

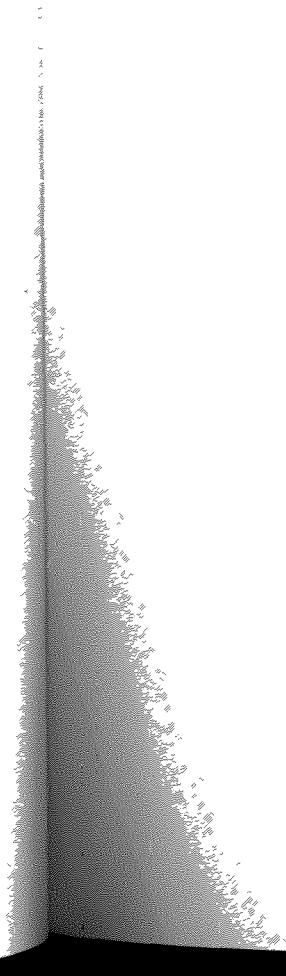
Transport Phenomena

The Art of Balancing

Harry Van den Akker
Robert F. Mudde

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Delft Academic Press

Preface

In 1956, Hans Kramers in Delft published his first lecture notes (in Dutch) on 'Fysische Transportverschijnselen' – to the best of our knowledge the first systematic treatment of the emerging discipline of Transport Phenomena. In 1958, Robert B Bird spent a period in Delft as a guest of Hans Kramers. This visit gave the two Professors the excellent opportunity to explore and improve the way of teaching Transport Phenomena. Bird published his 'Notes on Transport Phenomena' in the Fall of 1958, followed in 1960 by the first Wiley edition of the famous 'Transport Phenomena' textbook by Bird, Stewart & Lightfoot.

In Delft, the Dutch students kept using Kramers' shorter lecture notes in Dutch which in the course of the years were continuously improved, also by Kramers' successors Wiero J Beek and John M Smith. All those years the analogy of momentum, heat and mass transport remained the leading theme, just like in Bird's textbook. An essential element in the way Transport Phenomena has been taught in Delft has always been the emphasis on developing the students' ability of solving realistic engineering problems. Over the years, hundreds of challenging exam problems were devised.

In 1996, the current authors published a new version of the Delft lecture notes on Transport Phenomena for various reasons. Students, their interests, their prior education, and the way they prepare for exams were changing. In many curricula, the course got a different role and place. New applications in biotechnology, biomedical, smart materials and solar developed – remote from the traditional chemical industry. And Computational Fluid Dynamics (CFD) developed into a real analytical tool. All this required different didactic methods for teaching as well as different examples and exam problems.

Our new version of the Delft textbook 'Transport Phenomena' (still in Dutch) built on the earlier Delft lecture notes but was still based on the classical analogy of momentum, heat and mass transport, although the order of treatment was changed. fluid mechanics largely moved to the end, provoked by ideas developed by Kees Rietema at Eindhoven University of Technology. Most importantly, however, we put a much stronger emphasis on the basic method of drawing up balances, either about a particular device (a macro-balance) or about a differential element anywhere in a material or fluid (a micro-balance). In most cases, such a balance turns into a differential equation. We believe that teaching students as to how to draw up balances and solve differential equations is an excellent preparation for exploiting

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modern CFD techniques. The exam requirement that students should be capable of solving original problems was maintained.

Our textbook was quite successful. a 2nd edition was released in 2003-2005, a 3rd edition in 2008. In recent years, however, increasing numbers of foreign students arrived at Delft University of Technology for various MSc programs. This development has prompted the idea of publishing an English version of our Dutch textbook, simultaneously updating and improving a Dutch 4th edition. This textbook – Transport Phenomena: The Art of Balancing – is the result. We hope it will find its way to foreign universities as well.

We like to express our sincere appreciation for all suggestions for improvements we received over the years. In particular we like to acknowledge the contributions from A G N Boers, C Ouwerkerk, G C J Bart, C R Kleijn, J J Ph Elich, L M Portela, J A Battjes, R B Bird, and J E Schievink. We remain open for suggestions of further improvements.

Delft, August 2014

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Balances

1.1 The balance: recipe and form

The field of transport phenomena covers the transport of the three most important quantities – mass, energy, and momentum – in any (physical or chemical) process. The addition of the words ‘in any process’ in particular is an indication of one of the most important features of the field: transport phenomena is, above all, an engineering field with a wide range of applications.

Nonetheless, the field is also fundamental, given that it forms the basis for many other chemical engineering disciplines, such as reactor engineering, separation technology, and fluid mechanics. This makes transport phenomena a must for any chemical engineer. A good knowledge of the subject is also very useful to those in other professions, such as mechanical, mining, civil, and building engineers, physicists, chemists, and materials scientists.

The area covered by the field of transport phenomena and the discipline of chemical engineering is considerable. There are, for example, all kinds of processes in the chemical and petro-chemical industry, the flow of one or more phases through a pipeline, the behaviour of bubbles in a bioreactor, or the filling of a casting mould with liquid metal. At the other end of the scale, the field is also very important to more everyday matters, such as the heat emission of a radiator and the associated air flows in the room, and transport of oxygen by blood flow. Fortunately, these very different processes can be clearly understood and described with a limited number of rules.

Flow phenomena and heat and mass transfer are described in this field in terms of continuum properties, with only occasional references to molecular processes. This is how the basis is laid for chemical engineering: the expertise of designing and improving processes in which substances are transported, transformed, processed, or shaped. It is important here to fully understand the essence of a process – that is, to identify the essential stages in the transport of mass, heat, and/or momentum. The transport of these three quantities can, as it happens, be described in exactly the same way. Transport phenomena lays the basis for physical technology and provides the necessary tools. This textbook is about these tools.

First and foremost, transport phenomena is a subject of *balances* and *concepts* by which physical processes and phenomena can be described. In many cases, the subject is about deviations from a state of equilibrium and the subsequently occurring *resistances* to heat and mass transport. It frequently concerns a quantitative description of cause and effect. With the help of these still somewhat vague terms, it is possible to gain an outlined, but also very detailed, understanding and description of the aforementioned and countless other processes. This chapter will discuss the term *balance* in extensive detail.

For the description of the transport of any quantity, such as the transport of oxygen from bubbles to the liquid phase in a fermenter or the transport of heat through the wall of a furnace, the balance is an essential tool. The basic principle of the balance is the bookkeeping of a selected physical quantity. This concept is of particular importance when working with what are known as conserved quantities, these are quantities (like mass and energy) that are not lost during a process, but conserved.

The field of transport phenomena deals with steady-state or transient (time-dependent) processes in which mass, energy and momentum are exchanged between domains as a result of driving forces (differences in concentrations of mass, energy and momentum, and/or in pressure). Transport phenomena is therefore primarily about the ‘bookkeeping’ of the three physical quantities mass, energy and momentum.

This bookkeeping can refer to large control volumes, which involve *macrobalances*, however, balances can also be drawn up in relation to very small control volumes – these are known as *microbalances*, which provide information at a local scale. In almost all cases, solving problems such as about transport or transfer rates, or about changes in concentrations or temperatures, starts with drawing up one or more balances.

The next step is to derive from such balances proper equations, in many cases differential equations, the latter require initial and/or boundary conditions. The final step is about solving these (differential) equations to find the answer to the problem under consideration. In this approach, it is essential to denote all quantities with symbols!

The *general recipe* for drawing up a balance and solving the problem can be summarised as follows:

- 1) Make a sketch of the situation. Use symbols rather than numerical values to indicate quantities.
- 2) Select the quantity G that is being transported or transferred in the process under consideration.
- 3) Select the ‘control volume’ V about which information is to be obtained.

- 4) Find out whether and if so, how, the quantity of G in the control volume V changes during a brief period of time Δt . Draw up the balance (using symbols).
- 5) Solve the (differential) equation resulting from the balance.

The quantity of G in V can change in all kinds of ways. These should be examined systematically and, if applicable, included in the balance. For example, during Δt , G can flow into V from outside. As a result, the quantity of G inside V increases. It is also possible for G to flow outwards, from inside V . In this case, the quantity of G in V falls. We refer to “inflow” and “outflow”, respectively. Of course, it is also possible for *production* of G to occur inside V during period Δt : as a result, the total quantity of G in V increases. Negative production (= destruction, consumption, annihilation) is also possible, for example if G stands for the mass of a reagent that is being transformed in a chemical process.

Bear in mind that G may not necessarily be the quantity in which you are interested. In order to calculate temperature T , for example, a thermal energy balance has to be drawn up, and the thermal energy U must be selected for G .

The general structure for a balance is now as follows (see also Figure 1.1)

The change of G in V during Δt =

$$\begin{aligned} &= G \text{ (at time } t + \Delta t \text{) in } V - G \text{ (at time } t \text{) in } V \\ &= \text{quantity of } G \text{ that flows from outside into } V \text{ during } \Delta t + \\ &\quad - \text{quantity of } G \text{ that flows outside from inside } V \text{ during } \Delta t + \\ &\quad + \text{net quantity of } G \text{ that is produced in } V \text{ during } \Delta t \end{aligned}$$

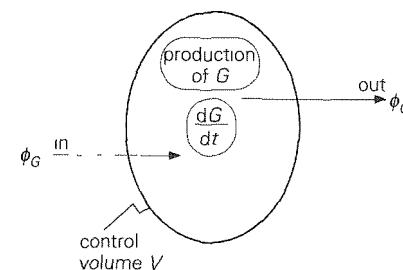


Figure 1.1

From now on, the symbol ϕ will be used to denote a transport (rate), with the dimension ‘quantity of G per unit of time’. Instead of transport rate, the term *flow rate* is used. The letter P stands for net production per unit of time, or net production rate. With the help of this notation, the quantity of G that flows ‘inwards’ (= from the outside to the inside) *during* the period of time Δt can, if Δt is very short, be written as the product of the flow rate ‘in’ *at time* t and the period of time Δt .

$$\phi_{G,\text{in}}(t) \Delta t$$

The same applies to the flow of G from the inside to outside and to the net production during Δt

$$\phi_{G,\text{out}}(t) \Delta t \text{ and } P_G(t) \Delta t$$

This means the balance is

$$G^{\text{in}V}(t + \Delta t) - G^{\text{in}V}(t) = \phi_{G,\text{in}} \Delta t - \phi_{G,\text{out}} \Delta t + P_G \Delta t \quad (1.1)$$

Dividing both sides of the Equation (1.1) by Δt and taking the limit $\Delta t \rightarrow 0$ produces

$$\frac{d}{dt} G^{\text{in}V} = \phi_{G,\text{in}} - \phi_{G,\text{out}} + P_G \quad (1.2)$$

Equation (1.2) is the basic form of the balance and is called the *balance equation*. The left-hand side therefore stands for the incremental change of the total quantity of G in V , while the three ways in which the total quantity of G in V can change are given on the right-hand side. The left-hand side is also known as ‘unsteady-state term’. All terms in Equation (1.2) have the same dimension – *should* have the same dimension: quantity of G per unit of time.

If, for a given quantity G , the net production *always* equals zero, in the case of mass, for example, then Equation (1.2) is simplified to

$$\frac{d}{dt} G^{\text{in}V} = \phi_{G,\text{in}} - \phi_{G,\text{out}} \quad (1.3)$$

Equation (1.3) is called a *conservation law*. Some quantities are indeed conserved – that is, they are only transported and/or (re)distributed.

It is very important to understand that the flows ‘in’ and ‘out’ actually have to cross the outer boundary of the control volume V .

Example 1.1. Population

The population of the Netherlands is known on 31 December of a particular year. Based on this number, describe a method for determining the number of people living in the Netherlands on 31 December of the following year, without counting them all over again.

The way of keeping track of the population is to use the balance method. To that end, use the general formula: first, the control volume has to be selected, with the number of people being the quantity for which the balance has to be drawn up. In this case, it is the Netherlands (see Figure 1.2).

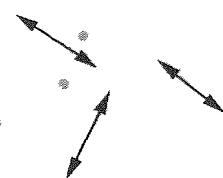


Figure 1.2

For the inflows and outflows during the year of interest, all the borders of the control volume have to be taken into consideration. This means that not only do the external borders with Belgium, Germany, and the North Sea have to be involved in the drawing up of the balance, but also individual transit points like airports and harbours. The borders should be defined here in the traditional sense of ‘passing through Customs’ (the fact that checks are no longer made on the internal borders of the European Union is not relevant here). Finally, the question of ‘production’ must not be overlooked: all births and deaths have to be counted up in order to arrive at the net production term in the balance equation, Equation (1.2).

Notice that a balance method of this kind also works for the number of people in the Netherlands aged between 20 and 30 years. However, extra care should be taken with regard to all the terms on the right-hand side of Equation (1.2): in the case of the inflows and outflows, the proportion of 20 to 30-year-olds in the flows should be used, while net production term should include all those who have turned 20 (counting positive) and 30 (counting negative) in period Δt as well as those who died between these ages.

□

Summary

The balance is an essential instrument in describing and calculating transport phenomena. Five basic rules are important when drawing up a balance and solving a problem. Together they may be considered as the recipe for solving transport issues:

- 1) make a sketch of the situation including all transports in and out, and the production inside, and use symbols;
- 2) select the quantity for which a balance has to be drawn up;
- 3) select the control volume about which the balance is to be drawn up;
- 4) draw up the balance in the form of which always is:

$$\frac{d}{dt} G^{\text{in}V} = \text{in} - \text{out} + \text{production}$$

5) solve the resulting (differential) equation

1.2 The mass balance

1.2.1 The total mass balance and the species balance

We will first deal with the balance for the total mass M . The total mass is typically a conserved quantity: the production or destruction of mass is impossible (except in the case of nuclear reactions), but it can be transported. This is why a conservation law applies to M . By substituting M for G , Equation (1.3) then becomes

$$\frac{d}{dt} M = \phi_{m,in} - \phi_{m,out} \quad (1.4)$$

The units of the different variables in Equation (1.4) offer a useful tool for checking the balance that has been drawn up. In Equation (1.4), all four terms have the unit kg/s.

Next is the mass balance for one of the species of a multiple-species system (see Figure 1.3). The bookkeeping is now concerned with mass M_A of substance A, which is present in control volume V . The general form of such a species-mass balance is

$$\frac{d}{dt} M_A = \phi_{m,A,in} - \phi_{m,A,out} + P_A \quad (1.5)$$

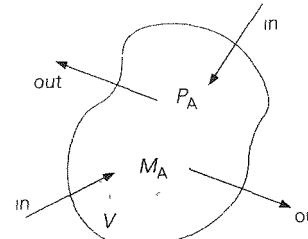


Figure 1.3

In the case of Equation (1.5), unlike Equation (1.4), we cannot talk of a conservation law anymore, on account of the production term P_A which is due to one or more chemical reactions. As in the case of chemical reactions working in terms of moles is to be preferred, all four terms in such a species-mass balance, Equation (1.5), have the unit mol/s or kmol/s.

It is often much more useful to draw up the balance with the help of concentrations. Later on, it will be shown frequently that it is concentrations and differences in

concentration that determine transport and not so much the quantity (the mass, in this case) itself. In general, a concentration is defined as the quantity G per unit of volume. Put another way, the concentration (g) of G is the quantity of G in volume V divided by the size of volume V , as a formula, this is

$$g = \frac{G}{V} \quad (1.6)$$

The concentration of the total mass is equivalent to density ρ , while the concentration of a species is represented by a c . Therefore, for a multi-component system consisting of species A, B, etc

$$\begin{aligned} c_A &= \text{mass of A per unit of volume} = M_A/V \\ c_B &= \text{mass of B per unit of volume} = M_B/V \\ &\text{etc} \end{aligned} \quad (1.7)$$

Naturally, for the total (mass) concentration ρ , the following applies

$$\rho = \frac{M}{V} = \frac{M_A + M_B + \dots}{V} = c_A + c_B + \dots \quad (1.8)$$

In order to draw up a mass balance for species A, which is present in the reactor in Figure 1.4, it is strongly advisable to use the general recipe consistently, as summarised at the end of § 1.1:

- 1) make a sketch and indicate all quantities and transports in symbols (see Figure 1.4)
- 2) quantity → mass M_A of A in reactor
- 3) control volume → whole reactor volume V
- 4) systematically check whether, by what means and how M_A changes in V , and draw up the *balance* for M_A in V

Step 5 of the recipe is not yet appropriate at this time

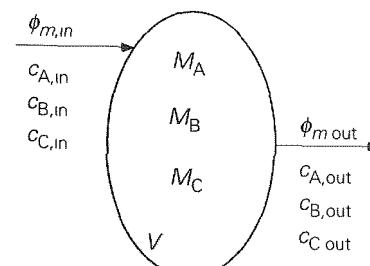


Figure 1.4

It is therefore a matter of systematically checking which effects can contribute to the increase or decrease of M_A in V . These effects will then become part of the right-

hand part of the balance equation, while dM_A/dt is on the left. The different terms on the right-hand side will be, in this case

flow in a mass flow $\phi_{m,\text{in}}$ goes into the reactor, which contains species A with a concentration $c_{A,\text{in}}$

$$\begin{aligned}\phi_{m,A,\text{in}} &= \text{mass of A that flows in per unit of time } V \\ &= (\text{volume that flows in per unit of time } V) \times (\text{mass of A} \\ &\quad \text{contained in a unit of volume of the ingoing flow}) \\ &= \phi_{V,\text{in}} c_{A,\text{in}}\end{aligned}\quad (19)$$

The symbol $\phi_{V,\text{in}}$ stands for the volumetric flow rate that goes into the reactor – that is, the number of cubic metres that flows into the reactor per second

flow out for this, by analogy, the following applies

$$\phi_{m,A,\text{out}} = \phi_{V,\text{out}} c_{A,\text{out}} \quad (10)$$

production as a result of a chemical reaction

$$P_A = r_A V \quad (11)$$

where r_A is the production of A per unit of volume (in mol/m³s). Because of this chemical reaction term, it is more useful to express all the concentrations in this balance equation in mol/m³

The species-mass balance for A in the reaction is therefore

$$\frac{d}{dt} M_A = \phi_{m,A,\text{in}} - \phi_{m,A,\text{out}} + P_A \quad (12)$$

and, as long as V is constant in time and with the help of Equations (17), (19), (10) and (11), can be rewritten as

$$V \frac{d}{dt} c_A = \phi_{V,\text{in}} c_{A,\text{in}} - \phi_{V,\text{out}} c_{A,\text{out}} + r_A V \quad (13)$$

Equation (13) is equivalent to

$$\frac{d}{dt} c_A = \frac{\phi_{V,\text{in}}}{V} c_{A,\text{in}} - \frac{\phi_{V,\text{out}}}{V} c_{A,\text{out}} + r_A \quad (14)$$

Notice that all the terms in Equation (14) now have the unit mol/m³s

If the corresponding Equations (13) for all the species present are written down and then counted up, the mass balance for the overall mass in V (the overall mass balance for short) is obtained

$$\begin{aligned}V \frac{d}{dt} c_A &= \phi_{V,\text{in}} c_{A,\text{in}} - \phi_{V,\text{out}} c_{A,\text{out}} + r_A V \\ V \frac{d}{dt} c_B &= \phi_{V,\text{in}} c_{B,\text{in}} - \phi_{V,\text{out}} c_{B,\text{out}} + r_B V \\ &\vdots \\ V \frac{d}{dt} (c_A + c_B + \dots) &= \phi_{V,\text{in}} (c_A + c_B + \dots)_{\text{in}} + \\ &\quad - \phi_{V,\text{out}} (c_A + c_B + \dots)_{\text{out}} + (r_A + r_B + \dots) V\end{aligned}\quad (15)$$

The left-hand side can be written as $V d\rho/dt = dM/dt$. The final term of the right-hand side is zero, as production of one species as a result of reactions entails the annihilation of other species. If $\phi_V \rho = \phi_m$ is also used, then Equation (15) does indeed cover the overall mass balance, see Equation (14)

Example 1.2. A chemical reactor under steady conditions

A chemical reaction takes place in a reactor. Substance A reacts, becoming a new product B. An aqueous solution of A flows into the reactor. The volumetric flow rate is 1 l/s, of which the concentration of A is $c_{A,\text{in}} = 100 \text{ kg/m}^3$. The reaction in the reactor is not complete, so that A is still present in the reactor exit. The volume flow at the exit is also 1 l/s, and the concentration here is $c_{A,\text{out}} = 20 \text{ kg/m}^3$. The situation is *steady* (that is, does not change over time). How great is the (negative) production of A in the reactor?

Clearly, in order to answer the question, a balance for the mass of A in the reactor will have to be drawn up. To do this, apply the recipe

- 1) sketch → see Figure 1.5.

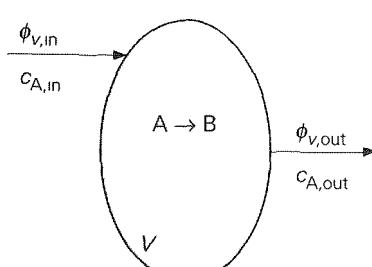


Figure 1.5.

- 2) quantity → M_A

3) control volume → whole reactor

4) steady → “ $\frac{d}{dt} = 0$ ”, the volumetric flow rates in and out are exactly the same → $\phi_{V,in} = \phi_{V,out} = \phi_V$

This means the balance is as follows

$$0 = \phi_V c_{A,in} - \phi_V c_{A,out} + P_A$$

For the production, this gives

$$P_A = \phi_V c_{A,out} - \phi_V c_{A,in} = 10^{-3} (20 - 100) = -8 \cdot 10^{-2} \text{ kg/s}$$

□

Incidentally, it is also possible to work with *mass fractions* instead of concentrations. These are written as an x and defined as the fraction of the species under consideration in relation to the overall mass

$$x_A = \frac{M_A}{M} \quad (1.16)$$

In terms of the mass fraction, the mass balance for species A is

$$\frac{d}{dt} (M x_A) = \phi_{m,in} \cdot x_{A,in} - \phi_{m,out} \cdot x_{A,out} + P_A \quad (1.17)$$

Notice that x has no dimension – that is, the unit is kg/kg

To simplify the balance equations and to arrive at (differential) equations that can be solved easily, some simplifying concepts have become quite commonplace in the chemical engineering world. First, the concept of an *ideally stirred tank*, or *ideally mixed tank*, has been introduced. This denotes a (flow) device in which the composition of its contents is always the same everywhere in the tank. This means that at all times the composition of the liquid that flows out of the tank is the same as that inside the tank. In the case of an ideally stirred tank being a chemical reactor operated with a continuous inflow and outflow, the term *Continuous Stirred Tank Reactor* (CSTR) is widely used.

For the first time in this textbook, first order linear differential equations have to be solved in the next example. The technique of solving this type of differential equation is presented in Appendix 1A.

Example 1.3. Coconut oil in an ideally stirred tank

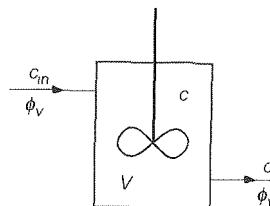


Figure 1 6

Look now at the situation in Figure 1 6 for an ideally stirred tank. There is a continuous and steady volumetric flow rate ϕ_V going into and out of the tank. This flow contains a certain concentration of palm seed oil c_{P0} . The tank is and remains completely full of palm seed oil. This is therefore a steady situation: flow rates and composition of the liquid do not change over time. At time $t = 0$, however, the supply of palm seed oil is stopped abruptly while at the same moment in time a liquid with a coconut oil concentration $c_{C,in}$ is supplied to the tank at the same volumetric flow rate.

The question is now: how do the concentrations of palm seed oil and coconut oil change at the exit as a function of time?

To find the answer, a mass balance has to be drawn up, in accordance with the formula – first, for the palm seed oil:

1) sketch → see Figure 1 6

2) quantity → mass of palm seed oil → $M_P = V \cdot c_P$

3) control volume → volume of the tank V

4) mass balance (for period $t \geq 0$)

$$V \frac{d}{dt} c_P = \phi_V 0 - \phi_V c_P + 0 \quad (1.18)$$

From $t = 0$ the entrance concentration $c_{P,in}$ of the palm seed oil equals zero. Equation (1.18) can now be rewritten as

$$\frac{d}{dt} c_P = -\frac{\phi_V}{V} c_P \quad (1.19)$$

Equation (1.19) now has to be solved as follows (as a boundary condition):

$$t = 0 \rightarrow c_P = c_{P0}$$

This produces

$$c_P(t) = c_{P0} \cdot \exp\left(-\frac{\phi_V}{V} t\right) \quad (1.20)$$

According to the same recipe, a mass balance can also be drawn up for the coconut oil for the period $t \geq 0$

$$V \frac{d}{dt} c_C = \phi_V c_{C,in} - \phi_V c_C + 0 \quad (1.21)$$

Equation (1.21) can be rewritten as

$$\frac{d}{dt} c_C = \frac{\phi_V}{V} (c_{C,in} - c_C) \quad (1.22)$$

Solving this differential equation along with the initial condition $c_C = 0$ at $t = 0$ results in

$$c_C(t) = c_{C,in} \left[1 - \exp\left(-\frac{\phi_V}{V} t\right) \right] \quad (1.23)$$

The latter equation expresses at which rate the concentration of coconut oil in the tank becomes equal to the concentration $c_{C,in}$ at the inlet after the switch

□

Summary

The general form of the species-mass balance for species A is

$$\frac{d}{dt} M_A = \phi_{m,A,in} - \phi_{m,A,out} + P_A$$

This balance can also be written in terms of concentrations and chemical reaction rate r_A :

$$\frac{d}{dt} V c_A = \phi_{V,in} c_{A,in} - \phi_{V,out} c_{A,out} \pm r_A V$$

The concentration of species A is denoted as c_A and, because of the chemical reaction(s), is in moles of A per unit of volume, with the rate r_A in moles of A per unit of volume and per unit of time.

Some examples (without chemical reactions) have shown how balance equations lead to first order linear differential equations which can easily be solved by the separation of variables method.

1.2.2 Chemical reactors

In Example 1.3, there was no production term. However, in chemical reactors, production (and/or consumption) of one or more species is an essential feature. In such cases, the production term will have to be specified in order to be able to solve the balance

This method will be illustrated for a *first order chemical reaction* in which the rate of transformation of species A per unit of volume, denoted as r_A (in mol/m³s), is directly proportional to the concentration c_A of A (in mol/m³)

$$r_A = k_r c_A \quad (1.24)$$

Here, k_r is the *first order reaction rate constant* (unit s⁻¹). For a reaction in which species A is consumed, the production rate of A is given by $P_A = -r_A V$ and is negative. For the simple reaction A → B, the positive production rate of species B depends on just the concentration c_A of species A and is given by $P_B = +r_A V$.

We will now examine different types of reactor

The batch reactor

Consider first an ideally stirred tank that is operated *batch-wise*, that is, the tank is filled in one go, after which nothing flows in or out. A is transformed according to a first-order reaction. This kind of reactor is known as a *batch reactor*. Given that there are no flows in or out of the reactor, the mass balance for substance A in the case of a constant reactor (control) volume is as follows

$$V \frac{d}{dt} c_A = 0 - 0 + r_A V = r_A V = -k_r c_A V \quad (1.25)$$

The solution to Equation (1.25) is obtained by using the pertinent boundary condition $c_A(t=0) = c_{A,0}$ representing the addition in one go of all reactive species to the tank.

$$\frac{c_A}{c_{A,0}} = \exp(-k_r t) \quad (1.26)$$

As was to be expected, quantity A in the tank reduces over time. After all, no A is supplied into the tank or withdrawn from the tank during the period in which A was being transformed.

The plug flow reactor

It is now the turn of the *ideal tubular reactor* for a chemical reaction to occur. In an ideal tubular reactor of this kind, each liquid package moves as quickly as all the others. This is known as *plug flow* and the reactor is denoted as a *plug flow reactor*. In our case, the reaction is again first order (with reaction rate constant k_r), where A is transformed into B.

Assuming that the concentration of substance A at the start of the reactor is $c_{A,0}$, what will the concentration be at the tube exit?

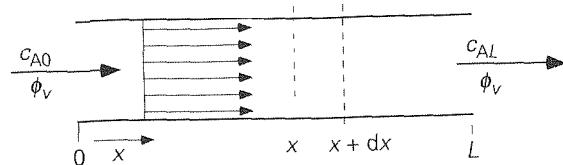


Figure 1.7

For the sake of simplicity, diffusion (will be covered later) is ignored and it is assumed that the liquid (in spite of the reaction) has a constant density. As a result of the chemical reaction, the concentration of A will steadily decrease towards the direction of the exit. To establish this pattern (the *profile*), a small slice of the tube somewhere in the reactor between x and $x + dx$ should be examined where x is the coordinate along the reactor in the direction of the flow (see Figure 1.7). Again, it is assumed that the condition is steady – that is, that there are no changes over time. A mass flow of A, quantity $\phi_v c_A$, comes into the control volume through the left-hand boundary plane. Of course, the concentration taken is the one as it is at position x . This is shown as $c_{A|x}$. Meanwhile, $\phi_v c_A$ flows out through the right-hand boundary plane, but now with c_A as it is at position $x + dx$ is $c_{A|x+dx}$. Finally, the consumption of A inside the slice as a result of the chemical reaction is again represented by $r_A V$ where now $V = Adx$. The mass balance over the plate is now

$$0 = \phi_v c_{A|x} - \phi_v c_{A|x+dx} - k_r c_A Adx \quad (1.27)$$

in which A is the surface of the cross section of the tube (perpendicular to the direction of the flow). Notice that the left-hand side of the equation is zero, given that the state is assumed to be steady, in the control volume, it is therefore not possible for the mass of A to change. By dividing all terms of the right-hand side of the equation by dx and taking the limit $dx \rightarrow 0$, Equation (1.27) can be written as follows

$$\phi_v \frac{dc_A}{dx} = -k_r A c_A \quad (1.28)$$

By using the method of separation of variables and thanks to the boundary condition $c_A(x=0) = c_{A0}$, the solution to this is:

$$\frac{c_A(x)}{c_{A0}} = \exp\left(-\frac{k_r A x}{\phi_v}\right) \quad (1.29)$$

This means the concentration at the exit is

$$\frac{c_A(L)}{c_{A0}} = \exp\left(-\frac{k_r A L}{\phi_v}\right) = \exp\left(-\frac{k_r V}{\phi_v}\right) \quad (1.30)$$

in which $V = A L$ is the volume of the tubular reactor

The above technique for drawing up a balance over a thin slice, of which the dimension goes to zero (limit $dx \rightarrow 0$), leads to a *micro balance*, see Equation (1.27), and provides detailed information (that is, a *profile*). As the local rate of the chemical reaction depends on the local concentration that decreases along the tubular reactor, this approach of drawing up a micro balance for a thin slice really is a must, although the original question was related only to the concentration at the reactor exit.

The Continuous Stirred Tank Reactor (CSTR)

Example 1.3 will now be expanded to include a chemical reaction. The reactor, a CSTR, contains a catalyst that accelerates the conversion of species A. The catalyst cannot leave the reactor. At first, a flow rate ϕ_v that does not contain any A passes through the reactor. From time $t = 0$, the incoming flow ϕ_v contains a concentration c_{A0} of A.

How does the concentration of A at the reactor exit progress as a function of time?

Again, a mass balance has to be drawn up and the resulting differential equation solved. Mass A is the quantity to be considered for the balance, and the control volume is the volume of the reactor. The balance is as follows

$$\frac{d}{dt} V c_A = \underbrace{\phi_v c_{A0}}_{\text{in}} - \underbrace{\phi_v c_A}_{\text{out}} - \underbrace{k_r c_A V}_{\text{production}} \quad (1.31)$$

For constant reactor volume and constant ϕ_v this balance equation can be rewritten as

$$\frac{d}{dt} c_A = -\left(\frac{\phi_v}{V} + k_r\right) c_A + \frac{\phi_v}{V} c_{A0} \quad (1.32)$$

This differential equation is a first order linear differential equation of the type

$$\frac{dy}{dx} = \alpha y + \beta \quad (1.33)$$

the solution of which is discussed in Appendix 1A.

With the initial condition that $c_A = 0$ at $t = 0$ (the reactor did not contain any A at the start), the solution to Equation (1.31) is

$$c_A(t) = \frac{\phi_v/V}{\phi_v/V + k_r} c_{A0} \left\{ 1 - \exp\left[-\left(\frac{\phi_v}{V} + k_r\right)t\right] \right\} \quad (1.34)$$

Notice that both ϕ_v/V and k_r have the unit s^{-1} . The eventual steady-state situation may be considered as a limit case and is obtained by substituting $t \rightarrow \infty$ into Equation (1.34)

$$c_A = \frac{1}{1 + k_r \frac{V}{\phi_v}} c_{A0} \quad (1.35)$$

This result can be directly derived from Equation (1.31), too in the eventual steady state the d/dt -term is zero

When comparing the performances of the ideal tubular reactor and the ideally stirred tank, both with the same ϕ_v/V -ratio, it is immediately clear that the transformation in the tubular reactor is much greater. This is caused by a difference in the average concentration $\langle c_A \rangle$ between both reactors. For a reactant that depletes the following applies in the tubular reactor, $\langle c_A \rangle$ is always greater than c_{A0} , while in the tank reactor $\langle c_A \rangle$ is actually always equal to the concentration at the exit. Given that the transformation is proportional to the concentration in the case of a first order reaction, the transformation in the tubular reactor will therefore be greater.

Example 1.4. A plug flow reactor with recirculation

For the purpose of exercise, we will now look at a practical situation in which part of the outgoing flow is fed back into the reactor. This is done in order to gain a better use of a reactant, if only a proportion of that reactant is transformed in a single passage, this means the length of the reactor does not have to be so long. It also means that in the case of an exothermic reaction (very common), the temperature at the entrance and consequently also the conversion of A in the reactor can be jacked up 'cheaply' using part of the heat in the exit flow (after all, most reactions take place more quickly with higher temperatures). In other cases, a heat exchanger is often placed in the recirculation duct that allows some of the reaction heat to be extracted from the flow and used elsewhere. This situation is illustrated in Figure 1.8

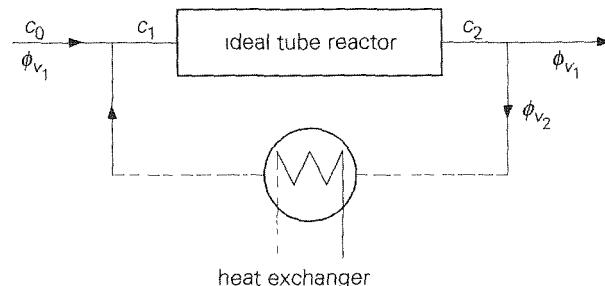


Figure 1.8

In the ideal tubular reactor, species A is transformed according to a first order chemical reaction. The volumetric flow rate of the inflow and outflow is ϕ_{v_1} . In order to remove the reaction heat, a volumetric flow rate ϕ_{v_2} is recirculated by a heat exchanger. The concentration of A in inflow ϕ_{v_1} is c_0 . The concentration that flows into the reactor is shown as c_1 ($\neq c_0$), while the concentration that leaves the reactor is referred to as c_2 . For the sake of simplicity, it is assumed that the reaction only occurs in the reactor. The volume of the reactor is V and the situation is steady. How great is c_2 compared with c_0 ?

The flow rate $\phi_{v_1} + \phi_{v_2}$ going into the reactor can be found by drawing up a total mass balance for the T-junction in the duct before the plug flow reactor. Similarly, the concentration c_1 follows from drawing up the mass balance for A for the same T-junction

$$0 = \phi_{v_1} c_0 + \phi_{v_2} c_2 - (\phi_{v_1} + \phi_{v_2}) c_1 \quad (1.36)$$

rearranging this equation, and introducing the *recirculation ratio* $a \equiv \frac{\phi_{v_2}}{\phi_{v_1} + \phi_{v_2}}$, all this gives

$$c_1 = \frac{\phi_{v_1} c_0 + \phi_{v_2} c_2}{\phi_{v_1} + \phi_{v_2}} = (1 - a) c_0 + a c_2 \quad (1.37)$$

From the earlier discussion on the plug flow reactor, it follows that for the current configuration the exit concentration c_2 obeys to

$$\frac{c_2}{c_1} = \exp \left(-k_r \frac{V}{\phi_{v_1} + \phi_{v_2}} \right) \quad (1.38)$$

Eliminating c_1 from Equation (1.38) with the help of Equation (1.37) results into

$$\frac{c_2}{c_0} = \frac{1 - a}{\exp \left[(1 - a) k_r \frac{V}{\phi_{v_1}} \right] - a} \quad (1.39)$$

Two limit cases merit closer examination

- 1) $a = 0$, that is, no recirculation. For this situation, it follows from Equation (1.39) that:

$$\frac{c_2}{c_0} = \exp \left(-k_r \frac{V}{\phi_{v_1}} \right) \quad (1.40)$$

Of course, this is the result for the ideal tubular reactor of Equation (1.30) after all, there is now no recirculation

- 2) $a \rightarrow 1$, that is, the recirculation flow is much greater than ϕ_V . Now, with the help of the series expansion $\exp x \rightarrow 1 + x$ for $x \rightarrow 0$, Equation (1.39) can be approximated as follows

$$\frac{c_2}{c_0} = \frac{1}{1 + k_r \frac{V}{\phi_V}} \quad (1.41)$$

This is precisely the result that was obtained before – see Equation (1.35) – for an ideally stirred tank in a steady-state situation! \square

Summary

In this Section, several chemical reactors have been examined: the batch reactor, the plug flow reactor (being the ideal tubular reactor), the Continuous Stirred Tank Reactor (CSTR), and the plug flow reactor with recirculation. A first order reaction was assumed in every case.

Every time, one or more mass balances has to be drawn up for a suitable control volume. In many cases, this control volume was the full reactor vessel and the balance was a macro balance. In the case of a tubular reactor, however, you have to draw up a micro balance for a thin slice somewhere in the reactor, the slice thickness being dx with $dx \rightarrow 0$, this procedure leads to a differential equation from which the concentration profile $c(x)$ inside the reactor follows

1.2.3 Residence time distribution

Consider a small liquid package which, as part of a volume flow ϕ_V , flows into and through a tube of volume V , cross-sectional area A and length L . At time $t = 0$ the package (or element) has just entered the tube. At time t it has covered a distance of $\ell = v t$ (see Figure 1.9), therefore, at time $\tau = L/v$ the element is at the end of the tube. Time τ is referred to as the *residence time*.

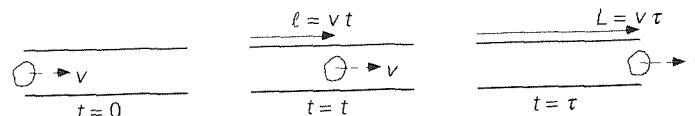


Figure 1.9

If every package in a flow has the same velocity $v = \phi_V/A$, then the same residence time τ applies to every package

$$\tau = \frac{L}{v} = \frac{AL}{\phi_V} = \frac{V}{\phi_V} \quad (1.42)$$

A flow in which every liquid package (or element) has the same residence time is described as *plug flow* (see also Figure 1.7)

In reality, the packages do not generally have one and the same residence time. After all, not every package has the same velocity and nor do they all cover the same route. In reality, the highest velocity in a tube is at the axis, while along the wall it is actually zero, this makes plug flow an ideal type of flow that in fact never occurs. In a stirred tank, the packages follow very different paths precisely because of the mixing. The result is that in reality, there is always a residence time distribution in every device, as well as a *mean residence time* $\bar{\tau}$, shown by

$$\bar{\tau} = \frac{V}{\phi_V} \quad (1.43)$$

Knowledge of this residence time distribution can be important for a successful operation of the process under consideration. An example that comes to mind is that of the sedimentation ('settling') of fixed particles in a sewage treatment plant. The residence time of *all* the packages of liquid has to be sufficiently long for all the particles in them to settle.

There are several functions by which the residence time distribution can be characterised, they will be discussed one-by-one below. The non-dimensional time $\theta = t/\bar{\tau}$ is used in every case, with τ defined through Equation (1.43).

The E-function

First of all, the residence time distribution can be characterised with the help of the 'ages' of the packages when they pass the exit. This way the age distribution at the exit can be obtained, which is known as the *E-function*. The definition of the *E-function* ('exit age function') is

$$E(\theta) d\theta = \text{volume fraction of the outgoing flow with a non-dimensional residence time of between } \theta \text{ and } \theta + d\theta \quad (1.44)$$

The recipe for determining $E(\theta)$ should be: take a sample from the outgoing flow and determine the fraction with a non-dimensional residence time of between θ and $\theta + d\theta$. Do this for every θ between 0 and ∞ . An example of an *E-function* is given in Figure 1.10.

Notice that the integral of $E(\theta)$ for interval $[0, \infty)$ is equal to 1. This can be understood by realising that

$$\int_0^{\theta_1} E(\theta) d\theta = \text{volume fraction of the sample of the outgoing flow with residence time } \theta \leq \theta_1 \quad (145)$$

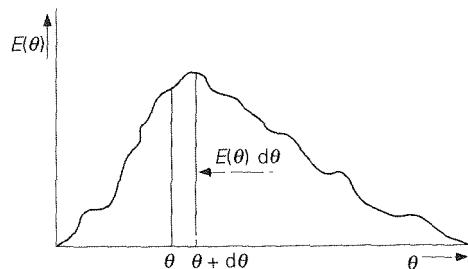


Figure 1.10

Every package that leaves the device via the outflow has only had a finite residence time in the device. For this reason, Equation (1.45) means

$$\int_0^{\infty} E(\theta) d\theta = 1 \quad (146)$$

The mean residence time τ can be calculated from the E -function according to

$$\tau = \int_0^{\infty} t E(\theta) d\theta \quad (147)$$

while the standard deviation of the residence time distribution can be described by

$$\sigma^2 = \int_0^{\infty} (t' - \tau)^2 E(t') dt' \quad (148)$$

This method of describing the residence time distribution is generally not very practical – after all, how do you determine how long a package has stayed in a device?

In practical situations, usually experiments are therefore conducted in which a known change is applied to the inflow of a device and the response to this at the exit is measured as a function of time, in order to find the residence time distribution that goes with that particular device. Incidentally, this procedure is not only used for a single device, but also for a combination of devices such as in a plant.

The most commonly-occurring entrance changes are the ‘step’ and the ‘pulse’ (see Figure 1.11). In the case of the step, a sudden change is applied to the concentration of some marked substance (marker, or tracer) in the inflow. This new level is then

maintained. The pulse scenario involves a brief ‘injection’ of the tracer in the inflow (the injection is so small in size and short in time that the flow rate ϕ_V remains more or less constant)

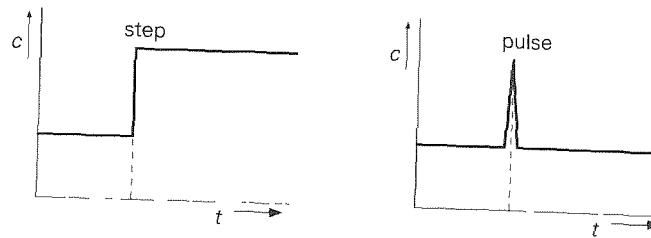


Figure 1.11

The C-function

The C -function shows the time-dependent response at the exit of a device to pulse-induced tracer material at the entrance. This process is illustrated in Figure 1.12.

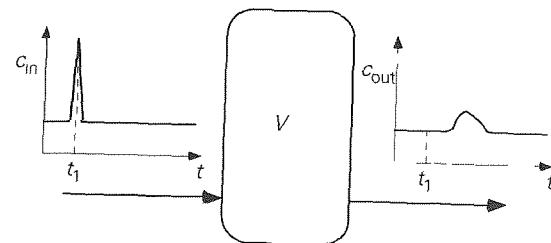


Figure 1.12

The total quantity of material A injected into the device amounts to M_A . For the average concentration c_0 of A in the device, if all of A is inside it, it then follows that $c_0 = M_A/V$ (where V is the volume of the device). The C -function is now defined as

$$C(\theta) = \frac{c_{\text{tr,out}}}{c_0} \quad (149)$$

$c_{\text{tr,out}}$ is the concentration of the tracer (denoted by index tr) at the exit. The mass balance (for $t > 0$) for the tracer material in the device is

$$\frac{d}{dt} M_{\text{tr}} = \phi_V c_{\text{tr,in}} - \phi_V c_{\text{tr,out}} = -\phi_V c_{\text{tr,out}} \quad (150)$$

In Equation (1.50), $c_{\text{tr,in}} = 0$ given that the tracer material is applied in a pulse at $t = 0$ and the balance is drawn up for $t > 0$.

The integral of the C -function from 0 to ∞ is also equal to 1. Proof of this follows from the integration of the left-hand side of Equation (1.50) from $t = 0$ to $t \rightarrow \infty$.

$$\int_0^{\infty} \frac{d}{dt} M_{\text{tr}} dt = M_{\text{tr}}|_0^{\infty} = -M_{\text{tr}}(t=0) = -V c_0 \quad (151)$$

where $M_{\text{tr}}(t \rightarrow \infty) = 0$ is used since all the tracer material will exit the device sooner or later. Combining Equations (150) and (151) produces

$$V c_0 = \int_0^{\infty} \phi_v c_{\text{tr,out}} dt \quad (152)$$

Dividing both the right-hand side and the left-hand side of this equation by $V c_0$ gives

$$1 = \int_0^{\infty} \frac{\phi_v}{V} \frac{c_{\text{tr,out}}}{c_0} dt = \int_0^{\infty} C(\theta) d\theta \quad (153)$$

The recipe for determining the C -function is therefore follow the tracer concentration change at the exit of the device after a tracer pulse has been applied at the entrance. The resulting curve should satisfy the condition of Equation (153).

It is possible to demonstrate that in a steady situation the E and C -functions are identical $C(\theta) = E(\theta)$. The methods by which they are determined are essentially different, however the E function is determined from a single sample, while in the case of the C function, the response at the exit has to be monitored for a sufficiently long period of time.

The F -function

The F -function is another function that can be found by following the concentration in the exit as a function of time. The F -function represents the response of the exit to a step function at the entrance – from e.g., $c = 0$ to $c = c_{\text{in}}$ (see Figure 113).

$$F(\theta) = \frac{c_{\text{out}}}{c_{\text{in}}} \quad (154)$$

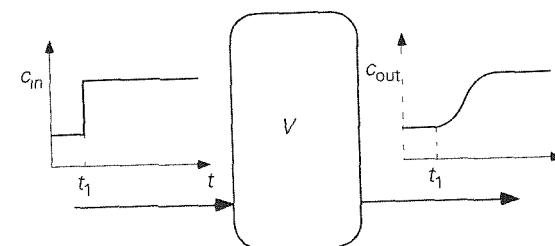


Figure 113

The F -function has some characteristic properties. For example, $F \rightarrow 1$ for $t \rightarrow \infty$, i.e. for $\theta \rightarrow \infty$ ultimately, the concentration in the exit is equal to that at the entrance. A possible shape of the F -function is shown in Figure 114.

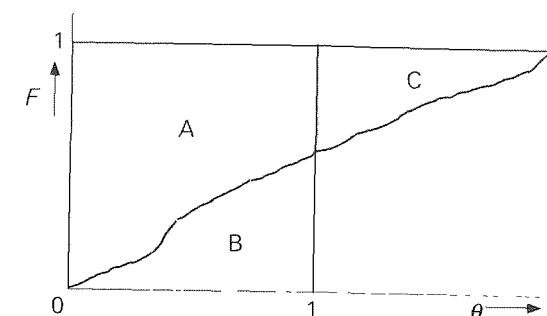


Figure 114

There is another characteristic that every F -function has. the shaded areas B and C in Figure 114 are of equal size. This can be derived as follows. the mass balance for the tracer material in the device is ($t \geq 0$)

$$\frac{d}{dt} M_{\text{tr}} = \phi_v c_{\text{in}} - \phi_v c_{\text{out}} \quad (155)$$

Integration from $t = 0$ to $t \rightarrow \infty$ produces

$$\int_0^{\infty} \frac{d}{dt} M_{\text{tr}} dt = \int_0^{\infty} \phi_v (c_{\text{in}} - c_{\text{out}}) dt \quad (156)$$

The left-hand side of this equation can again be rewritten as

$$\int_0^{\infty} \frac{d}{dt} M_{\text{tr}} dt = [M_{\text{tr}}]_0^{\infty} = V c_{\text{in}} \quad (157)$$

After all, at $t = 0$ the device does not contain any tracer yet, so $M_{\text{tr}}(t = 0) = 0$. Combining Equations (156) and (157) produces

$$1 = \int_0^{\infty} \frac{\phi_v}{V} (1 - \frac{c_{\text{out}}}{c_{\text{in}}}) dt = \int_0^{\infty} [1 - F(\theta)] d\theta \quad (158)$$

In other words, the sum of the areas A and C in Figure 114 is exactly equal to 1. $A + C = 1$. At the same time, the sum of areas A and B is equal to 1 (the length of both sides of the square AB is 1). The conclusion is therefore that areas B and C are equal, regardless of the form of the F -function.

The physical significance of the F -function is that F is equal to the volume fraction in the outgoing flow with a non-dimensional residence time of less than θ . From the definitions of C and E , it follows that $C(\theta)d\theta$ is the volume fraction in the outgoing flow with a residence time of between θ and $\theta + d\theta$, the following therefore applies

$$F(\theta) = \int_0^{\infty} C(\theta) d\theta = \int_0^{\infty} E(\theta) d\theta \quad (159)$$

The second equality applies only in a steady-state situation. An extremely practical relationship follows from Equation (159)

$$C(\theta) = \frac{dF(\theta)}{d\theta} \quad (160)$$

It is very useful since the discrete character of the pulse function prevents its use as a boundary condition when trying to calculate a C -function for an ideal type of flow device from the differential equation that results from a species mass balance. The step function, however, does make the use of a boundary condition in the calculation of an F -function feasible. The C -function can then be calculated from the F -function thanks to the property of Equation (160). See Examples 1.5 and 1.6 below.

Real-world and ideal flow devices

E -, C - and F -functions characterize, each in their own way, the state of mixing in a vessel, or system, and in this way how a system responds to changes from outside. In the real world, it is possible and rather easy to just measure the F - and C -functions. In Figure 1.15 some C -functions are presented. Figure 1.15a shows a response in which the distribution is rather nicely centred around the mean residence time τ – as a result of a rather sound flow or mixing state of the tank under review. In Figure 1.15b, however, the stepwise drop in the response for times longer than τ may be indicative of an internal circulation. A dual peak such as in Figure 1.15c may suggest that the liquid flow may get split upon entering the vessel with the two liquid streams reaching the exit via separate paths of unequal length. In Figure 1.15d, the maximum of the distribution function arriving earlier than τ as calculated with Equation (143) may be due to short-circuiting between entrance and exit, some parts of the vessel acting as ‘dead zones’ which do not really take part in the through flow.

By comparing a measured response with a set of calculated residence distribution functions, it might be possible to roughly characterise the flow or mixing state of a tank or system as ideally stirred, a plug flow, a number of ideally stirred tanks in series, or a combination of plug flow and ideally stirred tanks.

We will therefore now turn to various types of ideal flow devices – such as one of more ideally stirred tanks, or a plug flow – for which F and C -functions can be calculated. Remember that, since these functions characterise the residence time distribution, chemical reactions can and indeed must be disregarded. After all, the residence time distribution in a particular device is determined solely by the flow or mixing state.

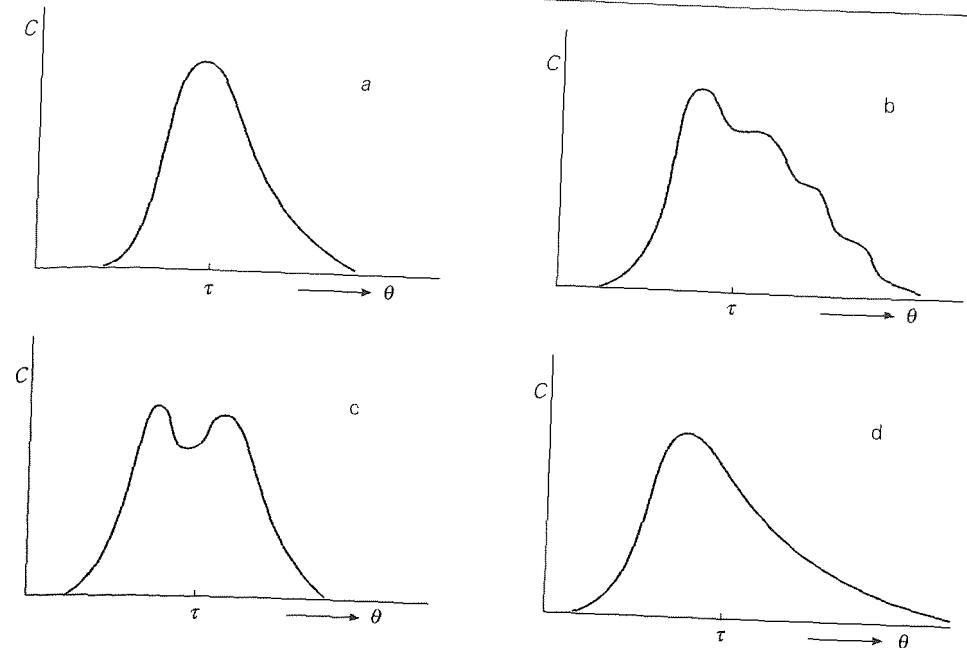


Figure 1.15

Example 1.5. F and C -functions for an ideally stirred tank

Calculate the F and C -functions for the ideally stirred tank. See Figure 1.6 and also Example 1.3.

In Example 1.3, coconut oil replaces palm seed oil at the entrance at, say, $t = 0$. In other words, this is a ‘step’ from 0 to c_m in the concentration of coconut oil at the entrance. In order for the F and C -functions to be determined, it is necessary to determine the concentration of the tracer (the coconut oil) at the exit as a function of the time. The mass balance for coconut oil is given by Equation (1.21) and can be shown to result in the expression for the exit concentration given by Equation (1.23). With $\tau = V/\phi_V$ and $\theta = t/\tau$ it follows for the F -function that

$$F(\theta) = \frac{c_{\text{out}}}{c_m} = 1 - \exp(-\theta) \quad (161)$$

and therefore, thanks to Equation (1.56), for the C -function that

$$C(\theta) = \frac{dF}{d\theta} = \exp(-\theta) \quad (162)$$

Example 1.6. F and C -function for two ideally stirred tanks in series

Consider two ideally stirred tanks in series, with inflow and outflow, connected as shown in Figure 1.16. The tanks have identical volumes V . When $t = 0$, and with a

constant volumetric flow rate ϕ_v , the concentration of some tracer at the entrance is suddenly changed stepwise from $c = 0$ to $c = c_0$

In order to be able to determine the F and C -functions of the system of these two tanks, it is necessary to know what the concentration at the exit is - that is, $c_2(t)$

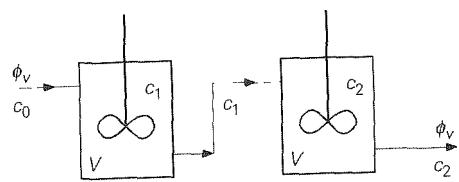


Figure 1.16

Mass balance of tank 1

$$V \frac{dc_1}{dt} = \phi_v (c_0 - c_1) \quad \text{with } c_1(0) = 0 \quad (1.63)$$

Mass balance of tank 2

$$V \frac{dc_2}{dt} = \phi_v (c_1 - c_2) \quad \text{with } c_2(0) = 0 \quad (1.64)$$

The solution to Equation (1.63) is

$$c_1 = c_0 \left[1 - \exp\left(-\frac{\phi_v}{V} t\right) \right] \quad (1.65)$$

Equation (1.64) is not so easy to solve, because c_1 is a function of the time. Substituting the solution for c_1 - Equation (1.65) - into Equation (1.63) results in

$$V \frac{dc_2}{dt} = \phi_v c_0 \left[1 - \exp\left(-\frac{\phi_v}{V} t\right) \right] - \phi_v c_2 \quad \text{with } c_2(0) = 0 \quad (1.66)$$

This is an inhomogeneous linear differential equation. Several methods for solving such an inhomogeneous differential equation are presented in Appendix 1B. The solution to Equation (1.65) is

$$c_2(t) = c_0 \left[1 - \left(1 + \frac{\phi_v}{V} t \right) \exp\left(-\frac{\phi_v}{V} t\right) \right] \quad (1.67)$$

With definitions $\tau = 2V/\phi_v$ (as the overall volume of this system is what matters *viz.* $2V$) and $\theta = t/\tau$, it follows for the F -function that

$$F(\theta) = \frac{c_2(\theta)}{c_0} = 1 - (1 + 2\theta) \exp(-2\theta) \quad (1.68)$$

and for the C -function that

$$C(\theta) = \frac{dF}{d\theta} = 4\theta \exp(-2\theta) \quad (1.69)$$

□

Example 1.7. F -function in the case of a plug flow

The ideal plug flow reactor was discussed in § 1.2.2 (see Figure 1.7). We are concerned here with the F -function of the ideal plug flow, without a chemical reaction taking place. In a plug flow, every liquid package has velocity v . Now, from $t \geq 0$, a marker substance is injected into the inflow (concentration c_0). Each liquid element has exactly the same residence time τ as given by Equation (1.42).

There is therefore no residence time distribution involved - no marker substance comes out before $t < \tau$, while for $t \geq \tau$ the marker substance always comes out with concentration c_0 . For the F -function, therefore, the following applies

$$F(\theta) = 0 \quad \text{for } \theta < 1 \quad (1.70)$$

$$F(\theta) = 1 \quad \text{for } \theta \geq 1$$

□

Summary

In a device through which a flow is passing, the packages do not take the same length of time from the point of entry to the point of exit. In this context, the terms residence time, mean residence time, non-dimensional (residence) time, and residence time distribution have been introduced. Knowledge of this residence time distribution is important in order to be able to properly operate the device. Three functions have been discussed for the purpose of showing the residence time distribution:

the E -function: shows the residence times of the parts of a sample from the outgoing flow *at one point in time*,

the C -function: shows the reaction at the exit to a *pulse* at the entrance,

the F -function: shows the reaction at the exit to a *step* at the entrance.

A relation between the F and C -functions can be derived:

$$C(\theta) = \frac{dF}{d\theta}$$

For a system consisting of one or more ideal devices, expressions can be derived for the F -function of the system. In the real world, C - and F -functions can be measured only.

1.2.4 Multiple tanks in series

The ideal tubular reactor of § 1.2.2 (Figure 1.7) can be mimicked by putting a large number of ideally stirred tank reactors in series (see Figure 1.17) and operating them in a steady state. This will be proven below by using balances

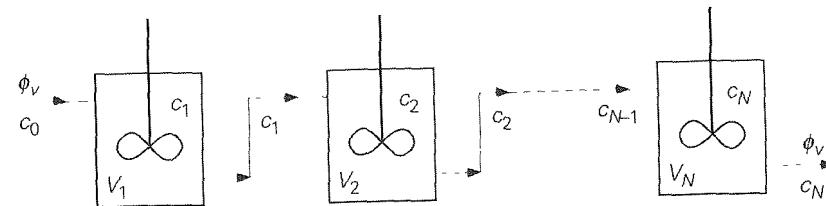


Figure 1.17

After the first tank, the time independent concentration is (see § 1.2.2)

$$\frac{c_1}{c_0} = \left(1 + k_r \frac{V_1}{\phi_V}\right)^{-1} = \left(1 + \frac{k_r V / \phi_V}{N}\right)^{-1} \quad (1.71)$$

$V_1 = V_2 = \dots = V/N$ (N is the number of tanks in series, V the volume of all the tanks combined). Concentration c_1 is the concentration of the inflow into tank 2, so the following applies

$$\frac{c_2}{c_1} = \left(1 + \frac{k_r V / \phi_V}{N}\right)^{-1} \quad (1.72)$$

or with the help of Equation (1.71)

$$\frac{c_2}{c_0} = \left(1 + \frac{k_r V / \phi_V}{N}\right)^{-2} \quad (1.73)$$

Finally, the concentration after the N^{th} tank is found as follows

$$\frac{c_N}{c_0} = \left(1 + \frac{k_r V / \phi_V}{N}\right)^{-N} \quad (1.74)$$

For greater N , the tank reactors in series will increasingly resemble the ideal tubular reactor. Each slice of a plug flow reactor may be conceived as a small ideally mixed reactor. Ultimately, in the limit $N \rightarrow \infty$, both systems are the same.

$$\lim_{N \rightarrow \infty} \left(1 + \frac{k_r \tau}{N}\right)^{-N} = \exp(-k_r \tau) \quad (1.75)$$

In Figure 1.18, the curves of c_N are shown as a function of $k_r \tau$, with $\tau = V/\phi_V$, for a number of values of N . The result of the ideal plug flow reactor is also shown

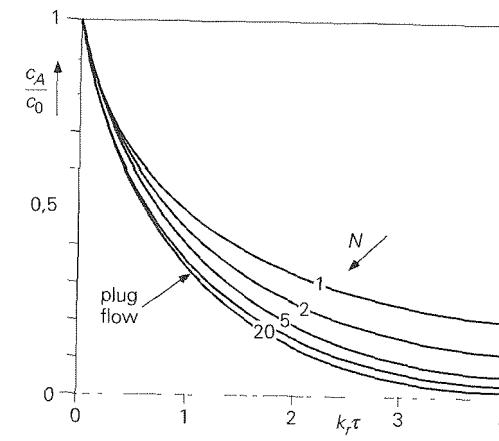


Figure 1.18

Example 1.8. F and C -functions for N ideally stirred tanks in series

In order to determine the F and C -functions of N tanks in series, N transient mass balances must be considered without a source term for chemical reactions. This situation is illustrated in Figure 1.19

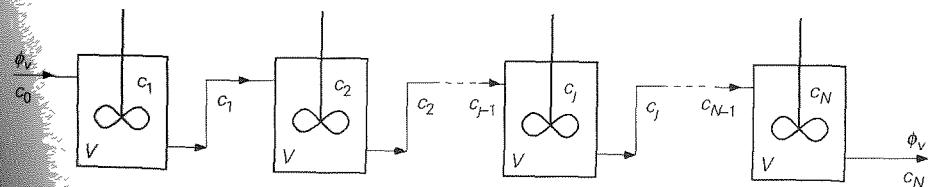


Figure 1.19.

The tanks all have an equal volume, V . When $t = 0$, and with a constant volume flow, the inflow at the entrance is suddenly changed from $c = 0$ to $c = c_0$ (step method). In order to be able to determine the F -function, it is necessary to know what the concentration at the exit is - that is, $c_N(t)$.

Mass balance of tank 1:

$$V \frac{dc_1}{dt} = \phi_V (c_0 - c_1) \quad \text{with } c_1(0) = 0 \quad (1.76)$$

Mass balance of tank j :

$$V \frac{dc_j}{dt} = \phi_V (c_{j-1} - c_j) \quad \text{with } c_j(0) = 0 \quad (177)$$

or

$$\frac{dc_j}{dt} - \frac{N}{\tau} c_{j-1} + \frac{N}{\tau} c_j = 0 \quad \text{in which } \tau = \frac{NV}{\phi_V} \quad (178)$$

The solution to Equation (178) is given by

$$c_j = \exp\left(-\frac{Nt}{\tau}\right) \int_0^t \frac{N}{\tau} c_{j-1} \exp\left(\frac{Nt}{\tau}\right) dt \quad (179)$$

In principle, applying this to a random tank in the series is not difficult, though it is laborious – after all, the concentration of all the tanks before it must first be calculated. By substituting $\zeta = \exp(Nt/\tau)$ and dividing by c_0 , Equation (179) is rewritten as

$$\frac{c_j}{c_0} = \frac{1}{\zeta} \int_1^\zeta \frac{c_{j-1}}{c_0} d\zeta \quad (180)$$

Making the calculation for one tank is easy

$$\frac{c_1}{c_0} = \frac{1}{\zeta} \int_1^\zeta d\zeta = \frac{\zeta - 1}{\zeta} = 1 - \frac{1}{\zeta} \quad (181)$$

It is not difficult for two tanks either

$$\begin{aligned} \frac{c_2}{c_0} &= \frac{1}{\zeta} \int_1^\zeta \frac{c_1}{c_0} d\zeta = \frac{1}{\zeta} \int_1^\zeta \left(1 - \frac{1}{\zeta}\right) d\zeta = \frac{1}{\zeta} (\zeta - 1 - \ln \zeta) \\ &= 1 - \frac{1}{\zeta} (1 + \ln \zeta) \end{aligned} \quad (182)$$

For three tanks, the task is a little more laborious, and produces this

$$\begin{aligned} \frac{c_3}{c_0} &= \frac{1}{\zeta} \int_1^\zeta \frac{c_2}{c_0} d\zeta = \frac{1}{\zeta} \int_1^\zeta \left[1 - \frac{1}{\zeta} (1 + \ln \zeta)\right] d\zeta \\ &= \frac{\zeta - 1}{\zeta} - \frac{1}{\zeta} \ln \zeta - \frac{1}{2\zeta} (\ln \zeta)^2 \\ &= 1 - \frac{1}{\zeta} \left[1 + \ln \zeta + \frac{1}{2} (\ln \zeta)^2\right] \end{aligned} \quad (183)$$

For N tanks, the pattern continues, fortunately, and the following applies

$$\frac{c_N}{c_0} = 1 - \frac{1}{\zeta} \left[1 + \ln \zeta + \frac{1}{2} (\ln \zeta)^2 + \dots + \frac{1}{(N-1)!} (\ln \zeta)^{N-1}\right] \quad (184)$$

The F -function follows by substituting $\theta = t/\tau$ and $\zeta = \exp(N\theta)$ in Equation (184)

$$F(\theta) = 1 - \exp(-N\theta) \left[1 + N\theta + \frac{1}{2}(N\theta)^2 + \dots + \frac{1}{(N-1)!} (N\theta)^{N-1}\right] \quad (185)$$

The C -function follows from $dF(\theta)/d\theta$

In Figure 1.20, $F(\theta)$ has been plotted as a function of θ , from which it appears that $F(\theta)$ becomes steeper and steeper as N increases. In the event that N is infinitely large, there is no longer any distribution in residence time – the F -function becomes equal to that for a tube with plug flow. The volume of every tank has to be infinitely small in that case, otherwise the residence time itself is infinite

□

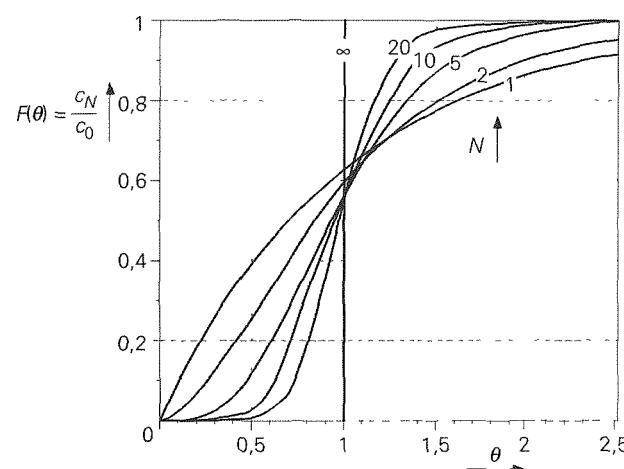


Figure 1.20.

Summary

A plug flow reactor can be approximated by a large number of ideally stirred tank reactors in series. Similarly, the F -function of a series of infinitely small ideally stirred tanks approaches the F -function of a plug flow.

1.3 The energy balance

1.3.1 Introduction

The main topic in § 1.2 was mass. In this Section, the focus will be on energy. Yet, we will exploit here the same technique and the same recipe of drawing up a balance about a control volume. In addition, an energy balance exhibits the same, familiar basic form

$$\frac{d}{dt} = \text{in} - \text{out} + \text{production}$$

Energy manifests itself in many forms, which can often be easily converted into each other, although in such transformation processes some energy is usually lost in the form of useless ‘heat’. To some extent, such an energy transformation is similar to a chemical reaction that converts one particular species into one of more other ones.

We will use capital letters to denote amounts of energy present in a control volume, just like we used M for the total mass (in kg) in a control volume. Here, we will use capitals for the so-called extensive variables: E for the total amount of energy in a control volume, H for the total enthalpy, U for the total amount of thermal energy, S for total entropy, all in J.

On the analogy of working with density ρ and with species concentrations c , all in kg/m³, in the context of mass balances, with a view to energy balances we will use small letters for *energy concentrations* such as e , h and u , all with the unit J/kg. We explicitly choose here for working on a mass basis, to bypass effects of temperature and pressure on the control volume.

The table below gives an overview of the most commonly occurring forms of energy in terms of such energy concentrations.

Form	Energy concentration (expressed per unit of mass)
kinetic energy	$\frac{1}{2}V^2$
potential energy	gz
internal energy	u
pressure energy	p/ρ
enthalpy	$h (= u + p/\rho)$

The *internal energy* (also known as *thermal energy*) stands for

- (i) the thermal movements that individual molecules make given their degrees of freedom for translation, rotation (including internal), and vibration, and

(ii) the short-range molecular interaction between individual molecules. This means the internal energy also depends on the form and composition of the molecules. Internal energy can therefore be regarded as a physical property.

Where there is a constant volume, $du = c_V dT$, and $c_V T$ is often filled in for u (see the intermezzo below). For liquids (because of their low thermal expansion coefficient), a good approximation is $c_V = c_p$, and therefore also $u = c_p T$.

Intermezzo

According to the first law of thermodynamics, the following applies (for a system of constant composition and mass):

$$dU = T dS - p dV$$

The entropy, S , of a system can be regarded as a function of $\{T, V\}$. This means that dS can be written as follows:

$$dS = \left(\frac{\partial S}{\partial T} \right)_V dT + \left(\frac{\partial S}{\partial V} \right)_T dV$$

So for changing the overall internal energy, U , we can also write:

$$dU = T \left(\frac{\partial S}{\partial T} \right)_V dT + \left[T \left(\frac{\partial S}{\partial V} \right)_T - p \right] dV$$

The first term on the right-hand side represents the specific heat at constant volume, defined as:

$$c_V = T \left(\frac{\partial s}{\partial T} \right)_V$$

where we have switched from the extensive variable S (in J) to the specific entropy s (in J/kg). For a system with a constant volume, it is of course only the specific heat that contributes towards to the change in specific internal energy:

$$du = c_V dT$$

Remember that for a system with constant volume this is an exact term, even if the specific heat is in principle a function of the temperature, for example. In integral form, the change in internal energy, again with a constant volume, is shown by:

$$u - u_{\text{ref}} = \int_{T_{\text{ref}}}^T c_V dT \approx c_V (T - T_{\text{ref}}) \quad \text{for constant } V$$

The first equality is again exact, while in the case of the second, a calculation is used whereby the specific heat is constant in the first order if T is not very different from

the reference temperature T_{ref}

For the internal energy concentration, u , we can therefore use the result $u = c_v T$. If a phase transition is involved, caution should be exercised however the latent heat (Δh , again in J/kg) of the phase transition should be taken into consideration in such cases.

The p/ρ term from the above Table allows for a sort of ‘potential’ energy and indicates the capacity of a gas or liquid to flow under the influence of differences in pressure. In terms of energy, pressure energy can be transformed into kinetic energy for example a liquid (or gas) starts flowing under influence of differences in pressure in the liquid (or the gas). This flow runs naturally from areas of high pressure to those of low pressure.

It can also be seen in the first law of thermodynamics that pressure is a kind of energy concentration $dU = TdS - pdV$. The change to the overall internal energy (dU) of the system is caused in part by the work term, pdV . In other words, p can be regarded as an energy concentration per unit of volume, and p/ρ therefore as energy concentration per unit of mass. By using intensive variables (T, p, \dots) and extensive variables (U, S, V, \dots), it is easy to derive in thermodynamics that $U = TS - PV$. So for the internal energy per unit of mass we find $u \equiv \frac{U}{M} = Ts - \frac{p}{\rho}$, which confirms

the above interpretation of p/ρ .

In many cases, the total energy of a system is the sum of the internal, potential, and kinetic energy. In terms of energy concentrations, we can define the following

$$e = u + gz + \frac{1}{2}v^2 \quad (1.86)$$

Remember that the energy concentrations are determined in relation to a suitably selected reference level. In the ‘case of balances, however, it generally concerns changes to energy concentrations, reference levels are often not relevant here. Nonetheless, it is necessary to be prepared for phase transitions and their associated specific energy (enthalpy) changes Δh (in J/kg). In addition, all energy concentrations in Equation (1.86) should preferably be expressed in the unit J/kg, this also applies to the kinetic and potential energy.

In most ‘transport phenomena’, the above definition of e is sufficient. Where chemical reactions play a role, consideration must also be given to the *chemical enthalpy* (often in J/mol) that accounts for the atomic structure of a molecule and the pertinent interactions of nucleus and electrons. When methane is burnt, for example, chemical enthalpy is released in the form of heat. The energy ‘stored’ in a CH₄ mole becomes available, as the products CO₂ and H₂O are ranked lower down the energy

ladder. Although chemical enthalpy changes are often dominant in chemical reactors, this form of energy will be disregarded from now on.

Another important concept has to be introduced *energy dissipation*. Dissipation stands for the fact that the transformation from one form of energy to another always naturally runs in one direction. The useful forms, like kinetic, potential, and (partly, see below) pressure energy, all ultimately end up as internal energy. In more general terms, dissipation is the transformation of (for us as people the mostly useful) ‘mechanical energy’ to ‘thermal energy’ (that is, to chaotic kinetic energy of individual molecules). The mechanism for dissipation is *friction*.

Example 1.9. The bouncing ball

If a tennis ball is released at a particular height above the ground, it loses potential energy on its way down and gains kinetic energy. At the same time, a small amount of the ball’s energy is transferred to the air, which then starts to flow and therefore also gains kinetic energy. In addition, energy is dissipated as a result of friction with the surrounding air. When the ball ‘collides’ with the ground, the kinetic energy is transformed into ‘elastic energy’ and some of it is dissipated.

After the bounce, the elastic energy is again transformed into kinetic energy which in turns changes again into potential energy (and a small part of which again ‘disappears’ into the air) until all the kinetic energy is exhausted and the ball reaches its new ‘highest’ point. The cycle repeats itself several times of course, until the ball eventually rests motionless on the ground and all the kinetic and potential energy has been dissipated.

□

Summary

There are many manifestations of energy which all can be converted into each other. The focus was here on internal, or thermal, energy u and on pressure energy p/ρ . The physical backgrounds of these two ‘types’ of energy have been discussed. The concept of ‘energy dissipation’ has also been highlighted – the one-way traffic through which mechanical energy is converted into useless thermal energy (heat) by friction.

As a preparation to drawing up energy balances, the concept of ‘energy concentrations’ has been introduced and the specific total energy concentration has been defined: $e = u + \frac{1}{2}v^2 + gz$.

We use small letters for energy concentrations (in J/kg), while capital letters denote extensive variables (in J).

1.3.2 The total energy balance

Energy is a *conserved quantity*, like mass. This is an important starting point in physics. For the balance equation it means that the production term equals zero, providing that the total energy really is considered – in other words, including types of energy (chemical, electrical, nuclear, ...) that are not part of Equation (1.86). If we therefore consider the total energy of a system with a given volume, the energy content can only change through the inflow or outflow of energy through the boundaries of this volume.

$$\frac{dE}{dt} = \text{energy flow in} - \text{energy flow out}$$

There is therefore no production term in this equation, because energy cannot be produced from nothing. The above equation is a *conservation law*, entirely comparable with Equation (1.3) for mass.

When drawing up an energy balance for a specific type of energy (or a combination of types) it is important not just to take the transport terms of the selected energy type into account, as in the energy conservation law above, but also to include the transformation (the production) of the type selected into other types (and vice versa) in the balance. The general form of a balance for a specific type of energy has the same structure as the species mass balance, Equation (1.5)

$$\frac{d}{dt} = \text{flow in} - \text{flow out} + \text{production} \quad (1.87)$$

From now on, we will concentrate on the total energy of a system defined as the sum of the internal, the potential, and the kinetic energy $E = U + E_{\text{pot}} + E_{\text{kin}}$, with the related energy concentration $e = u + gz + \frac{1}{2}v^2$. Figure 1.21 gives an illustration of a control volume, with the possible energy flows associated with it.

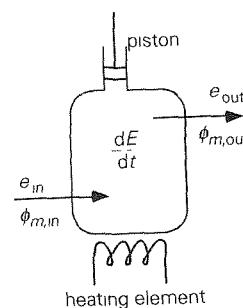


Figure 1.21

The unsteady-state (or transient) term of the left-hand side of the total energy balance which shows how quickly the total energy within the control volume V changes, is:

$$\frac{d}{dt} E$$

With the help of the energy concentration e (per unit of mass), this term can be written as

$$\frac{d}{dt} E = \frac{d}{dt} (\rho V e) \quad (1.88)$$

Several forms of *energy transport* are now possible.

- An energy flow as a result of *mass* flow rate into (or out of) the control volume. This mass itself contains energy. The mass flow carries the energy ‘under its arm’, as it were. Analogous to the transport terms ‘in’ and ‘out’ of species A in Equations (1.9) and (1.10), we also write the transport terms ‘in’ and ‘out’ for energy (in J/s) as the product of a flow rate and a concentration, that is, as a mass flow rate (in kg/s) times energy concentration (J/kg)

$$\phi_{m,\text{in}} e_{\text{in}} \quad \text{and} \quad \phi_{m,\text{out}} e_{\text{out}}$$

- An energy flow as a result of *heat* (via a heating element, for example) flowing into the control volume (or flowing out with the help of a cooling element). This energy flow does not involve a mass flow. We denote this flow as follows

$$\phi_q$$

- An energy flow, which also crosses the boundaries of the control volume, as a result of *work* performed per unit of time by or on the ‘outside world’. Such work may be performed from outside on the control volume by means of a piston, stirrer, pump, or compressor – that is, via piston rods or revolving axles. Work can also be performed by the outside world on the control volume as a result of a mass flow rate flowing inwards across one of the boundaries of the control volume against the prevailing pressure there. Conversely, work can also be performed from the control volume on the outside world, by means of a piston or a turbine (that operates a mill, for example, or generates electric power via a dynamo) or by a mass flow rate that flows across one of the boundaries of the control volume against the outside pressure. The overall (net) ‘flow’ as a result of *work* (on and/or from the control volume) is written as

$$W$$

Finally, *energy production* (per unit of time) P_e in the interior of V is possible. This could involve heat production, for example, as in a chemical reactor as a result of an exothermic chemical reaction or in a metal wire as a result of electric current. Actually, the presence of the production term P_e is the result of our own limitation that E does not cover all types of energy – only internal, potential, and kinetic energy. Without such a limitation, there would be no production term, of course. It is impossible to produce energy from nothing. After all, energy is a conserved quantity. If from now on we really limit ourselves to the types of energy listed in the table at the start of this Section, the production term P_e in the energy balance is equal to zero.

By substituting the above expressions for the various contributions in Equation (1.87) we arrive at the general form for the total energy balance:

$$\frac{d}{dt} E = \frac{d}{dt} (\rho V e) = \phi_{m,in} e_{in} - \phi_{m,out} e_{out} + \phi_q + W \quad (1.89)$$

It is also useful to divide the energy flow resulting from work, W , into two parts.

- one part ϕ_w , which stands for the work as a result of the pistons, stirrers, pumps, compressors, and/or turbines, and
- one part that is related to the mass flow rates that flow into and/or out of the control volume and then perform work against the prevailing pressure

If a ‘package’ of fluid flows into the control volume at velocity v in a time interval dt through a surface A , then during this dt a force pA will be exercised on the package, which will move over a distance $dx = v dt$. In other words, this involves an amount of energy $dE = F dx = pA v dt$. In the balance, we need the energy per unit of time (that is, the power) and that is exactly the same as pAv , or as $\phi_v p = \phi_m p/\rho$.

With respect to W , distinguishing between two types of work leads to three terms in the total energy balance, Equation (1.89).

$$W = \phi_w + \left[\phi_{m,in} \frac{p}{\rho} \Big|_{in} - \phi_{m,out} \frac{p}{\rho} \Big|_{out} \right] \quad (1.90)$$

This means that Equation (1.89) can be rewritten as

$$\frac{d\rho e V}{dt} = \phi_{m,in} \left(e + \frac{p}{\rho} \right)_{in} - \phi_{m,out} \left(e + \frac{p}{\rho} \right)_{out} + \phi_q + \phi_w \quad (1.91)$$

The work (per unit of time), ϕ_w , is therefore now just the work performed by the outside world through mechanical devices such as turbines and pumps.

In many cases, especially if the pressure in the system under consideration can be taken as a constant (using a reasonable approximation) and certainly if *phase transitions* are involved with the accompanying density changes and work performed, it is useful to work in terms of the specific *enthalpy* $h = u + p/\rho$ in the ‘in’ and ‘out’ flows (with all variables in J/kg).

Example 1.10. Transport of water through a tube

A constant flow of water flows through a horizontal cylindrical tube (see Figure 1.22) as a result of an imposed pressure difference. This difference in pressure amounts to 2 bar ($= 2 \times 10^5 \text{ N/m}^2$) and the mass flow rate is 1 kg/s. The tube has a (constant) diameter D of 2 cm and is well insulated. The water has a density ρ of 10^3 kg/m^3 , a specific heat at constant volume c_v of $4.2 \text{ kJ/kg}\cdot\text{K}$ and, as usual under this type of conditions, can be regarded as incompressible.

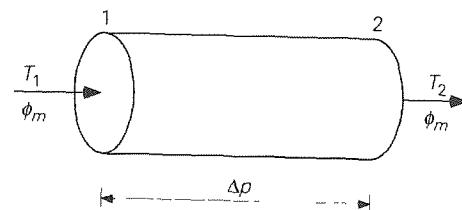


Figure 1.22.

Answer the following questions

- Give the energy balance and calculate the rise in temperature of the water
- What power must a pump have in order to be able to cause this rise in temperature?

Consider a control volume that extends from a point right after the pump, denoted as point 1, until point 2 at the open exit of the pipe (see Figure 1.22). Draw up a mass balance and a (total) energy balance for this control volume. Given that the situation is steady, the following applies:

$$\phi_{m,in} = \phi_{m,out} = \phi_m \quad \text{and} \quad \frac{dE}{dt} = 0$$

Additionally, $\phi_w = 0$ (no pump) and $\phi_q = 0$ (no heat exchange between pump and the outside world). This means that the energy balance for the whole tube is

$$0 = \phi_m \left[u_1 + \frac{p_1}{\rho_1} + \frac{1}{2} v_1^2 + g z_1 - \left(u_2 + \frac{p_2}{\rho_2} + \frac{1}{2} v_2^2 + g z_2 \right) \right] \quad (1.92)$$

Equation (1.92) becomes much simpler when $z_1 = z_2$ (horizontal tube), $\rho_1 = \rho_2$ (water is incompressible) and $v_1 = v_2$ (providing the diameter of the tube and the water density ρ are constant).

The energy balance then becomes

$$u_1 + \frac{p_1}{\rho_1} = u_2 + \frac{p_2}{\rho_2} \quad (1.93)$$

Due to the imposed pressure difference $p_1 - p_2 > 0$, it follows that $u_1 < u_2$. In other words *pressure energy is transformed into internal energy*. As we have seen, with a constant ρ , the following approximation applies, according to thermodynamics

$$u_1 - u_2 = c_v(T_1 - T_2) \quad (1.94)$$

From Equations (1.93) and (1.94) it then follows

$$T_2 - T_1 = \frac{p_1 - p_2}{\rho c_v} \quad (1.95)$$

Substituting the numerical data produces a rise in temperature of 0.048 K which is useless!¹

The rise in the temperature of the water is therefore an example of dissipation of mechanical energy. This energy (per unit of mass) is provided by the pump that raises the pressure of the water at the start of the tube. An energy balance for an ideal pump¹ in the case of incompressible liquid runs therefore as

$$0 = \phi_m \left(\frac{p_0}{\rho} - \frac{p_1}{\rho} \right) + \phi_w \quad (1.96)$$

If the water flows through the pipe only due to the pump action and the suction line is really short, then the pressure p_0 immediately upstream of the pump is equal to the pressure at the end of the tube $p_0 = p_2$. With this information, it follows that

$$\phi_w = \phi_m \frac{p_1 - p_2}{\rho} = 1 - \frac{2 \cdot 10^5}{10^3} = 200 \text{ W} \quad (1.97)$$

This result is of course equal to $\phi_m(u_2 - u_1)$ the power provided by the pump ultimately ends up as internal energy.

Example 1.11. Compression of a gas

With the help of a compressor (an 'air pump'), air is compressed from 1 bar to 5 bar under steady-state conditions. The power consumption of the compressor is

¹ An ideal pump only raises the pressure of a liquid without heat development inside the pump. We assume also $v_1 = v_2$.

$6 \cdot 10^3 \text{ W}$. The mass flow rate through the compressor is 108 kg/h and the diameter of the entrance and exit tubes is 5 cm. Room temperature is 20°C . How hot is the gas that leaves the compressor?

Because of the steady-state situation in the control volume (= the compressor, see Figure 1.23), dM/dt and dE/dt are both 0

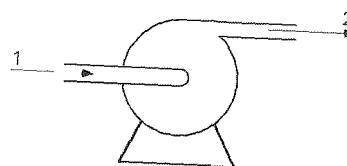


Figure 1.23

From the mass balance it follows that

$$\phi_{m,1} = \phi_{m,2} = \phi_m \quad (1.98)$$

If we assume that the compressor does not give off any heat via the wall directly to the ambient air (that is, $\phi_q = 0$), then the energy balance is

$$0 = \phi_m \left[u_1 + \frac{p_1}{\rho_1} + \frac{1}{2} v_1^2 - \left(u_2 + \frac{p_2}{\rho_2} + \frac{1}{2} v_2^2 \right) \right] + \phi_w \quad (1.99)$$

v_1 and v_2 can be expressed in ϕ_m , the local densities ρ_1 and ρ_2 , and the cross-sectional area A ($= \pi D^2/4$) of the entrance and exit

$$v_1 = \frac{\phi_m}{A} \frac{1}{\rho_1} \quad \text{and} \quad v_2 = \frac{\phi_m}{A} \frac{1}{\rho_2} \quad (1.100)$$

In these circumstances, air can be regarded as an ideal gas

$$p = \rho \frac{RT}{M} \quad (1.101)$$

$$u = \frac{5}{2} \frac{RT}{M} = \frac{5}{2} \frac{p}{\rho}$$

This latter equality has its origins in statistical physics. With temperatures that are not extremely high, that is, where the vibrations inside the molecules do not yet play a major role, any diatomic molecule, such as the oxygen and nitrogen molecules in air, has five degrees of freedom – three for translation and two for rotation. According to the equipartition theorem, every degree of freedom has an energy of $\frac{1}{2} RT$ per mole, or $\frac{1}{2} RT/M$ per kg.

After some substitutions, the energy balance is now

$$0 = \phi_m \left[\frac{7}{2} \left(\frac{p_2 - p_1}{\rho_2 - \rho_1} \right) + \frac{1}{2} \left(\frac{\phi_m}{A} \right)^2 \left(\frac{1}{\rho_2^2} - \frac{1}{\rho_1^2} \right) \right] - \phi_w \quad (1.102)$$

Substituting the numerical data then produces $\rho_1 = 119 \text{ kg/m}^3$, $\rho_2 = 354 \text{ kg/m}^3$, $T_2 = 492 \text{ K}$ and $\Delta T = 199 \text{ K}$. In practice, the outgoing gas flow is therefore often cooled - which again implies energy dissipation! \square

Example 1.12. The kettle

In this example, the balance technique will be used to develop an elementary description of the heating up and boiling of water in a kettle. Look at the kettle in Figure 1.24 and assume that the heating up process occurs through a constant heat supply ϕ_{q_1} . For the sake of simplicity, it is also assumed that the heat loss to the surroundings (ϕ_{q_2}) is constant. We will disregard the heating up of the kettle itself, for the purpose of convenience.

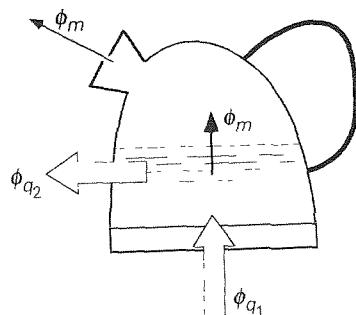


Figure 1.24

First look at the situation in which the water is being heated up (not boiling yet). In these circumstances, evaporation can be ignored, this involves only a minor error, depending on the water temperature. We will take the contents of the kettle as the control volume and look only at the liquid, ignoring the vapour. (Incidentally, the mass of all the water in the kettle including the vapour in the space above the liquid, and the mass of the liquid are more or less equal.) This means that the mass balance for the water (shown by subscript l for 'liquid').

$$\frac{d}{dt} M_l = 0 \quad (1.103)$$

As for an incompressible liquid $c_v = c_p$, and providing that c_p is independent of temperature, the energy balance for the liquid in rest in the kettle is

$$\frac{dE}{dt} = \frac{dU}{dt} = \frac{d}{dt} (M_l c_p T) = M_l c_p \frac{dT}{dt} = \phi_{q_1} - \phi_{q_2} \quad (1.104)$$

In other words, the temperature will rise at a constant rate

$$\frac{dT}{dt} = \frac{\phi_{q_1} - \phi_{q_2}}{M_l c_p} \quad (1.105)$$

With $T = T_0$ at $t = 0$, the above differential equation results in an expression for the liquid temperature as a function of time

$$T = T_0 + \frac{\phi_{q_1} - \phi_{q_2}}{M_l c_p} t \quad (1.106)$$

Then consider the situation in which the water is boiling. There is now a substantial mass flow rate (mostly vapour) coming out of the kettle that we really cannot ignore (you can hear the whistle!). This implies that we should no longer ignore the quantity (the mass) of vapour in the space above the liquid either. The mass balance for the control volume, that is, the contents of the kettle, now becomes (with subscript v for 'vapour', the vapour phase)

$$\frac{dM_l}{dt} + \frac{dM_v}{dt} = 0 - \phi_m = -\phi_m \quad (1.107)$$

Even if M_v were to be ignored, the result of Equation (1.107) is still of some value, because it is not unreasonable to assume that in the short term, the quantity of water vapour in the kettle remains constant during the boiling process at each moment, there is as much vapour leaving the kettle as there is liquid water changing into vapour.

This transition from liquid to vapour is accompanied by a change in volume. The vapour that is formed must therefore exercise work on the surroundings (the outside air), while the pressure in the kettle remains constant. These considerations play a role when we come to analyse the energy management of boiling. Again, we use what we know of thermodynamics. For a closed system (a system without mass flow rates in and/or out), thermodynamics tells us

$$\delta Q = dU + p dV \quad (1.108)$$

Instead of working with internal energy, U , we can also use enthalpy, H

$$H \equiv U + pV \quad (1.109)$$

This means that the conservation of energy can be written as

$$\delta Q = dH - Vdp \quad (1.110)$$

We therefore see that, for processes at constant volume ($dV = 0$) and constant pressure ($dp = 0$), as is the case in our kettle, enthalpy is a very useful quantity

because $dU/dt = dH/dt$. This is even more so given that on the right-hand side of Equation (1.91), enthalpy also occurs in the in and out terms (as a result of mass flow rates in and out). For the boiling process in the kettle (an open system, due to the outgoing flow of vapour), we arrive, based on Equation (1.91) and with $\phi_w = 0$, at the following enthalpy balance for the overall content of the kettle (liquid plus vapour phase)

$$\frac{dH}{dt} = \phi_{m,\text{in}} h_{\text{in}} - \phi_{m,\text{out}} h_{\text{out}} + \phi_q \quad (1.111)$$

In Equation (1.111), again all the effects of kinetic and potential energy are disregarded – both in the d/dt term on the left-hand side and in the ingoing and outgoing mass flow rates on the right-hand side of the equation – as they are very small in relation to the various enthalpy terms. For the overall enthalpy in the control volume, we can write

$$H = h_l M_l + h_v M_v \quad (1.112)$$

Finally, the ingoing mass flow rate is zero and the outgoing enthalpy is h_v . Because both pressure and temperature are constant during boiling, the enthalpy concentrations, h_l and h_v , are also constant. Equation (1.111) can therefore be written as follows

$$h_l \frac{dM_l}{dt} + h_v \frac{dM_v}{dt} = -\phi_m h_v + \phi_{q_1} - \phi_{q_2} \quad (1.113)$$

Combining Equations (1.107) and (1.113), and using the notation $\Delta h_v = h_v - h_l$ for the enthalpy of evaporation (in kJ/kg) results in

$$-\frac{dM_l}{dt} \Delta h_v = \phi_{q_1} - \phi_{q_2} \quad (1.114)$$

Starting from the original mass M_{l0} of liquid in the kettle, the expression for the mass of liquid in the kettle as a function of time then becomes

$$M_l = M_{l0} - \frac{\phi_{q_1} - \phi_{q_2}}{\Delta h_v} t \quad (1.115)$$

In other words, supplying heat to a kettle of boiling water only causes – not surprisingly – a reduction of the water mass through the phase transition when the atmospheric boiling point is constant and the atmospheric pressure is constant (if we ignore the very small, but constant pressure drop over the exit opening); this results (primarily because we are ignoring kinetic and potential energy contributions) in the removal of vapour via the discharge flow rate ϕ_m .

Bear in mind that throughout the analysis we have not taken the heat capacity of the kettle itself into account

□

Example 1.13. The refrigerator

The air in the food storage area of a refrigerator is cooled with the help of a coolant (or refrigerant, usually a freon) that is circulated in a closed circuit. This cooling can only take place when the refrigerant in the heat exchanger is at a lower temperature than the air in the food storage area. The coolant picks up heat from the food storage area and passes it to the air outside the refrigerator, and realises this with the help of phase transitions (evaporation, condensation) really a complex transport process

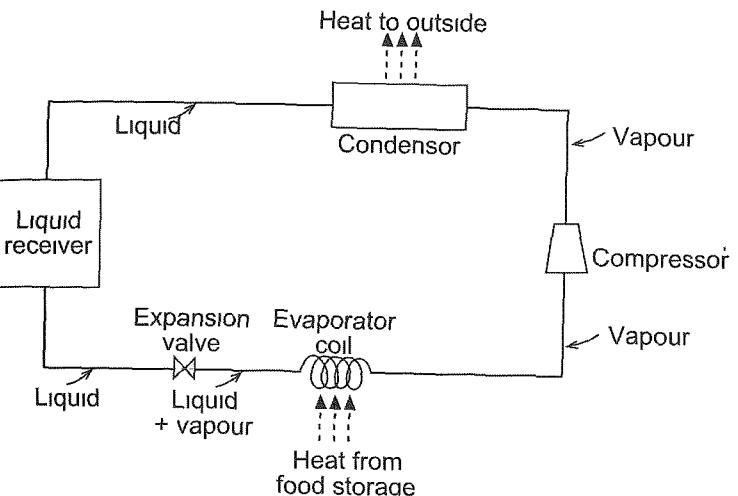


Figure 1.25

The closed cooling circuit (see Figure 1.25) comprises five essential components. The first component is a pressure vessel (also denoted as the liquid receiver) in which the refrigerant is a liquid due to a high pressure and temperature (say, 7 bar and 30°C). The liquid then expands through an expansion valve downstream of the valve, the pressure is lower (e.g., 1.8 bar) and, as a result, the liquid momentarily flashes (evaporates) partly by cooling to the boiling-point temperature (-15°C) at this lower pressure. The resulting vapour-liquid mixture then passes through the heat exchanger (also denoted as evaporator coil) that is in the food storage area to be cooled. By withdrawing heat from the air in the food storage area, the remaining liquid coolant may also evaporate, still at the low pressure and pertinent boiling-point temperature. The cold refrigerant emerging from the coil is then brought back to the original high pressure by a compressor, in this compression step, temperature also rises of course, e.g. to 45°C. The hot

vapour then passes through a heat exchanger, the so-called condenser (outside and at the rear side of the refrigerator), where it gives up heat to the ambient air such that the vapour condenses before it is returned to the liquid receiver.

Let's now focus on the expansion valve and draw up an energy balance for this valve during a steady-state operation. This valve is a passive component (no work ϕ_w performed) and we will ignore heat exchange with the ambient world ($\phi_q = 0$). That means Equation (1.91) reduces to

$$0 = \phi_{m,in} \left(e + \frac{p}{\rho} \right)_{in} - \phi_{m,out} \left(e + \frac{p}{\rho} \right)_{out} \quad (1.116)$$

For the valve, obviously $\phi_{m,in} = \phi_{m,out}$. As a phase change is involved, with a substantial change in density and with expansion work, a description in terms of enthalpy is needed. Then Equation (1.116) leads to

$$0 = \left(h + \frac{1}{2}v^2 + gz \right)_{in} - \left(h + \frac{1}{2}v^2 + gz \right)_{out} \quad (1.117)$$

As a result of the flashing, the vapour-liquid mixture leaving the valve with a much lower (mixture) density should have a much higher velocity than the liquid refrigerant entering the valve (to satisfy the above mass balance). The resulting change in kinetic energy, however, is still small in comparison with the enthalpy of the entering liquid refrigerant. Ignoring therefore – just like in the preceding example – the changes in kinetic and potential energy turns Equation (1.117) into the simple relation

$$h_{l,in} = [xh_v + (1-x)h_l]_{out} \quad (1.118)$$

in which x denotes the fraction of the refrigeration that has flashed (evaporated) – subscripts v and l denote vapour and liquid, respectively. By finding enthalpy data of the refrigerant of interest at the prevailing temperatures and pressures from thermodynamic property tables, one can calculate this fraction x , in the above case, x amounts to some 27%.

Summary

In principle, a total energy balance for a control volume has the same basic form as a species mass balance, and comprises transport and production terms. In drawing up a total energy balance, all three types of energy (internal or thermal, kinetic, and potential energy) should be taken into account:

$$e = u + \frac{1}{2}v^2 + gz$$

As a matter of fact, there is the convective transport of energy by mass flows into and out of the control volume. Also *enthalpy* $h = u + p/\rho$ plays a role in energy balances, with the flows entering and leaving the control volume as well as when a phase transition is involved. Further, work may be done by or upon the outside world that also may exchange heat with the control volume – all such effects have to be accommodated in an energy balance.

Through an energy balance, conversions of one type of energy in one or more other types can easily be demonstrated and accommodated. The general form of a total energy balance runs as:

$$\frac{d\rho Ve}{dt} = \phi_{m,in} \left(e + \frac{p}{\rho} \right)_{in} - \phi_{m,out} \left(e + \frac{p}{\rho} \right)_{out} + \phi_q + \phi_w$$

The concept of dissipation of mechanical energy into heat due to friction was illustrated with the help of some examples.

1.3.3 The thermal energy balance

So far, we have dealt with the total energy, but it is sometimes more helpful to look solely at a specific type of energy, such as thermal or internal energy U . The balance for U is

$$\frac{d}{dt} U = \frac{d}{dt} (\rho Vu) = \phi_{m,in} u_{in} - \phi_{m,out} u_{out} + \phi_q + P_u \quad (1.119)$$

As usual, the left-hand side of the equation represents the change over time in the internal energy U in the control volume. The first two terms of the right-hand side are the difference between inflow and outflow of internal energy by mass flow rates. The third term calculates the net heat flow that goes into or out of the volume. Finally, the last term P_u stands for production of internal (thermal) energy in the control volume as a result of *dissipation* (effects of friction) and for production of internal energy by *work* that is performed on the system.

Remember that it is not pistons, pumps, compressors and turbines that add and/or extract energy from the control volume, but ‘mechanical’ energy, a term resulting from the actions of pistons, pumps, compressors, and turbines is therefore not part of a thermal energy balance. But take note: thermal energy is certainly *not* a conserved quantity. The balance of Equation (1.119) is therefore not a *conservation law* either. The question now is to find an expression for production term P_u .

Consider again the overall energy balance, Equation (1.91) or, for a steady-state situation, Equation (1.92), in which the terms $\phi_m [u + p/\rho]_{in}$ and $\phi_m [u + p/\rho]_{out}$

occur, among others. These terms stand for the enthalpy decrease from entrance to exit. For this enthalpy decrease, the following applies

$$dh = du + p \cdot d\left(\frac{1}{\rho}\right) + \frac{1}{\rho} \cdot dp \quad (1.120)$$

The first two terms on the right-hand side are related to heat and should feature explicitly in a thermal energy balance after all, according to the first law of thermodynamics, the following applies, formulated on a mass basis

$$\delta Q = du + p \cdot d\left(\frac{1}{\rho}\right) \quad (1.121)$$

in which δQ stands for the change to the heat content (per kg). It is clear from this law that work performed on the system where pressure is constant and under adiabatic conditions, affects the internal energy of the system. Remember that Equation (1.121) relates to a *reversible process*: the kinetic energy of the molecules can be used to bring them closer together, and vice versa.

Owing to Equation (1.121), the term $\phi_m p d(1/\rho)$ should feature explicitly in a thermal energy balance such as Equation (1.119), in addition to the term $\phi_m du$. The term is the result of the difference in density between ingoing and outgoing mass flow rates. In a similar way to how energy production W due to work was divided into two terms in advance of Equation (1.90), in Equation (1.119) we now remove the *reversible* work term $\phi_m p d(1/\rho)$ from production term P_u and write it with the inflows and outflows. What remains of P_u is an *irreversible* energy transformation, the *dissipation* of mechanical energy in heat as a result of friction within the control volume. This friction, the production of thermal energy (heat), is the result of the resistance that is offered within the control volume to the flow *from entrance to exit*, and is therefore in proportion with the mass flow rate. For this dissipation term, we therefore write $\phi_m e_{fr}$, in which

e_{fr} = the quantity of mechanical energy that is irreversibly transformed into thermal energy (heat) per unit of mass

For a steady-state situation, in which the ingoing and outgoing mass flow rate are of course equal ($\phi_{m,in} = \phi_{m,out} = \phi_m$), Equation (1.119) can then be rewritten in the following form

$$0 = \phi_m \left[u_{in} - u_{out} - \int_{in}^{out} p \cdot d\left(\frac{1}{\rho}\right) \right] + \phi_q + \phi_m e_{fr} \quad (1.122)$$

which is known as the steady-state *thermal energy balance* or steady-state *heat balance*.

The above derivation of the steady-state thermal balance, together with the discussion about enthalpy changes, illustrates how carefully the production term in a balance should be treated when, as in the case of thermal energy, the quantity concerned *does not remain conserved*.

Summary

A thermal energy balance can be drawn up, analogous to the overall energy balance. With the help of the first law of thermodynamics, the production of internal energy can be divided into a reversible work part and an irreversible part, the dissipation. As a result, the steady-state internal energy balance runs as

$$0 = \phi_m \left[u_{in} - u_{out} - \int_{in}^{out} p \cdot d\left(\frac{1}{\rho}\right) \right] + \phi_q + \phi_m e_{fr}$$

It ties in nicely with the overall energy balance, with the dissipation, as a producer of thermal energy, featuring prominently.

1.3.4 The mechanical energy balance and the Bernoulli equation

Now that the overall energy balance and the steady-state thermal energy balance have been formulated, constructing the steady-state *mechanical energy balance* is simple, given that

$$E_{overall} - E_{thermal} = E_{mechanical} \quad (1.123)$$

Following on from this, subtracting Equation (1.122) from the steady-state version of Equation (1.91) leads to the steady-state mechanical energy balance

$$0 = \phi_m \cdot \left[\frac{1}{2} v_{in}^2 - \frac{1}{2} v_{out}^2 + g(z_{in} - z_{out}) + \int_{out}^{in} \left(\frac{1}{\rho} \right) dp \right] + \phi_w - \phi_m e_{fr} \quad (1.124)$$

This equation is usually written slightly differently, with indices 1 and 2 instead of 'in' and 'out' respectively:

$$0 = \phi_m \left[\frac{1}{2} (v_1^2 - v_2^2) + g(z_1 - z_2) + \int_2^1 \left(\frac{1}{\rho} \right) dp \right] + \phi_w - \phi_m e_{fr} \quad (1.125)$$

Notice that the production term has a minus sign here. This corresponds to the fact that dissipation destroys mechanical energy (both ϕ_m and e_{fr} are always positive, of course).

It should be noted here that the mechanical energy balance can be derived much more efficiently from the momentum balances (see further on in this textbook), by scalar multiplication with the velocity vector \vec{v} . The thermal energy balance is then arrived at by subtracting the mechanical energy balance from the overall energy balance.

It has been decided for this textbook to use the other method on the one hand to avoid the route via momentum balances and the associated mathematical manipulations, and on the other to familiarise the student with the idea that a balance equation can be drawn up for every quantity (conserved or not). Careful thought should be given to the physics of the production term, sometimes, it is useful or even necessary to model this production term (This is the case, for example, when describing and simulating turbulent flows.) For *conserved quantities* (such as mass and total energy) the production term is of course zero.

The Bernoulli equation

There now follows a number of examples of the use of the mechanical energy balance in the exceptional events that no work is performed on or by the system ($\phi_w = 0$) and that the dissipation is negligible ($e_{fr} \approx 0$). In such cases, and providing that ρ is constant, the steady-state mechanical energy balance, Equation (1.125), simplifies to what is known as the *Bernoulli equation*

$$\frac{1}{2}v_1^2 + gz_1 + \frac{p_1}{\rho} = \frac{1}{2}v_2^2 + gz_2 + \frac{p_2}{\rho} \quad (1.126)$$

or

$$\frac{1}{2}v^2 + gz + \frac{p}{\rho} = \text{constant} \quad (1.127)$$

In fact, this equation applies just along a flow line, the constant in Equation (1.127) will have different values for different flow lines. As a matter of fact, fluid parcels while following flow lines cannot change their mechanical energy under the pertinent conditions². The only possible transformation is from one form of mechanical energy to the other – in line with the conditions for which Equation (1.127) is valid. The terms in Equation (1.127) all have the dimension of energy per unit of mass.

Depending on the system of interest, Equation (1.127) is sometimes rewritten in terms of (pressure) heads, where all the terms have the dimension of length

² For a more detailed discussion, you are referred to e.g., Bird, R B, W E Stewart & E N Lightfoot, Transport Phenomena, Wiley, 2nd Ed., 2002

$$\frac{p}{\rho g} + z + \frac{v^2}{2g} = \text{constant} \quad (1.128)$$

Working in terms of heads is illustrated in Figure 1.26. Applying the Bernoulli equation successively to the points a, b, and c (all three on a single horizontal line) teaches us that

$$\frac{p}{\rho g} = \frac{p'}{\rho g} + \frac{v^2}{2g} = \frac{p}{\rho g} \quad (1.129)$$

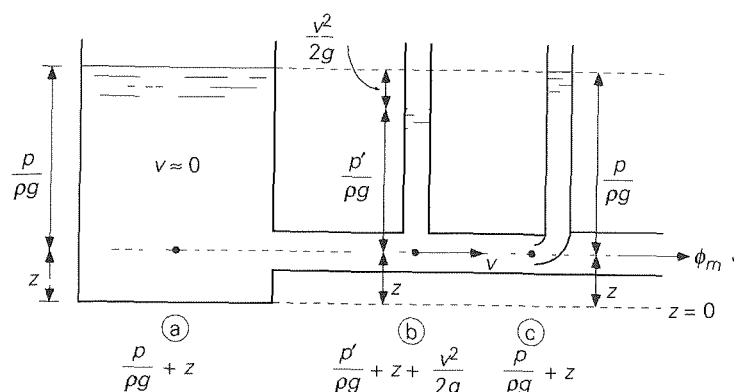


Figure 1.26

This is shown in the diagram the pressure p' at point b is lower than the pressure p at point a or point c. Indeed, at point b, the liquid has velocity, i.e. kinetic energy, and therefore pressure p' is less than pressure p at point a. At point c – exactly in the bent opening of the standpipe – the liquid is motionless again and therefore pressure is equal to that at point a again. Point c will therefore be able to ‘bear’ a greater column of liquid than will point b, put another way, the kinetic energy present in point b is transformed in point c entirely into pressure energy. Point c is a so-called *stagnation point*.

The two heads in the middle part of Equation (1.129) have their own name: *(static) pressure head* and *velocity head*, respectively. The ‘missing’ pressure at point b (see Figure 1.26) measuring $\frac{1}{2}\rho v^2$ – in line with the middle part of Equation (1.129) – is known as the *dynamic pressure*, while p is named *static pressure* and $\rho g z$ is denoted by the term *hydrostatic pressure*.

Pressure in the curved opening of the standpipe at point c is known as *stagnation pressure* and is the sum of the local static pressure and the local dynamic pressure. This terminology returns in the treatment of the flow around immersed objects and the pertinent forces, in § 2.3.1.

The Pitot tube

The aforementioned configuration can, in principle, be used to measure the velocity of the liquid. The most important precondition is that dissipation is indeed negligible. The *Pitot tube* (see Figure 1.27) shows how the principle of the configuration in Figure 1.26 takes shape in a compact device.

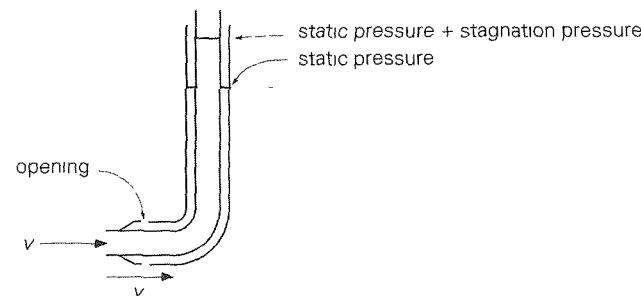


Figure 1.27

The device consists of two bent concentric tubes, the innermost of which measures the local stagnation pressure, being the sum of static pressure and dynamic pressure, and the outermost tube only the local static pressure. A 'long way' before the tube, the pressure is p , after all, and the velocity v , so the following applies (at a single height, along a flow line)

$$p + \frac{1}{2}\rho v^2 = \text{constant} \quad (1.130)$$

For the innermost tube, the flow is moving towards its opening. In order to prevent it (in a steady-state situation) from flowing in, a force in the opposite direction needs to be applied to the fluid. This is done by a higher pressure at the entrance – the local stagnation pressure. For the outermost tube, the fluid is flowing past the small opening at the side and does not try to flow into the outer tube. Hence, no force is needed to prevent fluid from entering. Consequently, no pressure difference is needed [On the contrary any pressure difference across the small hole would result in a flow in or out of the outer tube]. Thus, the difference between the two measured pressures is the dynamic pressure, $\frac{1}{2}\rho v^2$, which means it is a direct measure for the velocity of the liquid.

The Venturi tube

Another measuring instrument where, due to the nature of its construction, energy dissipation is negligible ($e_{fr} \approx 0$), is the Venturi tube. In the flow channel (see Figure 1.28), a gradual narrowing (apex angle $< 25^\circ$) is followed by an even more gradual widening (apex angle $< 8^\circ$) in order to comply with $e_{fr} \approx 0$. As long as the two criteria for the apex angle are met, then it can be relied on with certainty that the flow lines (along which the Bernoulli equation applies) will follow the shape of the

geometry and that no eddies or energy dissipation will occur. The Venturi tube should be set up horizontally in order to prevent any differences in potential energy between measuring stations 1 and 2.

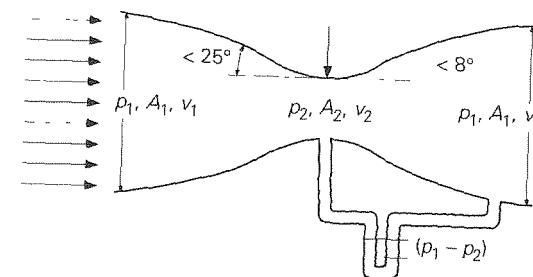


Figure 1.28

The mass flow rate ϕ_m , which runs through the flow channel in a steady-state situation, can now be derived from a mass balance, the Bernoulli equation, and the difference in pressure between point 1 a long way before (or a long way after) the throat (the narrowest passage) and point 2 in the throat. Denote the cross-sectional areas at points 1 and 2 by A_1 and A_2 respectively. From this, the mass balance for this steady-state condition can be obtained.

$$\phi_m = \rho v_1 A_1 = \rho v_2 A_2 \quad (1.131)$$

and from the Bernoulli equation (providing the liquid can be regarded as incompressible, that is, $\rho \approx \text{constant}$):

$$\frac{1}{2}v_1^2 + \frac{p_1}{\rho} = \frac{1}{2}v_2^2 + \frac{p_2}{\rho} \quad (1.132)$$

Combining the Equations (1.131) and (1.132) gives the expression for the mass flow rate:

$$\phi_m = \frac{A_2}{\sqrt{1 - \left(\frac{A_2^2}{A_1^2}\right)}} \sqrt{2\rho(p_1 - p_2)} \quad (1.133)$$

Notice that with this device, the possibility for transforming forms of mechanical energy has been exercised – pressure energy becomes kinetic energy, which again becomes pressure energy.

Example 1.14. Flue gases through a chimney

The flue gases from a furnace are fed to the base of a high chimney that is built on the ground. The diameter of the chimney is constant. The flue gases are at a constant temperature of 227°C , and the outside air is 20°C . Pressure p_1 at the

bottom of the chimney is Δp_m below the atmospheric pressure p_a of 1 bar (measured at ground level). The heat losses from the flue gas in the chimney are negligible. In addition, there is no dissipation of any note.

On the basis of this information, and for $\Delta p_m = 250$ Pa, how high is the chimney?

Before this question can be answered, an investigation should first be carried out to find out why the flue gas actually flows out of the chimney. After all, it surely comes into the chimney at a pressure lower than the ambient pressure of 1 bar? At the top of the chimney, however, the air pressure has also fallen below 1 bar. As a matter of fact, pressure in the ambient air drops if the column of air being 'carried' gets smaller. The ambient pressure at height H of the chimney exit is therefore not p_0 , but $p_0 - \rho_a gH$ (with ρ_a being the density of air at 20 °C = 1.2 kg/m³) and should be lower than the pressure $p_0 - \Delta p_m$ at the base of the chimney.

From Equation (1.125), with $\phi_w = 0$ and given the constant diameter of the chimney, it follows for the chimney that

$$0 = \int_0^H \frac{1}{\rho_g} dp + gH \quad (1.134)$$

The pressure drop from bottom to top is very small – check this afterwards with Equation (1.136) – and it is given that heat losses to the ambient air are minor. As a result, pressure and temperature of the flue gases hardly change if at all, and so the density ρ_g of the flue gases can also be regarded as constant (0.65 kg/m³ at 227 °C). This means Equation (1.134) simplifies to a Bernoulli equation

$$0 = \frac{1}{\rho_g} [(p_0 - \rho_a gH) - (p_0 - \Delta p_m)] + gH \quad (1.135)$$

$$\rightarrow H = \frac{\Delta p_m}{(\rho_a - \rho_g)g} \quad (1.136)$$

Substituting the data produces $H = 46.3$ m

A few trivial rules for designing a chimney follow from Equation (1.136): a greater Δp_m requires a higher chimney (when ρ_a and ρ_g are equal), hotter flue gases (lower ρ_g) mean a lower chimney will suffice (due to a better 'draught'). □

Summary

In this Section, the steady-state mechanical energy balance has been constructed by taking the difference from the steady-state overall energy balance and the steady-state thermal energy balance:

$$0 = \phi_m \left[\frac{1}{2}(v_1^2 - v_2^2) + g(z_1 - z_2) + \int \left(\frac{1}{\rho} \right) dp \right] + \phi_w - \phi_m e_{fr}$$

The production term in it is always negative: dissipation destroys mechanical energy. A number of cases were then examined in which no work was performed and the energy dissipation was negligible, while also $\rho = \text{constant}$. The steady-state mechanical energy balance then changes into the Bernoulli equation:

$$\frac{1}{2}v^2 + gz + \frac{p}{\rho} = \text{constant}$$

The latter shows conservation of mechanical energy: it is possible for pressure energy, kinetic energy, and gravitational energy to be transformed into each of the other types, but the sum of the three remains constant.

Finally, the Pitot tube and Venturi tube were dealt with, as were the terms pressure head, static head, velocity head, static pressure, hydrostatic pressure, dynamic pressure, and stagnation pressure.

1.4 The momentum balance

After the mass and energy balances we are left with the momentum balance. The quantity for which a balance now has to be drawn up is momentum P which usually is conceived as the product of the moving mass m (in kg) times velocity v (in m/s). The unit in which P is expressed is then Ns, analogous to Nm (or J) for energy E . As the notation shows, momentum involves an extra complication in relation to mass and energy. Like a force, momentum is a *vector* quantity, which means that three components have to be specified in order to establish the momentum. This is unlike mass or energy which are established with just one value (mass and energy are referred to as a scalar).

For momentum, therefore, three balances are needed. As a matter of fact, when using orthogonal axis systems like the much-used Cartesian coordinate system (x, y, z), the three momentum components (p_x, p_y, p_z – denoting momentum concentrations per unit of mass, in Ns/kg, or per unit of volume, in Ns/m³) only occur separately in these balances (note that p – with subscript! – does not refer to pressure here). In other words, the balance for momentum in the x -direction, p_x , contains no terms that include p_y or p_z .

First, we introduce the momentum balance in any direction x . The general form of the x -momentum balance is (for control volume V in Figure 1.29)

$$\frac{dP_x}{dt} = \text{flow of } x\text{-momentum in} - \text{flow of } x\text{-momentum out} + \text{production of } x\text{-momentum} \quad (1.137)$$

All terms of this equation have the unit Ns/s. The left-hand term represents the change over time of the overall amount of x -momentum in the control volume. The overall amount of x -momentum³ in the control volume can be written as $P_x = M v_x$, in Ns.

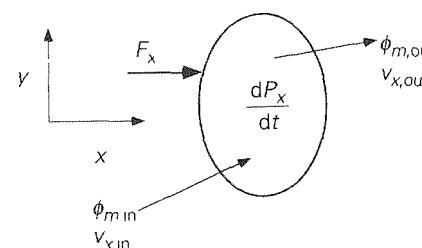


Figure 1.29

In this case, the flows in and out are the result of a mass flow rate that carries x -momentum with it. They therefore have the form of ϕ_m { x -momentum per unit of mass}. From classical mechanics, it follows that the x -momentum of a mass m is equal to mv_x . From this, it follows that the x -momentum concentration (per unit of mass) is equal to $(mv_x)/m = v_x$. The velocity in the direction of x can therefore be taken as the concentration (per unit of mass) of x -momentum, in Ns/kg. (From now on, the symbol p will no longer be used for momentum, only for pressure.) This means that, again entirely analogous to Equations (1.9) and (1.10) and to energy flows in and out in Equation (1.84), the flows of x -momentum in and out become

$$\phi_{m,\text{in}} v_{x,\text{in}} \quad \text{respectively} \quad \phi_{m,\text{out}} v_{x,\text{out}}$$

By analogy, the concentration of x -momentum per unit of volume is given by ρv_x , in Ns/m³.

All that remains now is the production of x -momentum. Here, too, classical mechanics can be invoked. In fact, Newton's second law

$$\frac{d}{dt}(mv_x) = \sum F_x \quad (1.138)$$

is already a simple form of the x -momentum balance that we are looking for. The left-hand side is the change to the x -momentum of the body. This change is the result

³ Velocity v_x is actually a mean velocity defined as

$$\langle v_x \rangle = \frac{\int \rho v_x dV}{\int \rho dV}$$

of the x -components of the forces that are working on the body. Therefore, the right-hand side of Equation (1.138), the sum of the forces in the x -direction, represents the momentum-production term. A force can therefore be regarded as a *producer of momentum* (Ns) per unit of time (s).

Classical mechanics further tells us that there are two types of force

- *body forces*, which work on the mass in the control volume, the best-known exponent of this is gravity,
- forces that affect the surface of the control volume, these include pressure forces and frictional force (or the shear stress – see next Chapter)

The momentum balances diverges from the mass and energy balance on this point. In the case of the latter two balances, production always takes place internally, while with the momentum balance it is possible for the production of momentum to occur on the surfaces. (It will be demonstrated below that this difference can be partly eliminated by introducing certain momentum flows that replace the frictional forces on the surface of the control volume.)

After all the above considerations, the general form of the x -momentum balance is now:

$$\frac{d}{dt}(Mv_x) = \phi_{m,\text{in}} v_{x,\text{in}} - \phi_{m,\text{out}} v_{x,\text{out}} + \sum F_x \quad (1.139)$$

It is useful to remember that the mass flow rates do not necessarily have to be in the direction of x (see Figure 1.29). If the situation is steady and the transport terms in Equation (1.139) compensate each other (or are equal to zero), the x -momentum balance reduces to a *force balance*

$$0 = \sum F_x \quad (1.140)$$

Similar balances for the y -momentum and z -momentum can of course be written down as well.

Example 1.15. The conveyor belt

Sand from a hopper lands on a horizontal conveyor belt moving at a velocity of $v_b = 1.0 \text{ m/s}$. The sand falls vertically at a mass flow rate of 225 kg/s . At first, the conveyor belt is empty and is gradually filled with sand (but does not fill up yet). Calculate the force needed to move the belt, assuming that it moves over its bearings without any friction.

The first question to be answered is this: why must a force be exercised on the belt if it is moving without any friction? The answer is that the sand that is falling continuously on the band has to be brought at the right horizontal velocity, i.e.

must receive momentum in the horizontal direction (the x -direction), for which a force in the horizontal direction is required! In order to calculate this force, a momentum balance has to be drawn up for a volume that covers all the sand that is lying on the belt (see Figure 1.30). Be sure to make the control volume so long at the right-hand side that no sand can leave the control volume in the time interval dt

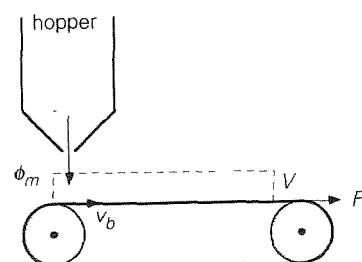


Figure 1.30

The balance for x -momentum runs as

$$\frac{d}{dt}(M_z v_b) = \phi_{p_{v,in}} - \phi_{p_{x,out}} + \sum F_x \quad (1.141)$$

M_z is the mass of sand that is lying on the belt. The balance becomes simple because there is no x -momentum flowing in or out of the control volume. The sum of the forces is F , the force that moves the belt. The unsteady-state term can be simplified with the help of a mass balance for the same volume

$$\frac{d}{dt} M_z = \phi_{m,in} - 0 = \phi_{m,in} \quad (1.142)$$

By combining the Equations (1.141) and (1.142), and conceiving v_b as a constant, it follows that

$$F = v_b \cdot \phi_m = 225 \text{ N} \quad (1.143)$$

It should also be pointed out that the same result is obtained if the sand has reached the end of the conveyor belt and is dropping down from the belt. Under these circumstances, the control volume should extend to the end of the belt, as a result, sand is flowing out of the control volume

Example 1.16. Filling a container

This example once more deals with the link between momentum flow and force as a producer of momentum

In a factory, containers are filled with liquid. This is an automated process, in which the weight of the containers is determined with the help of a weighing

scale. To give an idea, it takes about 20 seconds to fill a container and the velocity v of the vertical liquid jet that lands in the container is constant and amounts to 10 m/s.

What percentage of overweight must the scale show before the container contains the desired amount of liquid and the filling process can be stopped?

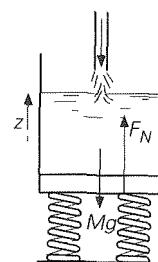


Figure 1.31

The control volume is an entire container. Although the liquid in a container may not be stagnant due to jet mixing during filling, on average the liquid in the container may be assumed to have virtually no vertical momentum, as a result, the left-hand side (the d/dt -term) of the balance for vertical momentum is zero and the balance then is (see Figure 1.31)

$$0 = -(\rho A v) v - 0 - Mg + F_N \quad (1.144)$$

where A is the surface of the diameter of the entrance and F_N is the force that the weighing scale exercises on the container. Equation (1.144) says that the weighing scale not only must carry the container (compensation of Mg), but also has to eliminate the momentum flow (the thrust) of the incoming liquid (negative production, or consumption, of vertical momentum). Mass M is a function of time, which can easily be determined from a mass balance for the tank

$$\frac{dM}{dt} = \rho A v \quad (1.145)$$

Integrating this equation with the initial condition $M = 0$ at $t = 0$ results in the following expression for the mass at filling time τ

$$M(\tau) = \rho A v \tau \quad (1.146)$$

For the overweight percentage, it then follows that

$$\frac{F_N - Mg}{Mg} = \frac{\rho A v^2}{\rho A v g \tau} = \frac{v}{g \tau} = 5\% \quad (1.147)$$

Example 1.17. A hanging droplet

Very slowly, individual water droplets are formed at the end of a vertically positioned glass capillary with an outer diameter of 2 mm. The flow through the capillary is negligibly small.

If the surface tension of water is $70 \cdot 10^{-3}$ N/m, use a force balance to calculate the diameter of the droplets that fall from the capillary.

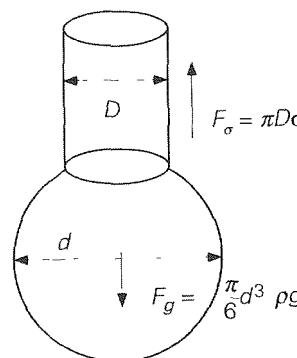


Figure 1.32

A momentum balance for the control volume (the droplet) will result in just a force balance because of the very low velocities both the increase in mass (the d/dt -term in the left-hand side of the momentum balance) and the inflow of momentum into the droplet during a time interval dt are insignificant. This simplification may be denoted as a quasi-steady-state approach.

The forces that dominate are gravitational force F_g and the surface tension force F_σ of the liquid that is in contact with the rim of the capillary, see Figure 1.32. The buoyancy of the air on the drop is ignored here. The two dominant forces have opposite direction and sign. This means that the force balance becomes

$$\sum F = 0 = F_\sigma + (-F_g) = \pi D \sigma - \frac{\pi}{6} d^3 \rho g \quad (1.148)$$

so that

$$d = \sqrt[3]{\frac{6D\sigma}{\rho g}} = 4.4 \text{ mm} \quad (1.149)$$

Comments about surface tension

The molecules in the bulk of a liquid encounter forces from the surrounding molecules which cancel each other out. This is not the case with molecules next to air, a resulting force operates here, which is aimed perpendicularly at the surface of the liquid. A quantity of liquid on which no external forces are operating

becomes spherical in shape, the surface energy has reached its minimum value at this point. It is as if the liquid were covered by an elastic film.

If the size of the surface of the liquid is increased, the number of molecules at the periphery also increases, and work is performed against the forces of attraction of the molecules in the liquid. The work (or energy), in joules, that is needed to increase the surface by 1 m^2 , is represented by *surface tension* σ , expressed in J/m^2 . Alternatively, the force required to increase a surface over a distance of b is σb (N), so that σ is also expressed in N/m .

At the rim of the capillary is a local and complicated force balance at the water-air-glass three-phase contact line. The liquid molecules in the boundary layer can be attracted more easily by a solid (*adhesion*) than by the liquid itself (*cohesion*), as a result of which, for example, the liquid rises in a capillary made from the solid in question.

In this example, the *adhesion force* is equal to the surface tension times the 'length' πD of the contact line.

□

Summary

Momentum, in Ns , is a vector. There are therefore three momentum balances, one for each component. It is recommended to think in terms of momentum concentrations: v , in Ns/kg , or ρv , in Ns/m^3 . The three momentum balances have the familiar basic form with a d/dt term, in and out terms, and production terms

$$\frac{d}{dt}(Mv_x) = \phi_{m,in} \cdot v_{x,in} - \phi_{m,out} \cdot v_{x,out} + \sum F_x$$

There are no terms involving y - or z -momentum in the x -momentum balance of course.

Forces can be seen as producers of momentum, in Ns/s . Here, too, there are no forces in the directions of y or z in the x -momentum balance.

Sometimes, a momentum balance simplifies to a force balance, e.g. when in a quasi-steady-state approach all other terms of the momentum balance compensate.

1.5 Examples of combined use of mass, energy, and momentum balances

Example 1.18. Flow through a bend

Water flows through a 90° bend in a well-insulated tube that has been positioned horizontally. Figure 1.33 shows a top view. The tube has a constant diameter A ,

and the water is assumed to be incompressible. The situation is a steady state. Draw up the mass balance, the energy balance, and the momentum balances for the whole bend.

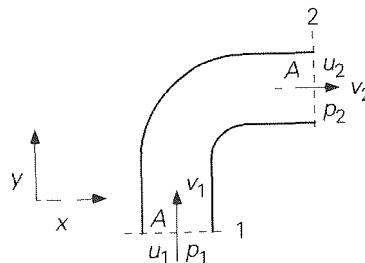


Figure 1.33

The situation is steady, so the left-hand side in all four balances is equal to 0 (Note: there are two relevant momentum balances¹)

- Mass balance

$$0 = \rho v_1 A - \rho v_2 A \rightarrow v_1 = v_2 \quad (1.150)$$

Clearly the magnitude of the velocity is unchanged, but the direction has changed, of course

- Energy balance

$$0 = \rho v_1 A \left(e_1 + \frac{p_1}{\rho} \right) - \rho v_2 A \left(e_2 + \frac{p_2}{\rho} \right) \quad (1.151)$$

Thanks to Equation (1.150), it then follows immediately that

$$u_1 + \frac{1}{2}v_1^2 + gz_1 + \frac{p_1}{\rho} = u_2 + \frac{1}{2}v_2^2 + gz_2 + \frac{p_2}{\rho} \quad (1.152)$$

Again because of Equation (1.150) and with $z_1 = z_2$, it follows that

$$\frac{p_1 - p_2}{\rho} = u_2 - u_1 \quad (1.153)$$

This result implies that the pressure drop can only be predicted if the extent of the energy dissipation is known, and vice versa

- Momentum balance in the x-direction

$$0 = \rho v_1 A \cdot v_1 - \rho v_2 A \cdot 0 + \sum F_x \quad (1.154)$$

The second term of the right-hand side states that no momentum is carried in the direction of y by the outgoing flow. The forces operating on the liquid in the y -direction are the pressure force $+ p_1 A$ exerted by the outside world in the positive y -direction on the liquid already inside the bend, and the reaction force of the wall to the liquid $+ F_{y,w \rightarrow f}$ (in either the positive or the negative y -direction that follows from the sign), therefore

$$F_{y,w \rightarrow f} = - \rho v_1^2 A - p_1 A \quad (1.155)$$

The wall must therefore supply a force in the negative y -direction and absorb a force $F_{y,f \rightarrow w}$ ($= -F_{y,w \rightarrow f}$) in the positive y -direction (action = reaction, Newton's Third Law). This force $F_{y,f \rightarrow w}$ stands for the sum of the pressure force on the liquid and the reaction force that arises when the momentum of the inflowing liquid is entirely absorbed by the wall

- Momentum balance in the x-direction

$$0 = \rho v_1 A \cdot 0 - \rho v_2 A \cdot v_2 + \sum F_x \quad (1.156)$$

The first term of the right-hand side states that no x -momentum is carried by the incoming flow

The forces working on the liquid in the x -direction are the 'pressure force' $-p_2 A$ exerted by the outside world on the liquid still within the bend and acting in the negative x -direction, and the reaction force of the wall to the liquid $+ F_{x,w \rightarrow f}$ (in either the positive or the negative x -direction that follows from the sign), therefore

$$F_{x,w \rightarrow f} = \rho v_2^2 A + p_2 A \quad (1.157)$$

The wall must therefore supply a force in the positive x -direction and absorb a force $F_{x,f \rightarrow w}$ ($= -F_{x,w \rightarrow f}$) in the negative x -direction (again, action = reaction, Newton's Third Law)

A nice illustration of the combined effect of $F_{x,f \rightarrow w}$ and $F_{y,f \rightarrow w}$ is a garden sprinkler revolving about a vertical axis where the liquid causes the centre piece to rotate in the reverse direction, or the wagging motion of a loose garden hose from which water is spurting

It has been assumed in the aforementioned that the velocity distributions at the entrance and exit are uniform (no differences in average velocity). In that case, the inflowing momentum in the direction of x is indeed $\rho A v_1 v_1$. If this is not the case, then the incoming momentum flow rate in the y -direction must be written as:

$$\rho \int v_i^2 dA \quad \text{or, for short} \quad \rho A \langle v_i^2 \rangle \quad (1.158)$$

where the brackets represent a cross-sectional average □

Example 1.19. The fire hose

A jet of water comes out of the round hole (diameter $D_2 = 4$ cm) in a flange situated at the end of a horizontally held fire hose (internal diameter $D_1 = 10$ cm). The velocity of the water in the round hole is 15 m/s. The jet of water enters the outside air unimpeded (see Figure 1.34). The situation is steady.

Determine the force F , in size and direction, that the flange exercises on the water. Assume that energy dissipation is negligible (The contraction of the water jet just after the outflow opening may also be disregarded.)

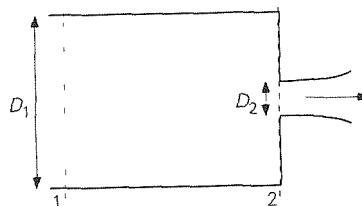


Figure 1.34

In order to determine F , it will be necessary to use the mass balance, the mechanical energy balance, and the momentum balance for the horizontal direction. All three balances have the same control volume, the whole tube section between the planes 1 and 2 in Figure 1.34. Plane 1 has to be chosen 'far' enough upstream of the flange, plane 2 runs precisely along the inside of the end flange. The calculation of F is as follows:

The mass balance for the control volume is:

$$0 = \rho A_1 v_1 - \rho A_2 v_2 \rightarrow \\ v_1 = \frac{A_2}{A_1} v_2 = \left(\frac{D_2}{D_1} \right)^2 v_2 = 2.4 \text{ m/s} \quad (1.159)$$

The mechanical energy balance for the same control volume is

$$0 = \rho A_1 v_1 \left(\frac{1}{2} v_1^2 + \frac{p_1}{\rho} \right) - \rho A_2 v_2 \left(\frac{1}{2} v_2^2 + \frac{p_2}{\rho} \right) \quad (1.160)$$

This results in a pressure drop between 1 and 2, the increase in kinetic energy is derived from the drop in pressure energy. Using the mass balance produces the following

$$p_1 - p_2 = \frac{1}{2} \rho v_2^2 - \frac{1}{2} \rho v_1^2 = 11.10^5 \text{ Pa} \quad (1.161)$$

which actually is the Bernoulli equation (remember steady state, no work, no heat exchange, constant ρ ; no energy dissipation). Because the pressure in the freely outflowing jet of water is equal to the pressure of the outside air ($p_2 = 1$ bar), the pressure in the hose is $p_1 = 21.10^5 \text{ Pa}$

These pressures also occur in the momentum balance in the flow direction

$$0 = \rho A_1 v_1 - \rho A_2 v_2 + p_1 A_1 - p_2 A_2 + F \quad (1.162)$$

All the quantities in this equation are now known, except F , entering the data produces $F = -1286 \text{ N}$. The force that the flange exercises on the water therefore operates in the opposite direction to that of the flow.

Notice that the pressure occurs in two equations both in the mechanical energy balance and in the momentum balance(s). In general which equation can or should be used for which purpose depends entirely on the nature of the problem under consideration. □

Example 1.20. Flow round an immersed obstacle

Two litres of water per second flow through a horizontal pipe with a constant diameter $D = 5$ cm. There is an obstacle in the pipe. This obstacle forms an (extra) element of resistance for the flow, conversely, the flow exercises a force F on the obstacle. The situation is steady. With the help of a pressure sensor, the pressure drop is measured for the (long) part of the pipe in which the obstacle is located. The friction on the wall of this part of the pipe may be ignored in relation to the flow resistance of the obstacle. The difference in pressure is 980 Pa.

First determine the force F that the water is exercising on the obstacle, and how much energy is dissipated per s.

To this end, draw up a balance for the momentum in the direction of the flow for the section of pipe over which the pressure drop is measured (see Figure 1.35). Note that the planes 1 and 2 should be located far enough from the obstacle to make sure that the flow in both planes should be free of effects associated with the presence of the obstacle. The momentum balance then is

$$0 = \phi_v \rho v_1 - \phi_v \rho v_2 + p_1 \frac{\pi}{4} D^2 - p_2 \frac{\pi}{4} D^2 - F \quad (1.163)$$

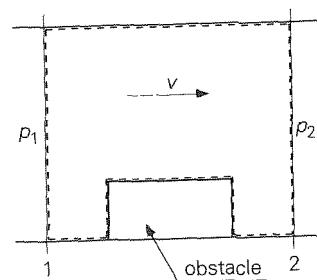


Figure 1.35

Because of $v_1 = v_2$ (because of the mass balance) and $p_1 - p_2 = 980 \text{ Pa}$ (measured) Equation (1.163) results in

$$F = \frac{\pi}{4} D^2 (p_1 - p_2) = 1.92 \text{ N} \quad (1.164)$$

As a result of friction along the surface of the obstacle and in the wake behind the obstacle (in eddies), mechanical energy is dissipated (transformed into heat). With the help of the mechanical energy balance, this energy dissipation is

$$0 = -\phi_m \frac{p_2 - p_1}{\rho} - \phi_m e_{fr} \quad (1.165)$$

From this, it is easy to see how much mechanical energy is destroyed per unit of time

$$\phi_m e_{fr} = 1.96 \text{ J/s} \quad (1.166)$$

It was possible to calculate the energy dissipation in this example, because the pressure drop over the obstacle was measured and therefore known. This will not generally be the case however, and it will be necessary to use a model for e_{fr} , so that *pressure drop calculations* for pipeline systems are possible. This will be dealt with in Chapter 5 □

Example 1.21. Outflow from a vessel through a hole

A large vessel is full of water up to height z_0 . A small hole with a diameter D which is much smaller than the vessel diameter, is located at height z in the wall of the vessel, below the water line. Water obviously pours out through the hole. Assume that the hole has a sharp edge so that – due to the absence of wall friction plays a subordinate role only.

How does the flow rate through the hole depend on the height of the liquid, z_0 ?

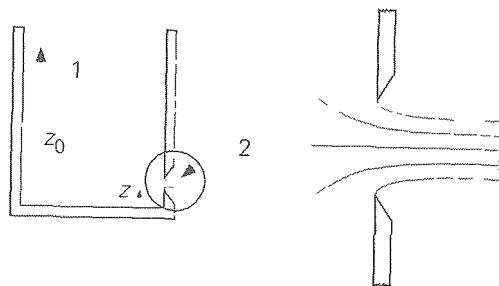


Figure 1.36

Application of the Bernoulli equation between points 1 and 2 (see Figure 1.36) – where both pressures are equal to the ambient pressure p_0 – produces for the velocity v in the hole (whereby $v = v_2$ and $v_1 \ll v_2$)

$$v = \sqrt{2g(z_0 - z)} \quad (1.167)$$

And therefore the following applies to the flow rate through the hole

$$\phi_V = \frac{\pi}{4} D^2 v = \frac{\pi}{4} D^2 \sqrt{2g(z_0 - z)} \quad (1.168)$$

In practice, the flow rate is less than calculated using Equation (1.168), as contraction of the discharging liquid jet occurs. The inertia of the liquid that from all sides flows radially towards the discharge hole does not allow the liquid to instantaneously give up this radial velocity (momentum) and to utilize the full cross-sectional area of the discharge opening. Only some distance downstream, outside the hole, do the flow lines become parallel and only at this downstream position does the pressure p_2 in the liquid jet become equal to the ambient pressure p_0 – this position therefore proves to be the point 2 presumed in view of Equation (1.167). At this position, the cross-sectional area of the liquid jet is therefore smaller than that of the discharge opening.

This contraction effect is usually taken into account by including a *discharge coefficient* C_d on the right-hand side of Equation (1.168), with $C_d < 1$ actually denoting the ratio of the cross-sectional area of the liquid jet at the position where the flow lines have become parallel, to that of the discharge opening.

$$\phi_V = C_d \frac{\pi}{4} D^2 \sqrt{2g(z_0 - z)} \quad (1.169)$$

The above phenomenon is generally denoted by the term ‘vena contracta’. Usually, the (sometimes very) small effect of friction losses is also included in the above discharge coefficient, but with sharp entrance edges of the discharge

opening the role of friction may safely be ignored. The lowest possible value of C_d is 0.6 and relates to turbulent flow (at a high value of the Reynolds number see Chapter 2) through a sharp-edged hole. The value of C_d increases as the entrance edges of the discharge opening are more rounded-off and the pertinent contraction of the discharging liquid jet decreases.

□

Appendix 1A

Many balance equations result in a first-order linear differential equation of the form

$$\frac{dy}{dx} = \lambda y \quad (\text{A } 1)$$

This differential equation is first order and linear because both the derivative of y and y itself only occur to the power of 1. The equation states that dy/dx , that is, the change of y by x , has a linear dependency on y itself. Notice that λ can be both positive and negative.

Because differentiating y versus x leads to a statement that gives the function y itself, $e^{\lambda x}$, which is also written as $\exp(\lambda x)$, is a solution to this differential equation. This means the general solution to the above differential equation is $y = C_1 e^{\lambda x}$, where C_1 is a constant yet to be determined – that is, that C_1 does not depend on x and therefore gives zero in the case of differentiating versus x . For a specific situation, C_1 is obtained with the help of the boundary (or initial) condition that $y = y_0$ when $x = 0$, resulting in the one solution, $y = y_0 e^{\lambda x}$. Wherever dy/dx depends on y itself, the solution to y is always an exponential function of x .

Another way of solving the above differential equation is the *separation of variables* method. This is particularly useful when the right-hand side – as is often the case – is a more complicated statement that is still a linear function of y . With the separation of variables, the dependent variable y and the independent variable x are separated. Every y goes to the left-hand side (as a result of division), and every x goes to the right-hand side (through multiplication). Equation (A.1) then becomes

$$\frac{dy}{y} = \lambda dx \quad (\text{A } 2)$$

Integrating this equation gives

$$\int \frac{dy}{y} = \ln y = \lambda x + C_2 \quad (\text{A } 3)$$

This result can be modified into an explicit outcome for y

$$y = \exp(\lambda x + C_2) = C_2' \exp(\lambda x) \quad (\text{A } 4)$$

where the integration constant C_2 – and therefore also C_2' – have to be found by substituting the boundary or initial condition $y = y_0$ at $x = 0$ – which is often written as $y(x=0) = y_0$ – into Equation (A 4), because the solution of Equation (A 4) also applies to $x = 0$, $C_2' = y_0$ then follows. Remember that every integration stage produces an integration constant for which a boundary or initial condition is required in order to arrive at a specific solution.

With transport phenomena, it is often necessary to work with a more complicated version of differential equation (A 1). This can be shown in general as

$$\frac{dy}{dx} = \alpha y + \beta \quad (\text{A } 5)$$

where α and β are constants. *Separation of variables* is a very suitable method for solving this differential equation. This separation step results in

$$\frac{dy}{\alpha y + \beta} = dx \quad (\text{A } 6)$$

The next step is to ensure that the same statement is made after the ‘ d ’ in the numerator on the left-hand side as in the denominator on the left-hand side, in order that the integration of the left-hand side produces $\ln(\alpha y + \beta)$. To that end, the left and right-hand side of Equation (A 6) are first multiplied by α

$$\frac{\alpha dy}{\alpha y + \beta} = \alpha dx \quad (\text{A } 7)$$

Then – providing that α and β are constants, that is, that they do not depend on y or x – the left-hand side is modified in stages:

$$\frac{\alpha dy}{\alpha y + \beta} = \frac{d\alpha y}{\alpha y + \beta} = \frac{d(\alpha y + \beta)}{\alpha y + \beta} \quad (\text{A } 8)$$

where it is handy to remember that the derivative of $(\alpha y + \beta)$ is precisely the α by which Equation (A 6) was multiplied. Substituting Equation (A 8) in Equation (A 7) and integrating results in

$$\ln(\alpha y + \beta) = \alpha x + C_3 \quad (\text{A } 9)$$

From this it follows

$$\alpha y + \beta = \exp(\alpha x + C_3) = C_3' \exp(\alpha x) \quad (\text{A } 10)$$

Then C_3' is obtained by entering $x = 0, y = 0$ into Equation (A 10)

$$C_3' = \alpha y_0 + \beta \quad (\text{A } 11)$$

This ultimately gives us the explicit solution for y

$$y = \frac{-\beta}{\alpha} + \frac{\alpha y_0 + \beta}{\alpha} \exp(\alpha x) \quad (\text{A } 12)$$

Appendix 1B

The field of transport phenomena sometimes involves *inhomogeneous linear differential equations*. They have the following form

$$\frac{dy}{dx} = ay + b(x) \quad (\text{B } 1)$$

This type of equation forms an extension of the differential equations of the type at (A 5), because the second term on the right-hand side is now a function of the independent variable x . There are several, closely related methods of solving this type of inhomogeneous differential equation (B 1).

First of all, the route via the homogeneous differential equation. the first step is to solve the homogenous variant of Equation (B 1), therefore

$$\frac{dy}{dx} = ay \quad (\text{B } 2)$$

The solution to this is

$$y = K_1 \exp(ax) \quad (\text{B } 3)$$

Note that K_1 may not be determined with the help of an initial or boundary condition, because every initial or boundary condition is part of the *overall* solution to Equation (B 1), and not of a partial solution. Equation (B 3) is not of course sufficient as a solution to Equation (B 1) when substituting the solution of Equation (B 3) on the left-hand side and right-hand side of Equation (B 1), we would find $0 = b(x)$. With solution (B 3), another term therefore has to be drawn up – one that does meet the requirements of Equation (B 1). Because the form of this extra term will strongly depend on $b(x)$, there is no generally valid form for the term, so a *particular solution* will have to be found *via trial and error*. This is a disadvantage of this method. Once the particular solution has been found, it has to be added to the partial solution of Equation (B 3), after which the integration constant follows through the application of the initial or boundary condition.

If $b(x)$ is an exponential function of x – say, $b(x) \propto \exp(\gamma x)$ – then the particular solution can be found by trying a solution of the form $k + h(x) \exp(\gamma x)$. It will then hopefully be possible to find k and $h(x)$ by substituting this trial function in Equation (B 1). If not, another trial function should be looked for. The result should be an equation in which a number of terms occur that contain $\exp(\gamma x)$, as well as several terms without $\exp(\gamma x)$. k is found from the terms without $\exp(\gamma x)$ – this is because they remain when every term with $\exp(\gamma x)$ disappears for $x = 0$ or for $x \rightarrow \infty$, depending on the sign of γ – after which $h(x)$ follows from the rest of the equation.

If $b(x)$ is a linear function of x , then the particular solution can be found by looking at the end situation (for $x \rightarrow \infty$) if at least dy/dx has then become very small.

A second way of solving differential equation (B.1) is through *variation of constants* where on the basis of solution (B.3)

$$y = K(x) \exp(ax) \quad (\text{B } 4)$$

is tested to see whether it can meet the requirements of Equation (B 1). Substituting Equation (B 4) into Equation (B 1) then gives

$$\begin{aligned} \frac{dy}{dx} &= \frac{dK(x)}{dx} \exp(ax) + aK(x) \exp(ax) \\ &= ay + b(x) = aK(x) \exp(ax) + b(x) \end{aligned} \quad (\text{B } 5)$$

from which it follows that

$$\frac{dK(x)}{dx} \exp(ax) = b(x) \quad (\text{B } 6)$$

and therefore

$$K(x) = \int b(x) \exp(-ax) dx \quad (\text{B } 7)$$

by which

$$y = \exp(ax) \int b(x) \exp(-ax) dx \quad (\text{B } 8)$$

Note that the integration constant that results from the integration on the right-hand side of Equation (B 8) should also be multiplied by $\exp(ax)$. The integration constant that results from integration on the right-hand side is again dealt with by the initial or boundary condition.

A third method for solving differential equation (B 1) is with an *integrating factor*. In this method, the differential equation is first rewritten as

$$\frac{dy}{dx} - ay = b(x) \quad (\text{B } 9)$$

The solution being sought $y(x)$ is then multiplied by a function $F(x)$, to which the following must apply

$$\begin{aligned} \frac{d}{dx} [F(x)y(x)] &= F(x)\frac{dy(x)}{dx} + \frac{dF(x)}{dx}y(x) \\ &= F(x)\left[\frac{dy}{dx} - ay\right] \end{aligned} \quad (\text{B } 10)$$

From this, it follows that $F(x)$ must satisfy

$$\frac{dF(x)}{dx} = -aF(x) \quad (\text{B } 11)$$

for which $F(x) = \exp(-ax)$ is a solution. Substituting this result in Equation (B 10) and combining it with Equation (B 9) gives

$$\begin{aligned} \frac{d}{dx} [\exp(-ax)y(x)] &= \exp(-ax)\left[\frac{dy}{dx} - ay\right] = \\ &= b(x)\exp(-ax) \end{aligned} \quad (\text{B } 12)$$

from which it follows, through integration, that

$$\exp(-ax)y(x) = \int b(x)\exp(-ax)dx \quad (\text{B } 13)$$

When $b(x)$ is also an exponential function in particular, the integration of the right-hand side is very straightforward. Thanks to Equation (B 13), the final solution to Equation (B 1) is

$$y(x) = \exp(ax) \int b(x)\exp(-ax)dx \quad (\text{B } 14)$$

Note that the integration constant that results from the integration on the right-hand side of Equation (B 14) should also be multiplied by $\exp(ax)$. The integration constant then follows through application of the initial or boundary condition

2 Mechanisms, non-dimensional numbers, forces

2.1 Molecular transport

2.1.1 Moving molecules

So far, we have looked primarily at flows of mass, energy, and momentum resulting from ‘collective’ behaviour. Mass of a certain species, energy of any type, or momentum flowed into (or out of) the control volume because it was carried, as it were, ‘under the arm’ of a mass flow rate that flowed into (or out of) the control volume. It could be said that this involved the molecules going ‘together’. The form of the expressions for the inflows and outflows is always a product of a mass (or volume) flow rate and a concentration in that flow rate (per unit of mass or volume). Such flows are forms of *convective transport*.

However, individual molecules are also able to effect transport of mass, energy, and momentum. At a molecular scale, molecules in a liquid or gas move around somewhat chaotically, criss-crossing and colliding with each other as a result of their thermal motion. Each molecule transports its own mass, momentum, and kinetic energy. Because they collide, they are able to transfer their momentum and energy wholly or partly to other molecules. In time, net transport over larger distances is possible. The mobility of individual molecules in a solid is, of course, much less, but here too, due to the fact they vibrate, they are perfectly able to pass, or conduct, heat by colliding with neighbouring molecules.

Notwithstanding the fact that this *molecular transport* is caused by the movements of individual molecules, it is useful to talk in terms of ‘mean quantities’ (continuum quantities) like density, (mass) concentration, and temperature. This Section describes the aforementioned transport in a phenomenological manner.

Diffusion

The following experiment serves to give us a greater understanding of the mechanism of molecular transport. A container is divided into two equal parts by a partition, in which there is a small hole (see Figure 2.1). The right-hand side of the tank is filled completely with distilled water, and the left-hand side with saltwater. The pressures on both sides are equal, which means no convective flow occurs from one compartment to the other. However, after a long enough period of time, both

sides will contain equal levels of saltwater. This equilibrium situation will never return to the first situation in which one side contained distilled and the other saltwater. What is the explanation for this? A close-up of the hole (see Figure 2.2) makes this clear.

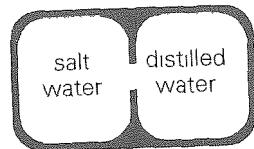


Figure 2.1

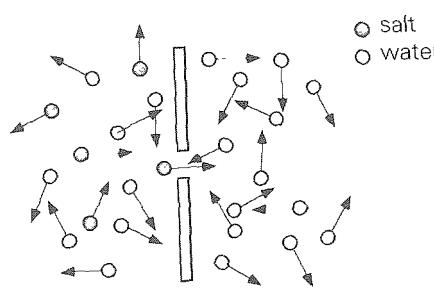


Figure 2.2

A veritable bombardment of molecules takes place from both sides onto the partition wall, and thus also onto the imaginary plane of the hole as a result, as many molecules find their way through the hole from left to right as they do from right to left, maintaining the zero pressure difference between the two compartments. However, if we look at the salt molecules⁴, things are different. The number of salt molecules approaching the hole from either side depends on the number density (concentration) of salt molecules on that side. At first, salt molecules only travel through the hole from left to right – there are no salt molecules on the right, after all. In time, the number of salt molecules in the right compartment increases, and so does the number of salt molecules that is able to return to the left. The *net* transport from left to right gradually decreases until the concentrations of salt are equal on both sides.

The process described above is known as *molecular diffusion* and originates in macroscopic differences in concentration. It is to be expected that the resulting net mass transport rate ϕ_m simply depends on this difference in concentration: the greater the difference, the stronger the net transport rate, and the greater the distance between the places of high and low concentration, the weaker the transport rate (as it may take the molecules longer to cover a larger distance).

Conduction

Molecular heat transport goes by analogy. The driving ‘force’ here is a difference in temperature. Temperature is actually the resultant of the kinetic energy of a very

⁴ It is actually incorrect to talk of salt molecules, as the dissolution of salt always involves dissociation into ions. This is a typical example of the use of an ‘engineering point of view’: the ‘removal’ of the physical reality and the introduction of all kinds of simplifications to the phenomenon under review in order to highlight and describe the essence of the phenomenon under consideration.

large number of atoms. An example in this context is that of a copper rod, the left side of which has a higher temperature than the right. This means on average that the molecules on the left have a greater kinetic energy than those on the right. In a solid, neighbouring molecules collide with each other all the time due to their vibrations about their fixed position. The effect of these collisions is that the fast-vibrating molecules transfer their kinetic energy to the slow vibrating ones. This is why the temperature on the left of the rod decreases slightly, while the temperature on the right increases. This continues until the temperature is equal on both sides and of course the net transport of energy (heat) is zero. The conclusion is that a difference in temperature gives rise to an energy flow – that is, transport of kinetic energy of molecules.

Looking at this phenomenon from a macroscopic perspective, there is simply transport, or ‘flow’, of heat. This mechanism of heat transport is not just confined to solids; the mechanism occurs within gases and liquids as well. In the case of the latter two, energy is passed on between neighbouring molecules not just via collisions, but also because of the criss-crossing movements of the molecules. ‘Warm’ molecules diffuse to a ‘cold’ location where they share their kinetic energy, while ‘cold’ molecules move away from that cold location and pick up some ‘heat’. The term used in the case of heat transport resulting from the activity of individual molecules is *conduction*. The net heat transport rate due to conduction is denoted by ϕ_q .

Momentum

Finally, it is also possible for momentum to be transported by individual molecules. Here, the molecules carry their own momentum. This effect can be easily understood by looking at the individual molecules in a *laminar* (= layered) flow. Conceptually, a flow of this type consists of adjacent layers (*in Latin laminae*, plural of *lamina*) where the velocity varies slightly from one layer to another (see Figure 2.3). For the sake of simplicity, it is assumed here that the substance involved is pure (that is, that all the molecules are the same). Molecules in layer 1 have, on average, superimposed a velocity $v_{x,1}$ on top of their criss-cross movement. For layer 2, of course, this is $v_{x,2}$ on average.

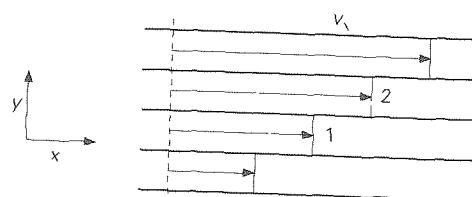


Figure 2.3

A molecule (with molecule mass m) that 'diffuses' from layer 1 to layer 2 will bring, on average, momentum $mv_{x,1}$ to it. Here, too, it is useful to conceive $v_{x,1}$ as an x -momentum concentration (in Ns/kg), as explained in § 1.4. As a result, $mv_{x,1}$ will then stand for the x -momentum of that molecule. A molecule from layer 2 will, on average, bring momentum $mv_{x,2}$ to layer 1. In the case of this diffusion, (about) as many molecules will go from layer 1 to layer 2 as they will vice versa. This will cause the overall momentum in layer 2 to fall; molecules richer in x -momentum will be replaced by more poor ones. For layer 1, it is the very opposite that is true. In addition, upon arriving in a new layer, molecules will collide with their new neighbours and exchange x -momentum – thus reducing the velocity differences between the *laminae*.

Viewed from a macroscopic perspective, a net momentum flow is involved once again, note that *x -momentum is now transported in the y -direction!* See Figure 2.4. This net x -momentum transport, denoted⁵ by ϕ_p , is in the negative y -direction in this case, from layers with a higher to those with a lower x -momentum concentration, as dv_x/dy is positive.

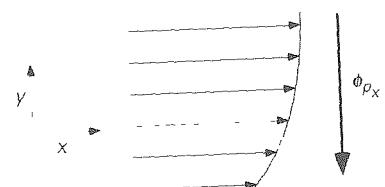


Figure 2.4

Summary

The following applies to molecular transport, based on the thermal movement of individual molecules:

- difference in concentration → net mass transport rate ϕ_m of a particular species
- difference in temperature → net energy transport rate ϕ_q (or heat 'flow')
- difference in velocity → net momentum transport rate ϕ_p

In the first case we speak of diffusion, in the second of (heat) conduction. In the third case, with laminar flow, we have to specify which momentum is transported by the individual molecules in which direction. In a laminar flow in the x -direction, the velocity gradient dv_x/dy results in a net x -momentum transport in the y -direction. When dv_x/dy is positive, the molecular transport is in the negative y -direction, while for negative dv_x/dy values the transport takes place in the positive y -direction.

⁵ In this elementary explanation, compliant with the use of the symbol P_y in § 1.4, we use the symbols p_x, p_y, p_z to denote momentum in the respective directions. Further on, we will switch to the usual v_x, v_y, v_z for momentum concentrations or velocities.

2.1.2 Fick, Fourier, Newton

With a view to arriving at practical descriptions of all three molecular transport mechanisms discussed above, simple equations have been drawn up – which are valid for a large category of substances – that link the driving forces, the above 'differences', to the transport rates. As mentioned in the discussion on mass diffusion, a greater difference in concentration Δc causes a greater flow (rate) while a greater distance L , over which the difference occurs, leads to a lesser flow (rate). It appears that the $\Delta c/L$ ratio is decisive. This proves to be true not only at finite distances but also locally.

To put it more accurately, the derivative of concentration c to position x , that is the local dc/dx , is decisive for the local mass flow rate. Of course, the mass is transported from a location with a high concentration to one with a low concentration, which is why the flow ϕ_m is a function of $(-dc/dx)$. A similar reasoning may be applied to both heat conduction and molecular momentum transport as a function of temperature gradient and velocity gradient, respectively.

It is easy to understand that, as with any flow or transport, the size of molecular transport is also directly proportional to the size of the plane through which the transport occurs. For this reason, it is useful to introduce the notion of a *flux*. A flux is a flow rate per unit of surface area (where the plane is perpendicular to the direction of transport). Therefore, if mass flow or transport rate ϕ_m passes through surface A (with A perpendicular to the direction of ϕ_m), then the flux is

$$\phi_m'' = \frac{\phi_m}{A} \quad (2.1)$$

The superscript '' indicates that it concerns⁶ a flux, that is, a flow rate per m^2 .

The equations for the molecular transport of a species, of heat, and of momentum are given in terms of their fluxes. In the simplest approach, each flux is assumed to be directly proportional to the pertinent gradient. The three equations, then, are

$$\text{mass flux} \quad \phi_{m,x}'' = -ID \frac{dc}{dx} \quad \text{Fick's law} \quad (2.2)$$

$$\text{heat flux} \quad \phi_{q,x}'' = -\lambda \frac{dT}{dx} \quad \text{Fourier's law} \quad (2.3)$$

$$y\text{-momentum flux} \quad \phi_{p,y,x}'' = -\mu \frac{dv_y}{dx} \quad \text{Newton's (viscosity) law} \quad (2.4)$$

⁶ Later, when dealing with ϕ , we will also use a single ' to indicate reference to a flow per unit of length – for example, ϕ_m' .

All three 'flows' are moving in the direction of x . Of course, Newton's law implies that also an x -momentum flux in the y -direction is possible. The minus sign in these laws means that the transport always runs from high to low concentration, the direction of the flux (in the positive or negative x -direction) always depends of course on the sign of the pertinent gradient (value less than or greater than zero).

The proportionality coefficient D is called the *diffusion coefficient*, the SI unit for D is m^2/s . The coefficient λ denotes the *thermal conductivity coefficient* and its SI unit is J/msK . The coefficient μ is the *dynamic viscosity* the SI unit of which is Ns/m^2 , the latter unit shows that μ stands for the momentum (in Ns) that in a laminar flow per unit of area is transported across the interface of two *laminae*.

Of the three laws, Fourier's law is the most generally applicable. Fick's law applies only to binary systems (these are system of just two components) and is also subject to other restrictions. This will be dealt with in detail in Chapter 4. Newton's law too is of limited validity. Liquids and gases that obey this law are referred to as *Newtonian liquids*. Liquids that fall into this category are more the exception than the rule. Liquids not obeying Newton's law are called *non-Newtonian liquids*. This will also be covered more extensively at a later stage (in Chapter 5).

In line with our earlier recommendation of working in terms of concentrations of species, energy and momentum, we would prefer to formulate the laws as follows:

$$\begin{array}{ll} \text{difference in mass concentration} & \rightarrow \text{mass flow rate} \\ \text{difference in energy concentration} & \rightarrow \text{energy flow rate} \\ \text{difference in } y\text{-momentum concentration} & \rightarrow y\text{-momentum flow rate} \end{array}$$

Fick's law of diffusion already meets this requirement. The other two can be rewritten for the special case of substances with a constant ρc_p or constant ρ respectively.

$$\text{Fourier } \phi_{q,x}'' = -\lambda \frac{dT}{dx} = -\frac{\lambda}{\rho c_p} \frac{d}{dx}(\rho c_p T) = -a \frac{d}{dx}(\rho c_p T) \quad (2.5)$$

If $\rho c_p = \text{constant}$

$$\text{Newton } \phi_{p_v,x}'' = -\mu \frac{dv_y}{dx} = -\frac{\mu}{\rho} \frac{d}{dx}(\rho v_y) = -v \frac{d}{dx}(\rho v_y) \quad (2.6)$$

If $\rho = \text{constant}$

The combination $\rho c_p T$ is the concentration of thermal energy (unit J/m^3). The coefficient $a \equiv \lambda/\rho c_p$ is called the *thermal diffusivity coefficient* and has the same unit as D m^2/s . The combination ρv_y is the y -momentum concentration (in Ns/m^3).

and its associated coefficient $v \equiv \mu/\rho$ is the *kinematic viscosity* (again, the unit is m^2/s). Note that the Equations (2.2), (2.5) and (2.6) are completely analogous, with all three of the respective coefficients D , a and v having the same SI unit m^2/s . This analogy between molecular mass transport, heat transport and momentum transport was already a key feature in the technique of drawing up balances and in describing convective transport in Chapter 1.

Note further that the numerical values of the dynamic viscosity μ and the kinematic viscosity v may differ by several orders of magnitude, for water, for example, $\mu = 10^{-3} \text{ Ns}/\text{m}^2$ and $v = 10^{-6} \text{ m}^2/\text{s}$ (at $T = 20^\circ\text{C}$ and $p = 1 \text{ bar}$). It is therefore important to keep these two viscosities firmly apart.

Example 2.1. Heat conduction in a copper rod

A copper rod (with a constant diameter and length L) is kept at a constant temperature at both ends T_0 at $x = 0$ and T_L at $x = L$ with $T_0 > T_L$. The rod is also thermally insulated from the surroundings.

In a steady-state situation, what is the temperature profile in the rod? How great is the heat flow through the rod, in that case?

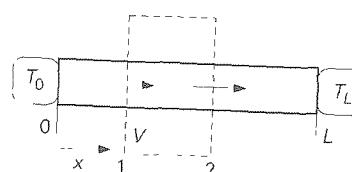


Figure 2.5

As the question is about the temperature profile in the rod, there is no point in selecting the whole rod as the control volume and drawing up a *macro heat balance*: this would at best link the mean temperature of the rod to heat flows in and out. Instead, you should select a small but representative control volume *inside* the rod, as illustrated in Figure 2.5, and draw up a *micro heat balance* for this small(er) control volume.

Because the rod is insulated, apart from the two ends, the heat transport will only occur lengthwise in the rod (from one end towards the other). The control volume can therefore cover the whole cross-sectional area of the rod – after all, nothing occurs transversely. This therefore concerns just a one-dimensional transport problem (without heat production).

In a steady-state situation, the heat balance for the control volume V in Figure 2.5 is therefore

$$0 = \phi_q \Big|_{x=x_1} - \phi_q \Big|_{x=x_2} \quad (2.7)$$

where, due to the given $T_0 > T_L$, the first term on the right-hand side stands for the 'flow in' and the second term for the 'flow out'. Because of the constant diameter of the rod

$$0 = \phi_q''|_{x=x_1} - \phi_q''|_{x=x_2} \quad (28)$$

As only heat conduction is involved, the fluxes can be written as follows

$$\phi_q''|_{x=x_1} = -\lambda \frac{dT}{dx}|_{x=x_1} \quad \text{and} \quad \phi_q''|_{x=x_2} = -\lambda \frac{dT}{dx}|_{x=x_2} \quad (29)$$

Substituting this in Equation (28) shows that the two heat fluxes through the planes 1 and 2 are equal, implying that – providing that λ is constant – the temperature gradient does not depend on position

$$\frac{dT}{dx} = C_1 = \text{constant} \quad (210)$$

Solving this very simple differential equation gives, with the help of boundary conditions $x=0 \rightarrow T=T_0$ and $x=L \rightarrow T=T_L$

$$T(x) = \frac{T_L - T_0}{L} x + T_0 \quad (211)$$

The temperature profile is therefore linear, which means the heat flow through the rod is

$$\phi_q = -\lambda A \frac{dT}{dx} = \lambda(T_0 - T_L) \frac{A}{L} \quad (212)$$

where A is the cross-sectional area of the rod

Remember how earlier, in § 1.2.2, also a small control volume *inside* the reactor was selected, the purpose of which was to arrive at a concentration profile along the reactor? There, we opted for a thin slice dx , because of the chemical reaction, with the view of obtaining dc/dx and the pertinent differential equation. In the above case, this is not necessary. The above case does illustrate again the use of a *microbalance* to derive a profile, in this case a temperature profile. □

Example 2.2. Evaporation of naphthalene from a tube

A long, narrow tube (length 25 cm, internal diameter $D = 1$ cm) is partly filled with solid naphthalene. The top of the tube is exposed to the air (see Figure 2.6). The length of the tube above the naphthalene is 20 cm. The ambient temperature is 20 °C.

How long does it take for a 1 mm layer of the naphthalene to evaporate?

Naphthalene details

diffusion coefficient in air	$D = 7 \cdot 10^{-6} \text{ m}^2/\text{s}$
density of solid naphthalene	$\rho = 1150 \text{ kg/m}^3$
molar mass	$M = 106 \text{ kg/kmol}$
vapour pressure at 20 °C	$p^* = 0.05 \text{ mm Hg}$

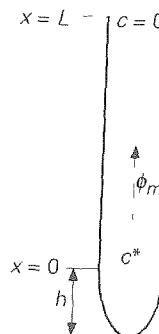


Figure 2.6

Drawing up a mass balance for the solid naphthalene in the tube produces

$$\frac{dM}{dt} = \rho A \frac{dh}{dt} = -\phi_{m,out} = -A \phi_{m,out}'' \quad (213)$$

A is the cross-sectional area of the tube. In order to progress further, it is necessary to determine the flux of naphthalene vapour. Naphthalene disappears only as a result of diffusion. At the interface between the solid naphthalene and air, the naphthalene concentration c^* in the gas phase may be estimated with the help of the ideal gas law from the local vapour pressure p^*

$$c^* = M \frac{p^*}{RT} \quad (214)$$

where p^* is the equilibrium vapour pressure above the solid naphthalene that depends on temperature. Because the top of the tube is exposed to the surrounding air, there is hardly any naphthalene present there: $c(L) \approx 0$. There is therefore clearly a driving concentration difference between $x=0$ and $x=L$, resulting in diffusive transport.

Given that solid naphthalene diffuses away only very slowly because of its extremely low vapour pressure at room temperature – the driving force for diffusion is very small – the diffusion in the tube can be regarded as quasi-steady. It is as if the situation is steady at any given moment (this has to be checked).

afterwards) Over a longer period of time, of course, this assumption becomes increasingly pointless

In a derivation entirely analogous to that leading to Equation (2.11), with the heat flux $\phi_q'' = -\lambda dT/dx$ replaced by the diffusive mass flux $\phi_m'' = -ID dc/dx$, the following result is obtained

$$c(x) = \frac{c(L) - c(0)}{L} x + c(0) = c^* \left(1 - \frac{x}{L}\right) \quad (2.15)$$

From this, it follows for the flux at $x = 0$ (at the surface of the naphthalene), that

$$\phi_m'' = -ID \frac{dc}{dx} = ID \frac{c^*}{L} \quad (2.16)$$

Combining Equations (2.13), (2.14), and (2.16) now produces

$$\frac{dh}{dt} = -\frac{ID M p^*}{\rho R T L} \quad (2.17)$$

Solving this differential equation gives $\Delta h = 1 \text{ mm}$ if

$$\Delta t = \frac{\rho R T L}{ID M p^*} \Delta h = 1.1 \cdot 10^8 \text{ s} \approx 3.6 \text{ years} \quad (2.18)$$

Notice that the earlier assumption about the diffusion rate was therefore correct. In fact, it is not entirely appropriate to use Fick's law in this situation – it is only because the vapour pressure of naphthalene is so low that Fick's law produces a satisfactorily accurate result. This situation will be dealt with again in § 4.3. \square

Convective transport is generally a much more effective way of transporting a particular quantity than is molecular (or diffusive) transport. Although the velocity of a liquid package is much lower than that of a molecule – a typical liquid velocity is 1 m/s, while the random velocity of a molecule in water at room temperature is of the order of 600 m/s – molecules move collectively in the case of convective transport. When it comes to molecular transport, the molecules behave as genuine individuals that each go their own way, and their movement is not in any particular direction. Finally, with convective transport, it is the quantity itself (for example, thermal energy) that counts, while with molecular transport it is all about gradients in this quantity.

Summary

For a large category of substances, molecular transport can be described with simple phenomenological laws. The transport of mass, thermal energy (heat), and momentum is described by Fick's, Fourier's, and Newton's law respectively.

$$\phi_{m,x}'' = -ID \frac{dc}{dx}, \quad \phi_{q,x}'' = -\lambda \frac{dT}{dx}; \quad \phi_{p,x}'' = -\mu \frac{dv_y}{dx}$$

All three laws link flow, or rather flux, to the driving gradients via a proportionality constant: the diffusion coefficient ID , the thermal conductivity coefficient λ , and the dynamic viscosity μ , respectively. Fourier's law is the most generally applicable, while the other two are subject to stricter requirements.

Providing that ρ and ρc_p are constant, all three laws can be written as

$$\text{flux of } \left\{ \begin{array}{l} \text{mass} \\ \text{thermal energy} \\ \text{y-momentum} \end{array} \right\} \propto -\frac{d}{dx} \left\{ \begin{array}{l} \text{mass concentration} \\ \text{thermal energy concentration} \\ \text{y-momentum concentration} \end{array} \right\}$$

for molecular transport in the x -direction. In this formulation, illustrating the firm analogy of molecular mass, heat and momentum transport, the proportionality constants are the diffusion coefficient ID , the thermal diffusivity α and the kinematic viscosity ν , respectively, all in m^2/s .

The minus sign in all these laws means that the transport always runs from high to low concentrations, the direction of the flux depends on the concentration gradient sign.

2.1.3 Transport coefficients

In the above naphthalene example, the rather high value for time Δt is attributable to a significant degree to the fact that the diffusion coefficient ID has such a low value. In order to be able to make a quick estimate of the size of the various flows in practice, it is useful to know the order of magnitude of the various transport coefficients (these are ID , λ , α , μ and ν). The following table could come in handy for this purpose:

	ID (m^2/s)	ν (m^2/s)	α (m^2/s)	λ (W/m K)
Gas	10^{-5}	10^{-5}	10^{-5}	10^{-2}
Liquid	10^{-8} to 10^{-9}	10^{-5} to 10^{-6}	10^{-7}	10^{-1}
Solid	10^{-11} to 10^{-15}			1 to 500

Remember that these transport coefficients are physical properties which in general depend on the atomic or molecular composition of a substance and on pressure and temperature.

The above estimates can be made for gases with the help of the *kinetic gas theory*, the kinetic gas theory can also be used to determine how, for gases, the transport

coefficients depend on pressure and temperature. For the diffusion coefficient, for example, the following simplified model can be set up.

Imagine that the molecules of a gas may be conceived as hard spheres. These spheres have a mean velocity v_m and travel on average a distance ℓ until they collide (ℓ being the average free path length). Suppose now that there are two types of molecule – A and B – both of about the same size and weight. Molecules B form the background with molecules A diffusing in between them, n_A denoting the number of molecules A per unit of volume. If we focus on a plane at position x (see Figure 2.7), let us assume that the number of A molecules to the left of the plane (n_{A-}) is slightly smaller than to the right of the plane (n_{A+}). The question now is how great the flow of A molecules through the plane is?

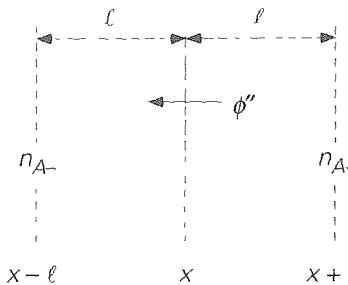


Figure 2.7

The movements of the molecules are random. For the sake of simplicity, we can say that $\frac{1}{3}$ of all molecules move in the x -direction (and $\frac{1}{3}$ in the y -direction and $\frac{1}{3}$ in the z -direction). Of this, half, that is $\frac{1}{6}$ of the total, move in the positive x -direction.

During a short interval of time τ , therefore, $\frac{1}{6}$ of all molecules located on the left-hand side within a distance $v_m \cdot \tau$ of plane x , pass this plane. The same applies to the molecules to the right of x . Net, this gives a flux (= number of particles per unit of surface and per unit of time) of

$$\phi'' = \frac{\frac{1}{6} n_{A-} v_m \tau - \frac{1}{6} n_{A+} v_m \tau}{\tau} \quad (2.19)$$

An estimate of the two particle densities can be obtained by attributing density n_{A-} at the plane $x - \ell$, that is, one mean free path length removed from plane x . The particles located here just pass by plane x without colliding. Similarly, put n_{A+} at plane $x + \ell$. This means that the following applies to the particle flux

$$\phi'' = \frac{1}{6} v_m [n_A(x-1) - n_A(x+1)] \quad (2.20)$$

Further,

$$n_A(x \pm 1) \approx n_A(x) \pm \frac{dn_A}{dx} \ell \quad (2.21)$$

So Equation (2.20) becomes

$$\phi'' = -\frac{1}{3} v_m \ell \frac{dn_A}{dx} \quad (2.22)$$

From this, it is easy to make a mass flux by multiplying it by molecule mass m

$$\dot{\phi}_m'' = -\frac{1}{3} v_m \ell \frac{dc_A}{dx} \quad (2.23)$$

Comparing Equations (2.2) and (2.23) gives for the diffusion coefficient

$$ID = \frac{1}{3} v_m \ell \quad (2.24)$$

(This result can also be obtained through a much more precise method.) Equation (2.24) expresses that in an ideal gas a diffusion coefficient (in m^2/s) may be described in terms of the product of a molecular velocity (in m/s) and the mean free path length (in m).

The mean velocity v_m can be determined from

$$\frac{1}{2} m v_m^2 = \frac{3}{2} k_B T \quad (2.25)$$

where k_B is the Boltzmann constant, and therefore it is found that

$$v_m = \sqrt{\frac{3RT}{M}} \quad (2.26)$$

Here, R is the gas constant and M the molar mass.

The free path length ℓ is inversely proportional to the particle density n , and the frontal surface area of the particles is $\pi \sigma^2$, where σ is the diameter of the hard spheres. Rewriting this with the help of Avogadro's number N_{avo} gives

$$\ell \propto \frac{1}{n \sigma^2} = \frac{m N_{\text{avo}}}{m n N_{\text{avo}} \sigma^2} = \frac{M}{\rho} \frac{1}{N_{\text{avo}} \sigma^2} \quad (2.27)$$

For the magnitude of ID and the variation of ID with T , p and ρ , it then follows that (for ideal gases, at least!)

$$ID \propto \frac{\sqrt{3RTM}}{\rho} \propto \frac{\sqrt{T}}{\rho} \quad (2.28)$$

It is also possible to estimate the other transport coefficients in ideal gases with the help of the same simple model⁷. After all, heat conduction involves the same flows that now carry, on average, $\rho c_p T$. In the case of molecular momentum transport, this is ρv on average. Here we assume that the exchange of energy and momentum during the collisions of the molecules is fast with respect to the molecular motions. The exact same as for ID therefore applies to λ and μ . Accordingly, we can write down immediately

$$\lambda \propto \left(\frac{1}{3} v_m \ell\right) \rho c_p \propto \sqrt{RTM} \quad c_p \propto \sqrt{T} \quad (2.29)$$

$$\mu \propto \left(\frac{1}{3} v_m \ell\right) \rho \propto \sqrt{RTM} \propto \sqrt{T} \quad (2.30)$$

It therefore appears that λ and μ are independent of pressure.

For liquids it can be deduced for the case of diffusion of molecules A through molecules B, that the following relation applies to the diffusion coefficient

$$ID_{AB} \approx \frac{k_B T}{6\pi \mu_B \sigma_A} \quad (2.31)$$

with k_B = Boltzmann constant, μ_B = viscosity of liquid B, and σ_A = diameter of molecule A.

The viscosity of liquids depends to a major degree on temperature. A rough approximation is given by Andrade

$$\log \mu \sim \frac{1}{T} \quad (2.32)$$

Summary

We have looked in this Section at the order of magnitude of the transport coefficients. The table in this Section gives a good overview of this. Using simple kinetic gas theory it has been found that, for ideal gases, the diffusion coefficient may be conceived as the product of a molecular velocity and a free path length. As a result of this model, the transport coefficients for ideal gases depend on temperature and pressure (density) as

⁷ The above analysis is based on the assumption that molecules are hard, inelastic spheres. A more complex analysis that takes a degree of elastic behaviour by molecules into account would lead to

$$\lambda \propto T^{0.70 \pm 0.75}, \quad \mu \propto T^{0.65 \pm 0.70}, \quad ID \propto T^{0.70 \pm 0.75}/\rho$$

These results, confirmed by experiment, apply to real gases when the pressures and temperatures are not too extremely high.

$$ID \propto \frac{\sqrt{T}}{\rho}, \quad \lambda \propto \sqrt{T}, \quad \mu \propto \sqrt{T}$$

For liquids, the transport coefficients are a function of temperature only: the diffusion coefficient is proportional to temperature while dynamic viscosity obeys to

$$\log \mu \sim \frac{1}{T}.$$

2.1.4 Shear stress: an alternative description of molecular momentum transport

In § 1.4 dealing with the momentum balance, it was stated that forces are producers of momentum. This idea can be used for developing an alternative view to molecular momentum transport. Let us again look at a control volume located in a neat, laminar (= layered) flow (see Figure 2.8)

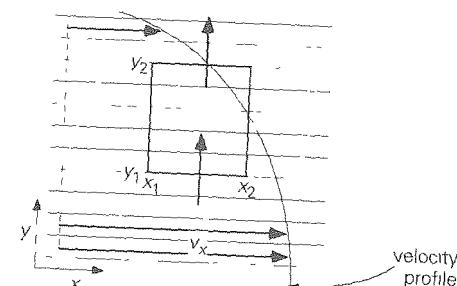


Figure 2.8

The flow is steady and is moving in the x -direction, where v_x is a function of the y -coordinate $v_x = v_x(y)$. The convective x -momentum flows through planes $x = x_1$ and $x = x_2$ are of the same magnitude (this can be easily shown with a mass balance!) and cancel each other out. Applying Newton's viscosity law to this situation implies that a molecular transport of x -momentum $\phi_{p_x, v}|_{y=y_1}$ is entering the control volume through plane $y = y_1$, due to the velocity gradient dv_x/dy in plane $y = y_1$, while similarly a transport $\phi_{p_x, v}|_{y=y_2}$ is leaving through plane $y = y_2$. Therefore, the x -momentum balance looks as follows in a steady-state situation

$$0 = \phi_{p_x, v}|_{y=y_1} - \phi_{p_x, v}|_{y=y_2} + \sum F_x \quad (2.33)$$

in which $\sum F_x$ stands for all forces acting in the x -direction, such as pressure forces driving the flow.

It is also possible, however, to look at this case from another perspective, given that adjacent layers interact due to molecular cross-overs a faster moving layer will drag a slower one, and a slower moving layer will retard a faster one. This interaction may be denoted by the terms ‘friction’, or ‘friction forces’. Such a frictional force is nothing more than a different interpretation (or model) of the net molecular momentum transport rate $\phi_{p_v,y}$. Along the plane $y = y_1$, a mutual frictional force acts between the layer directly under plane $y = y_1$ and the layer directly above it – the mutuality is because of Newton’s Third Law of Classical Mechanics (‘Action = Reaction’).

The frictional force is of course proportional to the size of the area A of the plane on which it acts. It is therefore better to look at the force per unit of area – just as the Equations (2.2), (2.3) and (2.4) relate to fluxes. Because the force acts parallel to the plane (and not normal to it), the force per unit of area is not referred to as a pressure, but as a *shear stress*, for which the symbol τ is used. In short

$$\tau_{yx} \equiv \phi_{p_v,y}'' \quad (2.34)$$

There is one very important convention associated with the term *shear stress*: the choice of the direction in which this force generally goes. The convention is

$\tau_{yx}|_{y=y_1}$ is the shear stress that acts in the x -direction in the plane $y = y_1$

and which the liquid layer with a y -coordinate of just less than y_1 exerts on the layer with a y -coordinate of just greater than y_1 .

Note that – for just the one-dimensional flows we are considering here – the first subscript of τ_{yx} refers to the direction normal to that of the flow, the second subscript relates to the x -direction in which either τ_{yx} or $-\tau_{yx}$ acts.

By definition, this shear stress appears in a force balance with a *plus* sign. Whether τ_{yx} acts in the positive or the negative x -direction, depending on the sign of τ_{yx} and – due to Newton’s viscosity law – on the sign of dv_x/dy , is not important when drawing up a force balance, but will be the result of the derivation that follows.

Therefore, for the situation considered here (Figure 2.8), it is possible to write $\tau_{yx}|_{y=y_1} A$ instead of $\phi_{p_v,y}|_{y=y_1}$. The momentum flux $\phi_{p_v,y}''|_{y=y_2}$ can also be replaced by a shear stress: the layer with $y < y_2$ exerts a shear stress $\tau_{yx}|_{y=y_2}$ on the layer just above it where $y > y_2$.

Again thanks to Newton’s Third Law, the layer just above plane $y = y_2$ exerts a shear stress $-\tau_{yx}|_{y=y_2}$ on the layer below it, which forms part of the control volume. The molecular ‘flow out’ of x -momentum $-\phi_{p_v,y}|_{y=y_2}$ in Equation (2.33) can therefore be replaced by the force $-\tau_{yx}|_{y=y_2} A$.

On the basis of the above alternative perspective (model) and the introduction of the concept of *shear stress*, the *momentum* balance of Equation (2.33) can also be written as a *force* balance.

$$0 = A\tau_{yx}|_{y=y_1} - A\tau_{yx}|_{y=y_2} + \sum \text{other forces in the } x\text{-direction} \quad (2.35)$$

Equations (2.33) and (2.35) are therefore completely identical and differ only through the model associated with them.

Equation (2.33) →

Equation (2.35) →

net molecular x -momentum transport as a result of individual molecule movements
shear stress as a result of layers exerting and feeling mutual friction

Summary

There are two ways of looking at molecular momentum transport:

1. as a kind of diffusion of momentum in terms of individual molecular motions, leading to fluxes such as $\phi_{p_v,y}''$,
2. as a frictional force per unit of area: a shear stress τ_{yx} that is exerted by two layers on each other as they move past each other at different velocities.

Due to these two interpretations, the *momentum* balance for a simple laminar flow in steady-state conditions can also be regarded as a *force* balance.

There is an important convention with regard to the signs used for the shear stress: the force exerted by the layer with the small coordinate on the layer with the large coordinate is given a ‘+’ sign in the balance.

2.2 Dimensional analysis

2.2.1 Non-dimensional numbers

After convective transport of mass, energy, and momentum were dealt with in detail in Chapter 1, molecular transport of mass, heat, and momentum were covered in

§ 2.1 In practice, many combined situations are present in fluids, in which both convective and molecular transport occur, though not necessarily in the same direction. In many cases, it is useful and usual to characterise processes or situations with the help of *non-dimensional numbers* that indicate the relationship of two such fluxes. This could concern the convective flux of a quantity (such as mass) in relation to the molecular flux of the same quantity, but also the ratio of the transport coefficients for two molecular fluxes is a commonly used non-dimensional number.

To start with the latter possibility the Equations (2.2), (2.5) and (2.6) give the molecular fluxes as a function of the gradients in the respective concentrations (providing that ρ and ρc_p are constant). The transport coefficients ID , a and v all have the same dimension (that is, m^2/s) and their values express how effectively the individual molecules of the relevant substance in the state of matter under consideration diffuse and transport heat and momentum respectively, given a certain value for the concentration gradients.

Consider the v/a ratio for an ideal gas. Thanks to the Equations (2.29) and (2.30), it is clear to see that molecules in an ideal gas transport heat as easily as they do liquid momentum $v/a = 1$. But for liquids, it appears that $v/a = 10$ to 100 . Liquid molecules obviously transport momentum more easily than they do heat. The v/a ratio is referred to as the *Prandtl* number, or *Pr* for short.

$$\text{Pr} = \frac{v}{a} \quad (2.36)$$

Similarly, the *Schmidt* (*Sc*) and *Lewis* (*Le*) numbers are defined thus

$$\text{Sc} = \frac{v}{ID} \quad (2.37)$$

and

$$\text{Le} = \frac{a}{ID} = \frac{\text{Sc}}{\text{Pr}} \quad (2.38)$$

For ideal gases, all three numbers have the value of one after all, the mobility of the molecules in an ideal gas is the limiting factor for molecular transport, rather than the effectiveness of exchange of energy or momentum between the colliding molecules. For liquids, however, *Pr* generally has values of between 10 and 100 , while *Sc* is often of the order of 10^3 .

As already discussed, however, for a certain quantity, the magnitude of the convective transport in a certain situation can be compared with its molecular transport to decide if one of the two may be ignored with respect to the other. If this occurs with a particular species in a multi-species system, the *Péclet* number is obtained

$$\text{Pe} = \frac{vL}{ID} \quad (2.39)$$

After all, when considering simultaneous convective and molecular (or diffusive) transport of a species C in the x -direction, the convective transport is equal to $A v c$ (in which v is the velocity, A is the cross-sectional area of the flow channel, and c is the concentration of C), while the molecular transport of C is given by $-A ID dc/dx$

$$\text{Pe} = \frac{\text{convective transport}}{\text{diffusive transport}} = \frac{Av c}{-A ID \frac{dc}{dx}} \quad (2.40)$$

If the concentration gradient (including the minus sign) may be approximated by c/L – where in the situation of interest L is the typical length scale or dimension over which the concentration varies see Equation (2.16) for example – Expression (2.39) is obtained

Example 2.3. Purging

A liquid containing a dissolved aggressive species B (concentration c_{B0}) is flowing through a tube. However, the pressure sensor that is being used to measure the pressure, is affected by corrosion due to contact with species B unless the concentration c_B is less than $c_{B0}/1000$. This can be resolved by mounting the sensor not in the wall of the (main) tube, but in a small branch away from the main tube (see Figure 2.9).

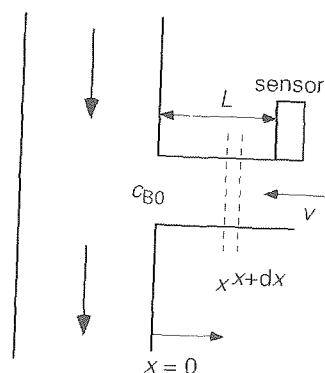


Figure 2.9

Nonetheless, B may still reach the sensor as a result of diffusion. By creating a low liquid flow (with velocity v) through the branch towards the main tube – this method is known as purging – it is possible to keep the concentration of B low and to limit the corrosion. The distance between the sensor and the junction of the branch and the main tube is denoted by L .

The question is this: how great must v be in order for $c_B(L) < c_{B0}/1000$?

The method that always works is that of the recipe from Chapter 1 draw up a mass balance for species B! In this case this should again be a micro balance, e.g. over a thin slice dx somewhere between $x = 0$ and $x = L$ – on the analogy of the plug flow reactor of § 1.2.2 – as we are interested in the decay of the concentration along the branch. From such a micro mass balance it then can be derived how c_B depends on x – from which it can be determined how great the distance L must be chosen to the effect that $c_B(L) < c_{B0}/1000$

Such a micro balance for a steady-state situation contains four terms a convective and a diffusive term at x and a convective and a diffusive term at $x + dx$, where it should be realised that the velocity v is in the negative x -direction

$$0 = -v A c_B \Big|_x - A ID \frac{dc_B}{dx} \Big|_x + \\ - \left\{ -v A c_B \Big|_{x+dx} \right\} - \left\{ -A ID \frac{dc_B}{dx} \Big|_{x+dx} \right\} \quad (2.41)$$

from which the second order differential equation

$$0 = v \frac{dc_B}{dx} + ID \frac{d^2 c_B}{dx^2} \quad (2.42)$$

follows. Integrating this equation once gives

$$v c_B + ID \frac{dc_B}{dx} = K_1 \quad (2.43)$$

The integration constant K_1 follows from the (boundary) condition that in the steady-state situation no net transport of B occurs over a randomly selected plane x between $x = 0$ and $x = L$

$$-A ID \frac{dc_B}{dx} + A (-v) c_B = 0 \quad (2.44)$$

After all, in this case it is also possible to immediately start with Equation (2.44), irrespective of drawing up a micro balance over a thin slice dx . As a matter of fact, Equation (2.44) expresses that in any plane, at position x , the diffusive transport to the right (the first term of the left-hand side) compensates the convective transport to the left (the second term of the left-hand side, the minus sign preceding v indicating the direction). The method of drawing up a balance for a thin slice dx , however, is the recommended procedure it always works.

The solution to the differential Equation (2.44) is obtained via the method of separation of variables, with the boundary condition $x = 0 \rightarrow c_B = c_{B0}$

$$\frac{c_B(x)}{c_{B0}} = \exp \left(-\frac{vx}{ID} \right) \quad (2.45)$$

The requirement for v therefore amounts to $v > (ID/L) \ln 1000$. In the event that $L = 10$ cm and $ID = 10^{-6}$ m²/s, this requirement is $v > 7 \cdot 10^{-5}$ m/s!

For $x = L$, Equation (2.45) can also be written in terms of the non-dimensional Péclet number $\text{Pe} \equiv vL/ID$

$$\frac{c_B(L)}{c_{B0}} = \exp(-\text{Pe}) \quad (2.46)$$

This is a good illustration of the fact that non-dimensional numbers are not just a conceptual nicety, but in many cases follow directly from an exact analysis (based on a balance!).

Summary

Various non-dimensional numbers have been introduced which all represent the ratio of two transport properties. The Prandtl ($\text{Pr} = \nu/\alpha$), Schmidt ($\text{Sc} = \nu/ID$) and Lewis ($\text{Le} = \alpha/ID$) numbers, for example, represent the ratio of two molecular transport coefficients

Another non-dimensional number introduced is the Péclet ($\text{Pe} = vL/ID$) number which shows how, in a certain situation, convective and molecular fluxes of a particular species relate to each other. These non-dimensional numbers very often show up when – starting from some macro or micro balance – a transport problem is solved.

2.2.2 The Reynolds number and the transition from laminar to turbulent flow

A similar thing as in § 2.2.1 for mass transport applies to the convective and molecular transport of momentum. We previously discussed the laminar flow $v_x(y)$ the flow runs in orderly, parallel (or in a cylindrical tube, coaxial) layers. For this situation and in the case of Newtonian fluids it is easy to estimate what the relationship is between convective x -momentum transport in the x -direction and molecular x -momentum transport in the y -direction

$$\text{molecular } \phi''_{p_x,y} = -\mu \frac{dv_x}{dy} \approx \mu \frac{v_x}{D} \quad (2.47)$$

$$\text{convective } \phi''_{p_x,x} = v_x \rho v_x \quad (2.48)$$

In the case of the molecular transport estimate in Equation (2.47), a typical dimension D has been introduced for the flow. This means that the gradient $d\nu_x/dy$ can be replaced (or estimated) by ν_x/D – in fact, the choice of D should be such that the estimate of the gradient is reasonable. The ratio of the convective momentum flux and the molecular momentum flux is known as the *Reynolds number* (Re)

$$\text{Re} = \frac{\text{convective transport}}{\text{molecular transport}} = \frac{\nu_x \rho v_x}{\mu \nu_x / D} = \frac{\rho v_x D}{\mu} \quad (2.49)$$

The subscript x is generally omitted from this definition of Re. Note that the concept and the definition of Re apply to both liquids and gases, *i.e.* to any fluid.

The momentum flux $\nu \rho v$ in the numerator of the Reynolds number is often denoted by the term *inertia* – the property whereby a fluid keeps moving straight ahead in the event of no force being exerted on it (see also the discussion on momentum and forces in § 1.4). The denominator of Re can be regarded as shear stress, that is, as friction or deceleration. This gives us

$$\text{Re} \approx \frac{\text{inertia}}{\text{friction}}$$

The Reynolds number can also be interpreted in terms of forces. The numerator $\nu \rho v$ can be read as ρv^2 – a quantity that – apart from a factor of $\frac{1}{2}$ – we already have encountered in the context of the Bernoulli equation (see § 1.3.4) as pressure energy and as *dynamic pressure*. In this perspective, Re may be conceived as the ratio of dynamic pressure and shear stress.

Note that in this typical example, the convective x -momentum transport and the molecular x -momentum transport occur in different directions. In other words, it concerns two competing transport mechanisms: convective transport thanks to – usually – a difference in pressure, and molecular (or diffusive) transport thanks to viscosity. The molecular transport mechanism aims to re-distribute the momentum as evenly as possible over the field of flow; after all, the molecules try and transport momentum from locations with a high momentum concentration (or velocity) to locations with a lower momentum concentration, even in a direction that is normal to the direction of the flow (the convective transport). This is of no interest to the inertia of the fluid: it wishes only to move straight ahead. The Reynolds number therefore characterizes a flow: it is a measure for how great the differences in velocity still can be in a direction normal to the convective momentum transport.

If Re is sufficiently small (that is, below a certain critical value), then the flow is *laminar*, as presupposed in the above example. The momentum concentration in a fluid element in some of the layers is in that case not so great that the shear stress is incapable of keeping this element or layer in check: the velocities are only relatively

low. However, if the Re number becomes too great, this will no longer be so. It will no longer be possible for the neat layered structure to be maintained. The differences in momentum concentration of adjacent fluid layers may then become so great that the molecules can no longer handle them – or, in other words: the shear stresses become too large. The result is that the fluid layers stumble over each other, as it were. The flow now turns *turbulent*. All kinds of *eddies* are then formed in the flow, and thanks to these eddies the momentum is distributed very effectively across the flow field.

These eddies derive their energy from the main flow and in turn pass it on to smaller eddies. In a completely developed turbulent flow, the kinetic energy in the eddies is passed on to ever-smaller eddies without any notable dissipation. After all, the viscosity (\rightarrow friction) is far too weak to resist the eddies. It is only with eddies with very small dimensions that the Reynolds number on the scale of such an eddy is low enough for the viscosity to be capable of exercising its dissipating effect. Ultimately, therefore, the mechanical energy is dissipated by friction in heat. To the human eye and mind, the dynamics of turbulent flow appears to be stochastic, but in reality it is chaotic. After all, the interactions between the fluid elements or packages are still governed by the laws of physics, but the effects of these laws in turbulent flows are many times more complex than in the case of laminar flow.

Flow through a cylindrical tube is *laminar* as long as the Reynolds number relating to the tube diameter D is less than around 2000. The transition to turbulent flow occurs when Re is somewhere between 2000 and 2500, depending on exactly how the experiment is carried out (the transition to turbulent is very sensitive to small disruptions, such as vibrations from pumps; these enhance the instability of the laminar flow). In other geometries, such as right-angled ventilation channels, and for the flow around immersed bodies, other critical values of the Reynolds number apply to the laminar-turbulent transition point.

Summary

The Reynolds number

$$\text{Re} = \frac{\rho v D}{\mu}$$

represents in a certain situation the ratio of a convective momentum flux (inertia) to a molecular momentum flux (friction) – in different directions, incidentally. This is most clear when Re is written as

$$\text{Re} = \frac{v \cdot \rho v}{\mu v / D}$$

Thus, the Reynolds number characterizes the state of the flow. Various interpretations of the Reynolds number have been discussed.

Whenever viscosity (or friction) is no longer capable of suppressing flow disturbances or instabilities, the flow sooner or later turns turbulent. Whether a flow is laminar or turbulent can be deduced from the value of the Reynolds number. The critical value of Re beyond which the flow is or becomes turbulent, varies from geometry to geometry, for a cylindrical pipe, the critical value is in the $2000 - 2500$ range.

2.2.3 Dimensional analysis: the concept

Several non-dimensional numbers have been introduced above, in which transport terms are compared with each other. The numerator and denominator of these non-dimensional numbers must of course have the same dimension in order for their ratio to be non-dimensional. It is in fact no different to the various terms in the balances in Chapter 1: every term in a balance has to have the same dimension (hint: this makes it an excellent checking mechanism⁸)

However, there is another way of using *dimensions*. It is possible to determine beforehand how the various quantities and physical properties that govern a process can be merged into a smaller number of non-dimensional groups. In the final solution to the problem under review, it will only be these groups that occur as variables. In general, this will mean far fewer variables than there were at the beginning. The technique for achieving this is known as *dimensional analysis*. How the technique works and the dangers that lurk in the technique of dimensional analysis will be covered in detail below⁸.

The problem in Example 2.3 can also be dealt with using dimensional analysis. The starting point of every dimensional analysis is the difficult question: what does $c_B(L)$ actually depend on?

As seen in Example 2.3, the answer is that it depends on c_{B0} , L , v and ID

$$c_B(L) = f(c_{B0}, L, v, ID) \quad (2.50)$$

The dimensional analysis technique works as follows: write the relationship between the dependent variable $c_B(L)$ and the independent variables c_{B0} , L , v and ID with the help of unknown exponents α , β , γ , δ and a non-dimensional constant k as

$$c_B(L) = k c_{B0}^\alpha L^\beta v^\gamma ID^\delta \quad (2.51)$$

Make sure that the right-hand side of Equation (2.51) only contains independent variables that you are able to choose separately from each other. This equation has to be in order dimensionally: the dimensions on the right-hand side must be equal to those on the left-hand side. This regulates the powers α , β , γ , δ . The SI units (or dimensions) of the five variables c_B , c_{B0} , L , v and ID are known of course, although the variables have to be expressed in their basic units of kg, m, s, K. In this case

c_B, c_{B0}	kg m^{-3}
L	m
v	m s^{-1}
ID	$\text{m}^2 \text{s}^{-1}$

Filling in the units into Equation (2.48) means the various basic units are as follows:

$$\begin{aligned} \text{kg} &= 1 = \alpha \\ \text{m} &= -3 = -3\alpha + \beta + \gamma + 2\delta \\ \text{s} &= 0 = -\gamma - \delta \end{aligned}$$

(remember that constant k is non-dimensional). This is a system of three equations with four unknowns. Three of the four unknowns in this system can be expressed in the fourth, for example

$$\alpha = 1, \delta = -\gamma, \beta = \gamma$$

With this result, Equation (2.51) is reduced to

$$c_B(L) = k c_{B0} \left(\frac{vL}{ID} \right)^\gamma \quad (2.52)$$

The first conclusion that can be drawn from Equation (2.52) is that the non-dimensional concentration $c_B(L)/c_{B0}$ is only a function of the non-dimensional group vL/ID which is recognized as the Peclet number Pe , known from Example 2.3. Formulated mathematically

$$\frac{c_B(L)}{c_{B0}} = f(Pe) \quad (2.53)$$

It is not possible to say anything about function f on the basis of this dimensional analysis. For that, it is necessary to find an exact solution to the problem. In this case, it is known from Example 2.3 that f is an exponential function.

In general, it is not the case that $c_B(L)$ can be calculated on the basis of Equation (2.52) with values for k and γ which apply to the entire domain of the Pe number. In practice, k and γ can be determined empirically for a limited Pe range only. In the case of Example 2.3, this amounts to determining a tangent on the curve of Equation

⁸ We prefer the 'exponent method' over the method of 'repeating variables'.

(2.46) for a certain value of Pe viewed this way, it is clear that k and γ are not constant in the entire domain of possible values for Pe

Nonetheless, a very useful conclusion can be drawn from Equation (2.52), that is, on the basis of the dimensional analysis as long as the number is constant, the non-dimensional concentration does not change. Even if a problem cannot be solved analytically and experiments are not possible (too dangerous, too costly, installation not yet built), it is possible with the help of experiments in a small-scale model, for example, to make a forecast about the process or phenomenon on a large scale, namely by letting the dominant non-dimensional number be of equal value in both situations.

With a view to experimenting at a different scale or under different conditions there is another application e.g., in the ‘purging’ case of Example 2.3 it is possible to replace the aggressive species B with a harmless species, X. Suppose then that the diffusion coefficient of X is eight times greater than that of B $ID_X = 8 ID_B$. And that in the case of substance X experimentally it is found that the velocity needed to get $c_X(L) = c_{X0}/1000$ is $v_X = 4 \cdot 10^{-4} \text{ m/s}$. The result of the dimensional analysis can then be used to determine what v_B should be in order to ensure that $c_B(L) = c_{B0}/1000$. This is because the following applies

$$\frac{c_X(L)}{c_{X0}} = f(\text{Pe}) \quad \text{and} \quad \frac{c_B(L)}{c_{B0}} = f(\text{Pe}) \quad (2.54)$$

In both cases, the function f is the same, and as here, too

$$\frac{c_X(L)}{c_{X0}} = \frac{c_B(L)}{c_{B0}} \quad (2.55)$$

should therefore be

$$f(\text{Pe}_X) = f(\text{Pe}_B) \rightarrow \text{Pe}_X = \text{Pe}_B \quad (2.56)$$

or, put another way

$$\frac{v_X L}{ID_X} = \frac{v_B L}{ID_B} \rightarrow v_B = \frac{ID_B}{ID_X} v_X = 5 \cdot 10^{-5} \text{ m/s} \quad (2.57)$$

Summary

Dimensional analysis is a technique for finding relations between the various quantities and physical properties that determine a problem, without having to solve the problem exactly, or analytically. However, the knowledge that is acquired is relatively approximate. A dimensional analysis condenses the variables into non-

dimensional groups that usually represent the ratio between two mechanisms, fluxes, or physical properties.

With the help of dimensional analysis, it is possible to compare different problems that relate to similar situations. In such situations, the non-dimensional groups should be kept constant. The rationale behind this approach is that the exact solution includes only the non-dimensional numbers that are found.

2.2.4 Dimensional analysis: technique and the Buckingham-Π theorem

For carrying out a dimensional analysis, some understanding of the problem under consideration is very important. This does not necessarily mean that already from the very beginning it should be understood *how* quantity A depends on a number of other quantities. Rather, the starting point is an analysis of *which independent variables* quantity A may depend on. This requires some physical insight as to causal relations between quantities.

As an example, physical insight regarding the mobility of molecules in an ideal gas – as embodied in the model leading to Equation (2.28) – tells us that in ideal gases the diffusion coefficient ID depends among other things on temperature and density which can be varied independently of each other. Indeed $ID = f(T, \rho)$. Pressure should not be added here, as – due to the ideal gas law – pressure, density and temperature are mutually dependent; the variables at the right-hand side should be independent of each other. In addition, it can be said *a priori* that in a dimensional analysis $ID = f(T, \rho)$ or, alternatively, $ID = f(T, p)$ will never lead to a decent result, as unlike ID both $f(T, \rho)$ and $f(T, p)$ contain the basic units K and kg. The gas constant R and the molar mass M of the species considered should be incorporated!

Further remarks and suggestions with respect to the selection of independent variables will be made in the context of the examples of § 2.2.5.

The general recipe for carrying out a dimensional analysis is as follows:

1. Select the quantity that is to be examined A .
2. Determine the independent physical variables B_1, B_{n-1} that determine A according to $A = f(B_1, \dots, B_{n-1})$. In total, there will now be n variables involved A, B_1, \dots, B_{n-1} .
3. Write the relation in the following form

$$A = k B_1^{\beta_1} B_2^{\beta_2} \dots B_{n-1}^{\beta_{n-1}} \quad (2.58)$$

where $\beta_1, \dots, \beta_{n-1}$ are unknown exponents (real numbers, not necessarily integers) and k a non-dimensional coefficient.

- 4 Express in both the left-hand side of the latter relation and the right-hand side all dimensions in the basic dimensions, or all (SI) units in the basic units. The basic dimensions (with their SI unit in brackets) are length (m), mass (kg), time (s) and temperature (K). As an example for energy $\rightarrow J = N \cdot m = kg \cdot m^2 \cdot s^{-2}$. In the remainder of this textbook we will work in SI units.
- 5 Make sure that this equation is dimensionally sound, which means that left and right in relation (2.58) the basic units should occur just as often. You do this by counting the basic units left and right and by then writing down with the help of the coefficients $\beta_1 \dots \beta_{n-1}$ for each basic unit an algebraic equation such that left and right this basic unit occurs just as often.
- 6 Solve the algebraic equations for $\beta_1 \dots \beta_{n-1}$ from stage 5. Whenever the number of unknowns $\beta_1 \dots \beta_{n-1}$ is greater than the number of algebraic equations (given the number of basic units), express then one or more of these β 's in terms of the other ones (just as in the *purging* example).
- 7 Substitute the values found in stage 6 into Equation (2.58), and combine $A, B_1 \dots B_{n-1}$ to non-dimensional groups or numbers.
- 8 It is usual to work towards the commonly known non-dimensional numbers, such as Pr, Sc, Le, Pe, and Re which were introduced earlier in this Chapter. This may be done by mutually multiplying or dividing the non-dimensional numbers found in stage 7. When transport terms such as fluxes and physical properties which occur in these common non-dimensional numbers, play a role with respect to a quantity A , these common non-dimensional numbers appear virtually automatically.

The number of non-dimensional groups that is found depends, among other things, on the number of independent variables that are considered. As to their number, it is hard to present a guideline, there should in any case be a sufficient number. The analysis at the start as to which independent variables B may play a role, is of crucial importance. As said, in the examples of § 2.2.5 ample attention will be paid to this issue.

There is a general rule, the *Buckingham II theorem*, that can be used to calculate in advance the number of non-dimensional groups (p) from the total number of variables (n) and the number of basic units (m) involved:

$$p = n - m \quad (2.59)$$

The number of non-dimensional (p) that is found therefore directly depends on the number of independent variables ($n-1$). This once more illustrates how important it is to identify the proper independent variables at the start of the analysis.

The proof of Equation (2.59) is simple, and is as follows. Equation (2.58) contains n variables (or parameters) $\{A, B_1, \dots, B_{n-1}\}$ and $n-1$ unknown powers $\{\beta_1, \dots, \beta_{n-1}\}$.

The number of different basic units that occur is m . In general, there are then m linear equations for $n-1$ unknown powers. This means that there must be $\{(n-1)-m\}$ unnamed powers and that m powers can be expressed in these 'unnamed powers'. If we now suppose that exactly every power $\{\beta_1, \dots, \beta_{n-1}\}$ can be calculated, then there would be precisely one non-dimensional group. Therefore, $\{(n-1)-m\}$ unnamed powers produce

$$p = 1 + \{(n-1)-m\} = n-m \quad (2.60)$$

non-dimensional groups

The Buckingham II theorem is a useful tool for quickly seeing how many non-dimensional groups a particular combination of variables will produce. Additionally, it is possible to make a quick check – after carrying out the dimensional analysis – whether the number of groups are in keeping with the theorem.

Example 2.4. Purging II

In Example 2.3, it was found that

$$c_B(L) = f(c_{B0}, L, v, ID) \quad (2.61)$$

So, there are 5 quantities, 3 basic units \rightarrow 2 non-dimensional groups according to the Buckingham II theorem. This is in line with the result of the above dimensional analysis. \square

Summary

An eight-stage recipe has been given for performing a dimensional analysis in which it is very important to carefully select the independent variables at the start of the analysis. A sound physical understanding of the problem is then very helpful. It is recommended to arrive at the commonly known non-dimensional numbers as much as possible.

The Buckingham II theorem is: the number of non-dimensional groups or numbers (p) that follows from a dimensional analysis with n parameters and m basic units is:

$$p = n - m$$

An important advantage of dimensional analysis is that for the problem at hand the number of variables is strongly reduced, *viz* from n to p .

2.2.5 Examples of dimensional analysis

Example 2.5. Pulling a wire

A smooth wire (diameter d) is pulled through a tank that is filled with a liquid. The wire is wetted over a length L . Consider the force F needed to pull the wire at a constant velocity v through the liquid.

Which variables does force F depend on? Using which non-dimensional groups can this process be described?

The answer to the first question is the diameter d and length L of the wire, the velocity v , and the density ρ and viscosity μ of the liquid. The reasoning behind this is that as a result of the movement of the wire ($\rightarrow v$) the liquid will also flow. In other words, the liquid will gain momentum, which is related to ρ . Finally, the transfer of momentum has to do with the frictional force ($\rightarrow \mu$) between the surface of the wire ($\rightarrow d$ and L) and the adjacent liquid. The effect of temperature on density and viscosity may be ignored as being a secondary effect, in addition, the condition that the variables have to be mutually independent, excludes this dependence being taken into account. As long as the velocity of the wire is constant, the density of the material of the wire is irrelevant.

The answer to the second question can be found with the help of dimensional analysis. We will use the aforementioned recipe.

1) quantity force $F \rightarrow \text{kg m/s}^2$

2) physical variables $d, L \rightarrow \text{m}$
 $v \rightarrow \text{m/s}$
 $\rho \rightarrow \text{kg/m}^3$
 $\mu \rightarrow \text{kg/m s}$

3) the relation $F = k d^\alpha L^\beta v^\gamma \rho^\delta \mu^\varepsilon$

4) in basic units $\frac{\text{kg m}}{\text{s}^2} = \text{m}^\alpha \text{m}^\beta \left(\frac{\text{m}}{\text{s}}\right)^\gamma \left(\frac{\text{kg}}{\text{m}^3}\right)^\delta \left(\frac{\text{kg}}{\text{m s}}\right)^\varepsilon$

5) for the various basic units, it follows that

$$\begin{aligned} \text{kg} &= \delta + \varepsilon \\ \text{m} &= \alpha + \beta + \gamma - 3\delta - \varepsilon \\ \text{s} &= -2 - \gamma - \varepsilon \end{aligned}$$

6) These are three equations with five unknowns. Of these, two can be 'chosen at will' in order that they can be used to express the other three. The choice of these two 'free options' is determined by two considerations. The first of these is this: in the three equations, is it possible to see what a sensible choice would

be? If so, make that choice. If not, ask the question of whether it is possible to predict which groups will occur on the basis of the stages 2 and 3 of the recipe, and base your choice on this (a matter of experience).

In this example, at stage 2, the variables d and L can be seen which together form a non-dimensional group, so don't choose β and α together as this would result in a conflict, but just β , for instance. Stage 2 also includes the variables ρ, v, d (or L) and μ , which together form a Reynolds number. Choose ε in this case, for example. Solving the equation now produces

$$\delta = 1 - \varepsilon$$

$$\gamma = 2 - \varepsilon$$

$$\alpha = 2 - \beta - \varepsilon$$

7) Substituting the above values for α, γ and δ into the equation of stage 3 gives

$$F = k d^{2-\beta-\varepsilon} \rho^\beta v^{2-\varepsilon} \rho^{1-\varepsilon} \mu^\varepsilon$$

Combining now produces the non-dimensional groups

$$\frac{F}{\rho^2 v^2 d^2} = k \left(\frac{L}{d}\right)^\beta \text{Re}^{-\varepsilon} \quad (2.62)$$

8) Incidentally, if β and δ were to be chosen at stage 6 rather than β and ε , then the following would have resulted, instead of Equation (2.62)

$$\frac{F}{d v \mu} = k \left(\frac{L}{d}\right)^\beta \text{Re}^\delta \quad (2.63)$$

This result is also correct and can be derived from Equation (2.62) by multiplying left and right by Re , clearly, $\delta = 1 - \varepsilon$.

This is generally applicable with dimensional analysis: the groups that are found can be multiplied with each other in order to make a new group, and one of the old groups may be replaced by the new one. Of course, the non-dimensional groups describing the process or phenomenon should be mutually independent, just like the dimensional variables of step 2 (see also § 2.2.4). \square

Dimensional analysis is a very powerful technique for reducing the number of variables used for describing a problem. However, dimensional analysis is not without danger: the selection of independent variables in stage 2 of the recipe determines the outcome. The selected variables must actually completely cover the

relevant physical processes – otherwise, dimensional analysis may result in senseless, non-physical results. If, for instance, heat transfer is to be analysed, then in stage 2 the temperature difference driving the heat transfer should be taken as a variable rather than the two individual temperatures, in the latter case, one would arrive at the ratio of these temperatures (in K, or in °C?) but such a ratio does not govern heat transport (see further Chapter 3). Now, the need of selecting a proper set of variables will be demonstrated in the next example.

Example 2.6. A stirred tank

A polymerisation reaction occurs in a stirred tank, during which the liquid viscosity μ increases. The impeller is linked to an engine, which ensures the impeller rotates at a constant number of impeller revolutions per unit of time, N . How does the power P , which the engine supplies to the stirrer, depend on N and μ and other relevant variables?

First attempt

Suppose that P is only dependent on μ and N

$$P = k N^\alpha \mu^\beta$$

so that the basic units involved should obey to

$$\frac{\text{kg m}^2}{\text{s}^3} = \left(\frac{1}{\text{s}}\right)^\alpha \left(\frac{\text{kg}}{\text{m s}}\right)^\beta$$

The equations as to the individual basic units run as

$$\begin{aligned} \text{kg} & 1 = \beta \\ \text{m} & 2 = -\beta \\ \text{s} & -3 = -\alpha - \beta \end{aligned}$$

The first and second equations *conflict!* This attempt, therefore, is, erroneous there are not enough physics in the equation for P , which anyhow should also be scale sensitive.

Second attempt

P depends on μ , N , and the diameter of the stirrer, D

$$P = k N^\alpha \mu^\beta D^\gamma$$

so that

$$\frac{\text{kg m}^2}{\text{s}^3} = \left(\frac{1}{\text{s}}\right)^\alpha \left(\frac{\text{kg}}{\text{m s}}\right)^\beta \text{m}^\gamma$$

Then, the equations are

$$\left. \begin{aligned} \text{kg} & 1 = \beta \\ \text{m} & 2 = -\beta + \gamma \\ \text{s} & -3 = -\alpha - \beta \end{aligned} \right\} \rightarrow \alpha = 2, \beta = 1, \gamma = 3$$

Therefore, $P = f(N, \mu, D)$ leads to a single non-dimensional group which is a constant

$$\frac{P}{N^2 \mu D^3} = \text{constant} \quad (2.64)$$

In the example, therefore, when $N = \text{constant}$ and $D = \text{constant}$ $P \propto \mu$

Third attempt

N , μ and D were chosen in the second attempt, and by combining ND , so was implicitly a velocity. These are three of the four variables that determine the Re. For that reason, let us also include ρ . It is likely to be of importance as far as the power is concerned whether the liquid being stirred is ‘light’ or ‘heavy’. Try

$$P = k N^\alpha \mu^\beta D^\gamma \rho^\delta$$

Equations

$$\begin{aligned} \text{kg} & 1 = \beta + \delta \\ \text{m} & 2 = -\beta + \gamma - 3\delta \\ \text{s} & -3 = -\alpha - \beta \end{aligned}$$

This gives

$$\begin{aligned} \alpha &= 3 - \beta \\ \gamma &= 5 - 2\beta \\ \delta &= 1 - \beta \end{aligned}$$

It therefore follows that

$$P = k \rho N^3 D^5 \left(\frac{\rho ND^2}{\mu} \right)^{-\beta} \quad (2.65)$$

The latter group is the predicted Reynolds number. The velocity at the edge or at the tip of the stirrer can be taken as the typical velocity, to which $v = \pi D N$ applies in any case. It therefore follows that

$$\rho \frac{ND^2}{\mu} = \frac{1}{\pi} \rho \frac{(\pi ND)D}{\mu} \propto \frac{\rho v D}{\mu} = \text{Re} \quad (2.66)$$

In a dimensional analysis, the factor $\frac{1}{\pi}$ is of no importance. With the help of the

non-dimensional group $Po = P/(\rho N^3 D^5)$ – which is known as the *Power number* – Equation (2 65) can therefore be written in non-dimensional form as

$$Po \equiv \frac{P}{\rho N^3 D^5} = k \left(\frac{\rho N D^2}{\mu} \right)^{-\beta} = k Re^{-\beta} \quad (2 67)$$

Notice that for $\beta = 1$, density drops out of Equation (2 67) and the result obtained is the same as that of attempt 2, where no effect of the density and therefore of inertia was included. In the $\beta = 1$ regime, the viscous effects, which are in the denominator of the Reynolds number, evidently predominate over the inertia forces which are in the numerator of the Reynolds number see Equation (2 49). Clearly, $\beta = 1$ is associated with low Reynolds number values which correspond with the laminar flow regime. For $\beta = 0$, the viscosity drops from Equation (2 64), $\beta = 0$ is therefore associated with turbulent flow conditions where viscosity does not play a role (at the macro-scale). Experimentally, the diagram in Figure 2 10 has indeed been found

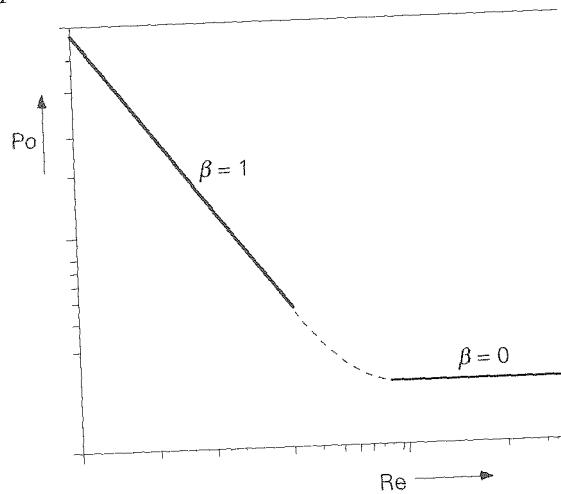


Figure 2 10

Fourth attempt

$P = f(N, \mu, \rho)$ the length scale has been omitted from the problem. This produces

$$P \propto \left(\frac{N \mu^5}{\rho^3} \right)^{1/2} \quad (2 68)$$

It will be clear that this result does not tally with the experiments. The reason for this is that the physics of the problem *can* not be properly described through proposition $P = f(N, \mu, \rho)$ according to this description, it does not matter as

far as the power is concerned whether the tank in question is large or small, while the density cannot occur in the denominator either, from a physics point of view!

Next, an examination could be carried out into how the power of the engine depends on the geometry of the stirrer (such as the height and thickness of the stirring blade, or the degree of curvature of the stirring blade) and the position of the stirrer in the container. According to the Buckingham II theorem, the addition of a variable keeps resulting in a new non-dimensional number – in geometric numbers in this case. Figure 2 11 shows how the power number of so-called turbine stirrers also depends on the size of the disk and on the ratio of the height, w , of the vertical or tilted impeller blades mounted onto the disk, and the impeller diameter

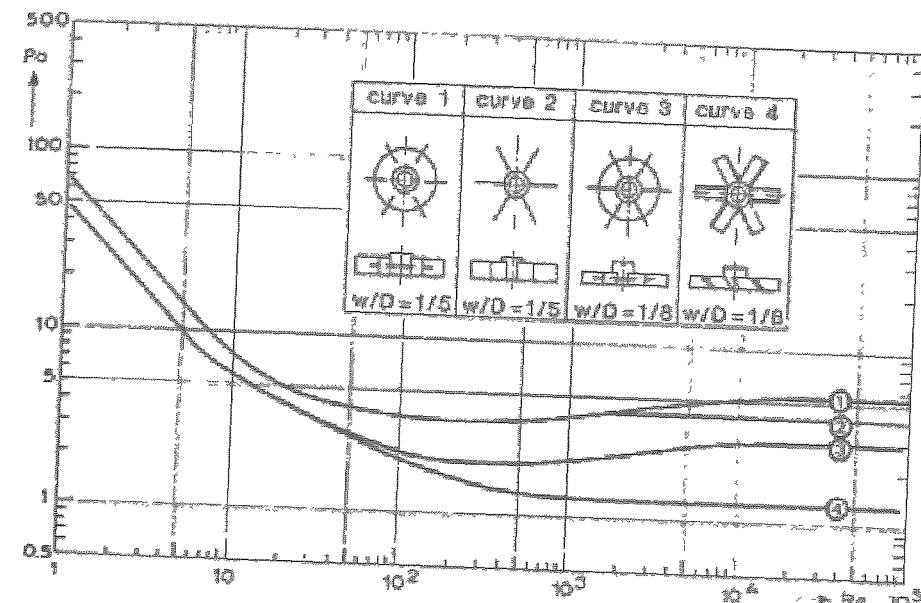


Figure 2 11

The above example shows that incorporating both μ and ρ as independent variables results in finding the Reynolds number. If from the outset it is clear, however, that under the conditions of interest the flow is laminar, i.e. viscosity dominated, then ρ can be ignored in the analysis (providing gravity can be ignored as well) and Re will not show up. Similarly, if from the outset it is clear that in a specific case the flow is turbulent, or inertia dominated, viscosity can be ignored and Re will not show up either. Just in the general case, with no *a priori* information about the type of flow, the Reynolds number will be one of the non-dimensional numbers found, indicating the variable of interest may be (very) different in laminar and turbulent flows. This

observation not only applies to stirred vessels, but to any case where convection plays a role

In vertical laminar flows, gravity may play a dominant role as the force driving the flow. In such cases, ρ might be better combined with the gravitational acceleration g to the new variable $\gamma = \rho g$ (in $\text{kg/m}^2\text{s}^2$) – to restrict the number of variables and the number of non-dimensional numbers, and to prevent Re from appearing

Example 2.7. Slot coating⁹

Figure 2.12 shows a cross-sectional view through the die of a specific coating machine. The very viscous Newtonian liquid (usually a polymer) is supplied via the vertical channel and is then entrained by the lower plate or belt (web) that moves to the right with velocity U . The result is that the web gets a coating of thickness δ_∞ which is smaller than the gap height δ .

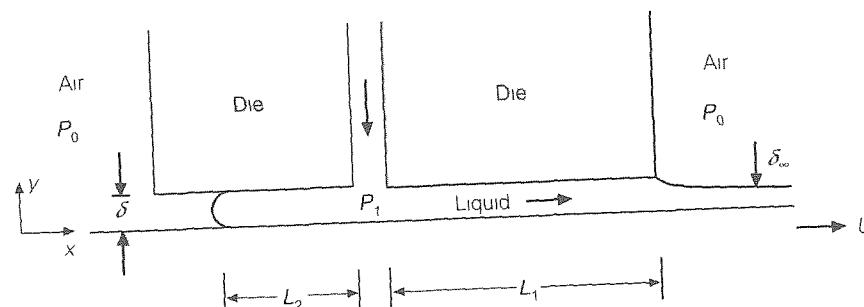


Figure 2.12

Consider a steady-state one-dimensional flow in the horizontal x -direction. As pressure P_1 is higher than the atmospheric ambient pressure P_0 , the viscous liquid will not only flow to the right – in the same positive x -direction as the web is dragging it – but also to the left – in the ‘wrong’ negative x -direction opposing the drag exerted by the web in the positive x -direction. The question is to find out by a dimensional analysis how in a steady-state operation the distance L_2 to which the liquid is capable of reaching to the left, depends on, among other things, the web velocity U .

In a dimensional analysis, an inventory has to be made of all, or at least several, highly relevant independent variables that have an effect on the variable of interest, in this case L_2 . The most relevant parameters are

- the web velocity U ,
- the pressure difference $\Delta P = P_1 - P_0$ rather than the individual pressures P_1 and P_0 see the remark in the paragraph preceding Example 2.6,

⁹ This problem has been derived from a problem in W H Deen, *Analysis of Transport Phenomena*, Oxford University Press, 2nd Ed., 2011

- the channel height δ a larger δ would leave more room for the flow in the ‘wrong’ direction, and
- the viscosity of the liquid not only because the overall flow is viscous, but also owing to the viscous drag or shear stress exerted on the liquid by the moving web

These four independent variables together determine L_2 . That makes five variables in total, leading (according to Buckingham’s theorem) to 2 non-dimensional numbers (given the three basic units involved)

Following the recipe of the dimensional analysis may result in the finding that the ratio L_2/δ depends on the non-dimensional group $\delta \Delta P / \mu U$ that stands for the ratio of ΔP to $\mu U / \delta$, where the latter – given Newton’s viscosity law – is a measure of the viscous drag force (per unit of area), or the shear stress exerted by the moving web on the viscous liquid. Of course, L_2 increases with increasing ΔP and h , and decreases with increasing μ and U .

This example will be revisited in Chapter 5 to derive an analytical expression for L_2 which is fully in line with the above result of the dimensional analysis. Note that the fluid density does not play a role in this coating process – as the flow is viscous.

□

Conclusion

A significant difficulty when applying dimensional analysis is that there is almost always something that emerges from the analysis, regardless of the choice of parameters. However, making the wrong choice of independent variables that ‘stretch’ the problem will result in failure: anyone putting insufficient physics into the analysis phase or not inserting enough common sense into the analysis will eventually find themselves in conflict with the laws of physics. Great care should therefore be taken when selecting quantities and physical properties.

The conclusion, then, is this dimensional analysis is very useful, but needs careful consideration.

2.3 Flow around immersed objects and net forces

2.3.1 Flow field and flow resistance

Any object that moves through a liquid or a gas experiences – and exerts – a force the fluid tries to resist the motion of the object, and conversely the object tries to entrain fluid. Mutatis mutandis this is also the case if the object is at a fixed position and the fluid flows around it. The ‘relative motion’ of the immersed object with

respect to the fluid is what matters and evokes a particular flow field and a related pressure field around the immersed object

The analysis will remain restricted to rectilinear (relative) motions of (more or less) spherical and cylindrical particles through fluids which overall either are stagnant or move at a uniform velocity. The focus is on the interaction force, or *drag force*, in the same, and just the opposite, direction as the particle or the fluid moves. Only steady-state situations will be considered here – that is, particle velocity and/or background velocity of the fluid being taken constant. Lateral forces, such as the lift force on an airplane wing or on a red blood cell in the laminar flow in a vein, as well as particle rotations are left out of consideration.

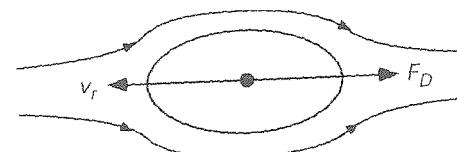


Figure 2.13

With the help of dimensional analysis (!), it is possible to gain an understanding of the groups that determine the *drag force* F_D on the object. F_D will depend on the velocity of the object with respect to the fluid (see Figure 2.13). For this, therefore, the relative velocity (v_r) must be taken. This is the difference between the velocity of the object and the velocity of the ‘undisturbed’ part of the liquid (that is, the velocity of the liquid a long distance from the object). It is this relative velocity that determines the flow field and the pressure field around the object. Obviously, the viscosity, μ , and the density, ρ_l , of the fluid will play a role, and the dimensions of the object will determine the magnitude of the force as well. For this, we take a typical ‘diameter’ D , therefore

$$F_D = F(v_r, \mu, \rho_l, D) \quad (2.69)$$

The result of the dimensional analysis is

$$\frac{F_D}{\rho_l v_r^2 D^2} = k \text{ Re}^\alpha \quad (2.70)$$

Therefore, the following applies to the drag force F_D

$$F_D = f(\text{Re}) D^2 \rho_l v_r^2 \quad (2.71)$$

The latter factor on the right-hand side of this equation stands for the inertia of the flow, although we will see in § 2.3.2 that it is usually rewritten as $\frac{1}{2} \rho_l v_r^2$. We can

also recognize it as a *dynamic pressure*, see the discussion about Equations (1.129) and (1.130). At the nose of the immersed object, i.e. at the so-called *stagnation point*, the fluid is ‘stopped’ locally, as a result, in line with the Bernoulli equation, kinetic energy is converted there into pressure energy, rendering pressure highest there, called the *stagnation pressure* p_{stagn} .

$$p_{\text{stagn}} = p + \frac{1}{2} \rho_l v_r^2 \quad (2.72)$$

where the first term on the right-hand side denotes the local static pressure. The idea here is that there is a pressure drop on the object that can be estimated with the help of the dynamic pressure.

The second factor on the right-hand side of Equation (2.71) has the dimension of a surface. This is hardly surprising after all, the drag force acts on the surface of the object. The function of the Reynolds number on the right-hand side of Equation (2.71) accounts for the ‘details’ of the area of flow around the object, where of course it matters whether the flow around the object is laminar or turbulent.

In order to elucidate all this, two contributions to the overall *drag force* F_D must be distinguished, namely, the form drag and the friction drag (or skin friction).

The term *form drag* can be understood from the example below. Consider a flat plate (surface area A) that is perpendicular to the flow of a fluid (see Figure 2.14). The fluid approaching the plate will be slowed down and will build up a *dynamic pressure* of the order of magnitude of $\frac{1}{2} \rho_l v_r^2$. However, behind the plate, in its wake, the liquid contains numerous eddies. As a result, this stagnation pressure is absent here. After all, there is kinetic energy in the eddies, which is deducted from the pressure energy according to the Bernoulli equation, and in addition substantial energy dissipation takes place. Consequently, there is a pressure drop over the plate. This results in a force on the plate in the direction of the flow.

$$F \propto A \Delta p = A \frac{1}{2} \rho_l v_r^2 \quad (2.73)$$

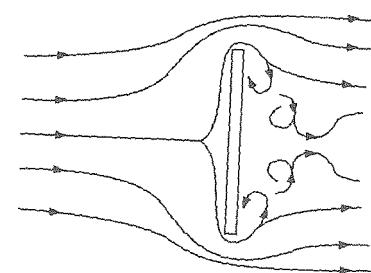


Figure 2.14

Friction drag (or *skin friction*) occurs in particular if the flow passes parallel to the surface of the object. The flat plate is a good example of this, too. Now, though, it concerns a motionless plate parallel to the flow. On the plate, the velocity of the liquid is equal to that of the plate – zero, in other words. In the *boundary layer* (see Figure 2.15), the velocity builds up in the direction of y until value v_r is reached at the edge of the boundary layer. This profile (which depends on both x and y) can be calculated with the help of the x and y -momentum balance, the mass balance, and boundary layer theory. From this, we can determine what is important to us – the shear stress between the liquid and the plate. The result is

$$\tau_w = 0.644 \left(\frac{\rho_l v_r x}{\mu} \right)^{1/2} \frac{1}{2} \rho_l v_r^2 \text{ providing that } Re_x < 3 \cdot 10^5 \quad (2.74)$$

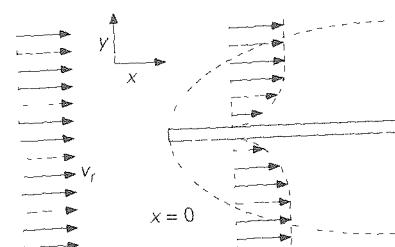


Figure 2.15

The overall force on the plate (length L in the direction of x , breadth B) can now be determined by adding up the contribution of the bottom and the top of the plate

$$F_{\text{friction}} = 2 \int_0^L \tau_w B dx = 2.66 \left(\frac{\rho_l v_r L}{\mu} \right)^{1/2} BL \frac{1}{2} \rho_l v_r^2 \quad (2.75)$$

With the help of the above illustrations of *form drag* and *friction drag* in extreme situations, it is easy to understand that the overall drag force on a random object in a flow is determined by the result of all the local pressure and shear stress values to which every part of the surface of the object is subjected. In principle, therefore, the overall drag force can be calculated by taking the component in the flow direction of all those local forces and integrating them across the entire surface of the object – as written explicitly for a flat parallel plate exposed to a flow in the first part of Equation (2.75). The *form drag* is then the resultant of integrating all the pressure forces on the object, while the *friction drag* results from integrating all the skin friction contributions.

We should also keep in mind that the velocity field around the object (from which all the local values of the shear stress are calculated) and the pressure field are generally

time-dependent and three-dimensional. The current state of technology makes a numerical calculation of the overall interaction force as described above possible for an increasing number of flow conditions, but in general, very simplified calculations are still widely used.

Summary

Immersed objects that move through and with respect to the surrounding fluid experience a counteracting force – the drag force. This force attempts to have the body move at the same velocity as the liquid. There are two distinctive effects: form drag and friction drag which have been explained extensively. Together, they form the drag force.

By means of a dimensional analysis, an expression has been derived for this drag force

$$F_D = f(\text{Re}) \cdot D^2 \rho_l v_r^2$$

In this context, the concept of stagnation pressure was discussed again, along with the contribution of shear stresses acting between object and fluid. Of course, the drag force strongly depends on the exact way the fluid flows around the object, and therefore on the particle Reynolds number.

2.3.2 Drag force and drag coefficient

Only in very exceptional cases can the drag force be calculated analytically. For example, this is the case with *creeping flow* around a sphere, that is, the flow with low Reynolds number values ($\text{Re} < 1$) round a sphere, if the fluid is incompressible – that is, if it has a constant density. For such low Reynolds numbers, the flow around the sphere is symmetrical. However, this does not mean that there is no form drag, because there is loss of pressure over the sphere as a result of dissipation. The analytical solution leads to an expression for F_D that is known as *Stokes' law*

$$F_D = 6\pi\mu R v_r \text{ providing that } \text{Re} < 1$$

$$(\text{or, for more precise results, } \text{Re} < 0.1) \quad (2.76)$$

with R being the radius of the sphere. Splitting this into form and friction drag gives

$$F_{\text{form}} = 2\pi\mu R v_r \quad (2.77)$$

$$F_{\text{friction}} = 4\pi\mu R v_r \quad (2.78)$$

In the engineering world, the overall drag force on an object is generally modelled on the basis of the following empirical equation

$$F_D = C_D(\text{Re}) A_{\perp} \frac{1}{2} \rho_l v_r^2 \quad (279)$$

in which A_{\perp} is the largest cross-sectional area of the object normal to the direction of flow or motion. In using Equation (279) a uniform approach velocity of the fluid or a stagnant fluid is tacitly assumed (see the introduction of § 2.3.1). Equation (279) shows, unsurprisingly, much similarity with Equations (270), (273) and (275). Note that the case of a plate being parallel to a fluid flow is not covered by Equation (279) because A_{\perp} approaches zero in that case.

According to Newton's Third Law, it is not just the medium that exerts a drag force on a particle, as modelled by Equation (279), but such a particle also exerts a reaction force on the medium. The force in Equation (279) is given a minus sign. Note that a minus sign also means that the force works in the opposite direction. A particle that moves through a medium at velocity v_r experiences a counteracting force from this medium. This is apparent from the following reformulation of Equation (279) in vector notation:

$$\vec{F}_D = - C_D A_{\perp} \frac{1}{2} \rho_l |\vec{v}_r| \vec{v}_r \quad (280)$$

in which $|\vec{v}_r|$ stands for the modulus of the velocity, i.e., stands for the magnitude of the velocity (regardless of the direction). It is always true that \vec{v}_r and \vec{F}_D by definition have opposite directions (see also Figure 2.13); after all, \vec{v}_r stands for the velocity of the object with respect to the fluid, while \vec{F}_D represents the force of the fluid on the object.

Coefficient C_D is called the *drag coefficient* and is therefore a function of Re , as follows from the dimensional analysis. Apart from liquid properties and the relative velocity, Re includes a typical dimension (size) of the object. For a sphere or a cylinder in a cross flow, the characteristic size is the diameter. The shape of the object also shows up in the precise form that function C_D (Re) has. Figure 2.16 shows C_D for several types of object.

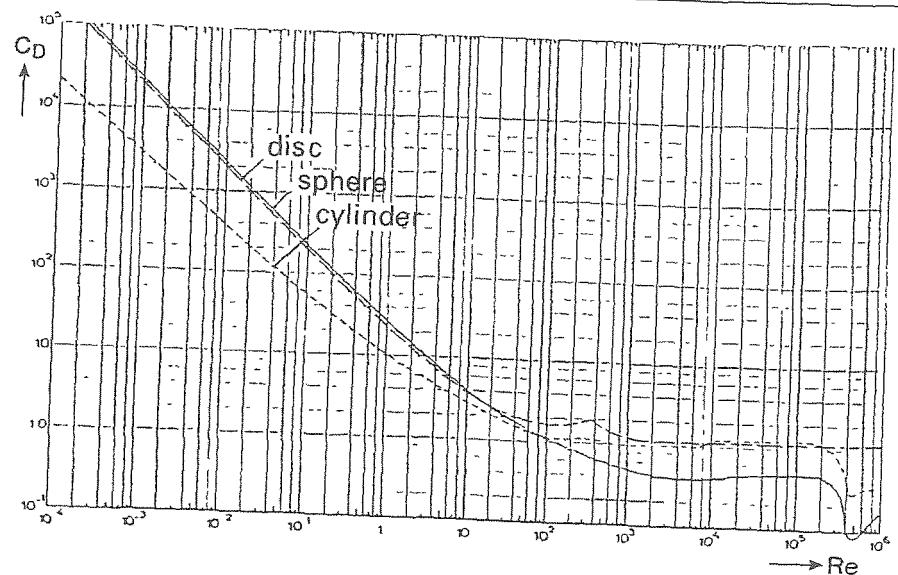


Figure 2.16

Stokes' law can also be written in terms of a drag coefficient. Combining Equations (276) and (279) produces (with diameter $D = 2R$)

$$C_D = \frac{24\mu}{\rho v_r D} = \frac{24}{\text{Re}} \quad (\text{providing that } \text{Re} < 1, \text{ or even better } \text{Re} < 0.1) \quad (281)$$

If the Re number becomes any greater, eddies form on the rear side of the sphere. A wake is then formed behind the sphere, when the boundary layer separates from the object as a result of the inertia of the fluid that prefers to carry on moving straight ahead. In the case of greater Re numbers, the eddies become bigger, and the point at which the boundary layer separates shifts further forward. Where the Re numbers are greater still, the wake becomes irregular and turbulent. Eddies are then carried by the flow and new ones are produced behind the sphere. Finally, with very high Re numbers, the boundary layer becomes turbulent and the point where it separates shifts once again to the rear of the sphere. This is all illustrated in Figure 2.17.

It is also possible to give an analogous description for the flow around cylinders in a cross flow. Another notable phenomenon occurs here, for $10^2 < \text{Re} < 5 \cdot 10^3$. The eddies behind the cylinder – there are two, in the form of cylinders – then become unstable. The cylinder now sheds off eddies to the left and right, alternately. A so-called Kármán vortex street now occurs behind the cylinder (named after Von Kármán). Such a street is schematically shown in Figure 2.18.

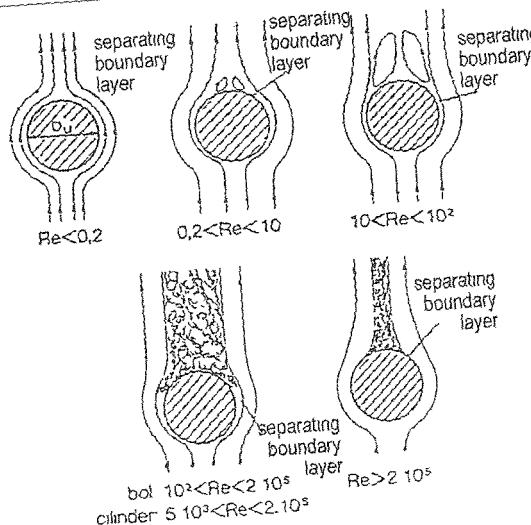


Figure 2.17

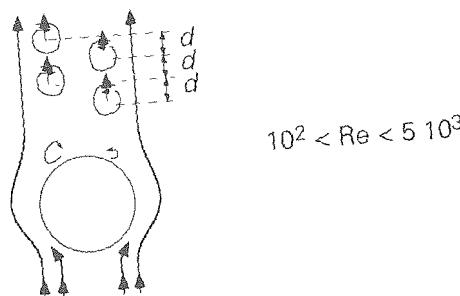


Figure 2.18

Summary

Generally, the drag force exerted by a flow on an immersed object is modelled (in a steady state situation) with the stagnation pressure and the projection of the surface of the body on a plane that is perpendicular to the relative velocity of the body and liquid

$$F_D = C_D(Re) \cdot A_{\perp} \cdot \frac{1}{2} \rho_l v_r^2$$

The coefficient C_D in this expression is called the drag coefficient and is a function of the particle Reynolds number and of the form of the body

For creeping flow round a spherical particle (for preferably Re smaller than 0.1) Stokes' law applies:

$$F_D = 6\pi\mu R v_r$$

which is in agreement with the previous equation for $C_D = 24/Re$.

Fluid flow around immersed spheres and cylinders in cross-flow has been discussed qualitatively. One should distinguish between laminar and turbulent flow. An important aspect is the separation of the boundary layer from the object and the exact position where this happens

2.3.3 Force balance and terminal velocity

The above concepts relating to the drag force that an object is subjected to in a flow field can be used for calculating (relative) particle motions. The behaviour of a particle is, after all, determined by the resultant of all the forces acting upon it. If the resultant does not equal zero, the particle is accelerating (Newton's Second Law), if the resultant is equal to zero, then the particle is motionless or it is carrying out a uniform movement (Newton's First Law)

The magnitude of the resultant is determined by a force balance. The drag force is one of the forces that features in such a balance and depends on the relative velocity v_r . If the result of the forces is zero, the relative velocity can be derived directly from the force balance

Consider a particle falling through a fluid at a constant velocity. It is known from classical mechanics that then the sum of the forces on the particle must be equal to zero. This also follows from a steady-state momentum balance over the particle, of course no momentum flows convectively into or out of the particle and therefore the steady-state momentum balance for the particle as the control volume – see Equations (1.139) and (1.140) – reduces to a force balance

$$\sum F_z = 0 \quad (2.82)$$

For a falling particle, this means the sum of gravity, buoyancy, and drag force is zero (see Figure 2.19)

$$F_g + F_{buoy} + F_D = 0 \quad (2.83)$$

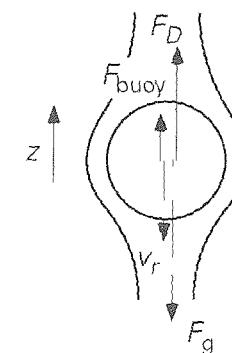


Figure 2.19

With the z -coordinate and the forces taken positive in the upward direction, the following applies to the buoyancy

$$F_{\text{buoy}} = \frac{\pi}{6} D^3 \rho_a g \quad (2.84)$$

to the gravity

$$F_g = -\frac{\pi}{6} D^3 \rho_p g \quad (2.85)$$

and to the drag force

$$F_D = C_D A_{\perp} \frac{1}{2} \rho_a v_r^2 \quad (2.86)$$

where ρ_a denotes the density of the ambient fluid and $A_{\perp} = \frac{\pi}{4} D^2$ (and not πD^2 , as that is the entire surface of the sphere, while the drag force is concerned with the projected area!) It should also be pointed out that the drag force is positive, directed upwards as the particle falls, the surrounding fluid exerts a force in the opposite direction (in other words, the fluid flows upwards in relation to the particle and so the drag force is directed upwards)

Substituting the Equations (2.84), (2.85), and (2.86) into the balance of Equation (2.83) produces

$$C_D \frac{\pi}{4} D^2 \frac{1}{2} \rho_a v_r^2 = \frac{\pi}{6} D^3 (\rho_p - \rho_a) g \quad (2.87)$$

from which follows

$$v_r = - \left(\frac{4}{3} g D \frac{\rho_p - \rho_a}{\rho_a} \frac{1}{C_D} \right)^{1/2} \quad (2.88)$$

where the minus sign accounts for the fact that the particle is moving downwards - that is, against the upward direction of z

A problem when determining the uniform velocity from such a balance is that in order to determine the velocity, it is necessary to know what the C_D from Equation (2.75) is for the drag force. Now C_D is a function of Re , and therefore of the relative velocity. It is possible to break out of this dilemma through *iteration*. This will be illustrated through two examples.

Example 2.8. A hailstone

Consider the uniform free fall of a spherical hailstone (diameter $D = 4$ mm, density $\rho_p = 915 \text{ kg/m}^3$) through motionless air. How great is the terminal velocity v_r ?

It is now possible to read in Figure 2.16 a value of C_D for an initial guess of Re . Using Equation (2.88), a v_r can then be calculated with which a new Re is calculated. This is then used in turn to read a new C_D value and to calculate a second v_r . This process of iteration is repeated until v_r no longer changes (to any notable degree).

On the basis of commonplace experience, you might expect with the hailstone that v_r would be so great that $\text{Re} \gg 1$ (this is rapidly the case, as the air viscosity is very low $\mu_a = 1.8 \cdot 10^{-5} \text{ Ns/m}^2$). On the basis of the initial guess that $\text{Re} > 10^4$ the iteration may proceed as follows

$$\begin{aligned} \text{Re} > 10^4 &\rightarrow C_D = 0.43 \text{ enter in Equation (2.88)} \rightarrow v_r = 9.6 \text{ m/s} \rightarrow \\ \text{Re} = 2570 &\rightarrow C_D = 0.40 \rightarrow v_r = 10.0 \text{ m/s} \rightarrow \\ \text{Re} = 2660 &\rightarrow C_D = 0.40 \end{aligned}$$

Further iteration is no longer necessary - the terminal velocity is some 10 m/s \square

Example 2.9. An air bubble in glue

A spherical air bubble (density $\rho_a = 1.2 \text{ kg/m}^3$, with subscript a for air) is slowly rising in a bottle of glue at a constant slip velocity, v_s . The bubble has a diameter of 3 mm and rises 2.5 cm in five seconds (easy to measure!). The density of the glue is $\rho_l = 10^3 \text{ kg/m}^3$.

Find the viscosity of the glue

Again, the solution is derived from a force balance, see Equation (2.83). With the positive z -axis vertically upwards, now the drag force is negative, as the air bubble moves upwards. Then Equation (2.83) becomes

$$-\frac{\pi}{6} D^3 \rho_a g + \frac{\pi}{6} D^3 \rho_l g - C_D \frac{\pi}{4} D^2 \frac{1}{2} \rho_l v_s^2 = 0 \quad (2.89)$$

From this, it follows for the drag coefficient that

$$C_D = \frac{4}{3} \frac{g D}{v_s^2} \frac{\rho_l - \rho_a}{\rho_l} \quad (2.90)$$

From the data it then follows that $C_D = 1570$. Such a high C_D means that $\text{Re} < 1$ (see Figure 2.16). But then it is also true that $C_D = 24/\text{Re}$ (the bubble is spherical in shape) and so it follows that $\text{Re} = 24/C_D = 1.53 \cdot 10^{-2}$. With the data, the velocity of the bubble $v_s = 5 \cdot 10^{-3} \text{ m/s}$. It is then established that the viscosity of the glue is

$$\mu_l = \frac{\rho_l v_s D}{\text{Re}} = 0.98 \text{ Ns/m}^2 \quad (2.91) \quad \square$$