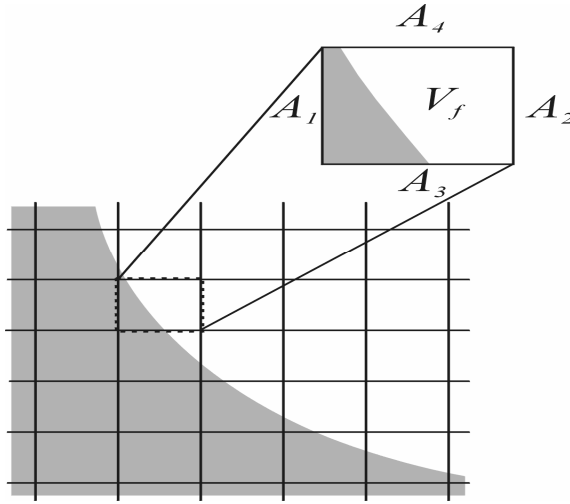


Figure 2.6. Geometric representation (shaded area) in the finite difference mesh using fractional area and volumes

The area and volume fraction are subsequently incorporated into the numerical equations and are also used to define boundary conditions. The resulting model provides significantly better accuracy in the numerical solution than the traditional stair-step approach.

2.7.4 Free Surface Tracking

Free surface exists in most metals flows and, certainly, during filling. It is challenging to model a free surface in any computational environment because flow parameters and materials properties, such as density, velocity and pressure, experience a discontinuity at it. Moreover, the motion of the free surface is the result of a combination of dynamic and kinematic flow conditions. Proper account of these conditions is critical to accurate modelling of free surfaces.

One of the commonly used methods to model free surfaces is the *Volume-of-fluid* (VOF) method [Hirt, 1981; Rider, 1998]. It consists of three main components: the definition of the volume-of-fluid function F , a method to solve the transport equation for F and the proper boundary conditions at the free surface.

Volume-of-fluid Function

The VOF function F is defined equal to one in the fluid and to zero outside. Averaged over a cell volume, it becomes the *fractional* volume of fluid, that is, the amount of fluid in the cell divided by the cell's total volume. Thus $F=1.0$ in a cell that is full of fluid and $F=0.0$ in an empty cell. A cell with free surface would have a value of F in the range between zero and one as shown in Figure 2.7.

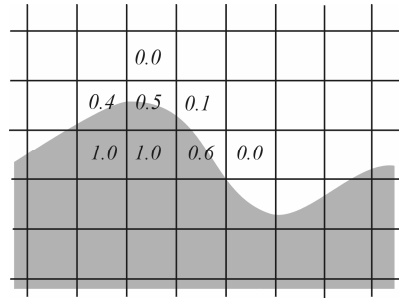


Figure 2.7. Illustration of the calculation of the Volume-of-fluid function in selected cells. The shaded area represents fluid

The VOF Equation

The VOF function can be interpreted as a kind of a tracer ink added to a fluid. Then it should be carried through space by the fluid. This consideration leads to a transport equation for the volume-of-fluid function:

$$\frac{\partial F}{\partial t} + \frac{\partial Fu}{\partial x} + \frac{\partial Fv}{\partial y} + \frac{\partial Fw}{\partial z} = 0. \quad (2.54)$$

Equation 2.54 is similar to Equation 2.29 for gas density. It is often called the *kinematic* equation because there are no forces present. It just states that the values of F move around according to the velocity field, like smoke in the air. This applies to the free surface itself making Equation 2.54 automatically include the kinematic free surface boundary condition given by Equation 2.15.

Tracking Free Surface

If conventional computational methods described earlier in this section are applied to the VOF equation the result will most likely be unsatisfactory because the free surface represents a boundary between the values of F in the fluid and outside. The derivative of F across the free surface is effectively infinite since its value changes from one to zero on an infinitely small length scale, that is, across the “thickness” of the free surface. Therefore, any attempt at approximating this variation with the finite difference method, *e.g.*, using Equation 2.52, is bound to be very inaccurate.

The most viable way to solve Equation 2.54 numerically is to use the *geometric* method, where the shape and location of the free surface within a computational cell are reconstructed using the values of the VOF function in its vicinity before computing the fluxes of the fluid volume at the cell faces. For example, if we know that fluid is filling the left portion of a cell, as shown in Figure 2.8, it will be some time before it crosses into the neighbour on the right.

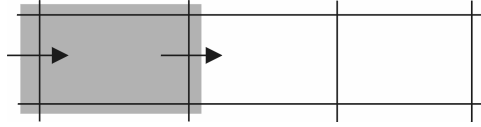


Figure 2.8. The calculation of fluid volume fluxes using the geometric method. The shaded area represents fluid, while vectors represent the direction of fluid motion. The cell in the middle must fill completely before fluid can cross into its neighbour on the right

Typically, the segment of the free surface within a computational cell is represented in three dimensions in a piecewise linear fashion, that is, with a section of a plane. Then its slope can be computed from the gradient of the VOF function, and its location is pinned by the value of F inside the cell. Then the respective amounts of fluid moving in or out of the cell at each of its six faces can be evaluated. This particular approach is sometimes called *piecewise linear interface calculation* or the PLIC method.

Free Surface Boundary Conditions

The components of the VOF method described so far can be applied to both two-phase (metal and air) and one-phase (metal and void) flows. In the former case, the space outside the $F = 1.0$ region is filled with air, and flow equations are solved for both fluids.

In the one-phase case, the inertia of the air is neglected and the $F=0.0$ space is effectively empty, void of mass, represented only by uniform pressure and temperature. This approach has the advantage of not wasting CPU time on modelling air since in most cases the details of its motion are unimportant for the motion of the much heavier metal. However, in this case, free surface becomes one of the fluid external boundaries and requires the definition of dynamic boundary conditions. These boundary conditions are contained in Equations 2.16 - 2.20. A proper definition of the boundary conditions is important for accurate capture of free surface dynamics.

2.7.5. Summary

The finite difference/finite volume approach to numerically solving the equations of fluid motion, combined with the FAVORTM and VOF methods provide the basis of the CFD calculations for incompressible and compressible flows in this book. The numerical solutions also contain turbulence, heat transfer and solidification. These and other numerical models are part of a general-purpose CFD code **FLOW-3D[®]** [FLOW-3D, 2006]. This code has been used through this book to validate analytical models and to provide transient, three-dimensional solutions that are beyond those simplified approaches.

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