TRANSPORT PHENOMENA

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CONTENTS

1. DIMENSIONAL ANALYSIS

> No investigator should allow himself to proceed to the detailed solution of a problem until he has made a dimensional analysis of the nature of the solution which will be obtained, and convinced himself by appeal to experiment that the points of view embodied in the underlying equations are sound.
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> — PERCY WILLIAMS BRIDGMAN,
> DIMENSIONAL ANALYSIS [YALE UNIVERSITY PRESS, 1922]

> We believe that technology is at its very best and it's more empowering when it simply disappears.
>
> — JOHNY IVES,

Dimensional analysis is an invaluable tool when dealing with physical phenomena, specially complex phenomena, since it helps to simplify complexity by stressing the important physical relationships of their parts instead of diffusing physics into complex maths.

In transport processes, a useful guide to perform dimensional analysis is the following:

(1) identify relevant transport properties, like fluid velocity, thermal energy flux, mass flux and so on;
(2) identify relevant material properties, such as viscosity, thermal conduction, specific thermal capacity, density and so forth;
(3) choose an independently dimensional set according to the phenomenon class; *i.e.*, mechanics, $\{\mathsf{M}, \mathsf{L}, \mathsf{T}\}$ or alternatively $\{\mathsf{F}, \mathsf{L}, \mathsf{T}\}$, thermal transport $\{\mathsf{E}, \mathsf{L}, \mathsf{T}, \Theta\}$;
(4) express the quantities using their dimensions in the chosen set;
(5) find the number of dimensionless quantities using the π-theorem:

$$n = p - r\,,$$

where n is the number of dimensionless quantities, p the number of physical quantities to be modeled and r the number of elements of the dimensional set;

(6) form the first π quantity using the physical quantity being seek as the base;

(7) form the rest of the π quantities using the rest of the physical quantities and their correspondent dimensions;

(8) find the model general equation:

$$\psi\left[\pi_i\right] = 0\,,$$

where the index i runs from 1 to n.

(9) propose the final model equation by isolating the first π quantity, the one containing the quantity being seek; *i.e.*,

$$\pi_1 = \psi\left[\pi_{i-1}\right]\,;$$

(10) replace the dimensionless quantities, $\{\pi_i\}$, with known dimensionless numbers, like the Reynolds number, if possible;

(11) finally, seek the particular mathematical form of the function ψ by guessing, using approximations, extreme cases and so forth.

Example. Consider the case of a sphere of diameter d and mass m falling vertically in a tank of side l containing a fluid of density ρ_{fl}. The equation of motion for the sphere velocity u reads [1]

$$m\dot{u} = mg - f_{\mathrm{d}}\,,$$

where g represents the acceleration due to gravity and f_{d} the drag force.

When the sphere attains its terminal velocity, u_{t}, then the drag is exactly balanced by the gravitational force. The task is thus to obtain an expression for the drag as a function of the sphere and fluid properties.

Solution. The motion of the sphere disturbs the fluid around it and causes fluid flow. This fluid flow results in friction causing a frictional drag that exerts a force on the sphere. Since the frictional resistance to flow is due to viscous stresses, it is expected that the fluid dynamic viscosity μ will be important in determining the frictional force. In addition, the force is expected to depend on the sphere velocity u, since a higher speed would result in a larger force. The length scales that could affect the flow are the tank width l and the sphere radius r. The fluid density ρ_{fl} could also be important, since a higher force is required for accelerating a fluid with a higher density.

It is important to note that the sphere mass or its density should not be relevant determining the flow, once the sphere velocity is specified. This is because the fluid velocity around the sphere, which results in the frictional force, is determined by the velocity with which the sphere is moving, and the sphere mass or density does not affect the fluid velocity. Similarly, the acceleration due to gravity determines the gravitational force on the sphere, but does not directly affect the fluid velocity around the sphere, once the sphere velocity is specified. Therefore, it is necessary to apply some judgment at the start of dimensional analysis to distinguish the material and dynamical properties that influence in the desired quantity. It is essential to ensure not to include irrelevant quantity in the analysis.

Now that all the relevant dimensional quantities for the drag force have been determined, it is necessary to isolate the *important* ones. This is a skill that can be developed by practice. In this particular case, let us look at the length scales that are likely to be important. If the tank width and height are large compared to the sphere radius, it is likely that only the sphere radius is a relevant length scale. On the other hand, if the sphere is very close to one of the walls of the container, say within a few radii, then the distance from the wall as well as the sphere radius could be important. For definiteness, let us proceed with the assumption that only the sphere radius is important in this case. This results in a set of important quantities:

(1) sphere radius, r;

(2) sphere velocity, u;

(3) fluid dynamic viscosity, μ; and

(4) fluid density, ρ_{fl}.

So an equation for the force has to have the form

$$f_{\mathrm{d}} = \psi\left[r, u, \mu, \rho_{\mathrm{fl}}\right]\,.$$

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[1] The complete model takes into account buoyancy; *i.e.*, $m\dot{u} = mg - f_{\mathrm{d}} - f_{\mathrm{b}}$, where f_{b} represents the buoyancy force. In this example, however, in order to stress the exposition of the dimensional analysis principles, buoyancy is ignored.

Since this is a dynamical problem and a force is being sought, then the chosen set of dimensional quantities is $\{\mathsf{F}, \mathsf{L}, \mathsf{T}\}$. In such a system, the chosen quantities have the dimensions:

- sphere radius, $\dim r = \mathsf{L}$;
- sphere velocity, $\dim u = \mathsf{L}/\mathsf{T}$;
- fluid dynamic viscosity, $\mu = \mathsf{F}\mathsf{T}/\mathsf{L}^2$; and
- fluid density, $\rho_{\text{fl}} = \mathsf{F}\mathsf{T}^2/\mathsf{L}^4$.

Since there are five dimensional quantities and three dimensions involved in the above relationship, there are two dimensionless groups, according to the π-theorem. One of these quantities has to involve the drag, while the other is a combination of the sphere diameter and velocity and of the fluid properties (density and viscosity).

Let us construct the first dimensionless quantity, called a scaled force π_f, as a combination of the drag, viscosity, velocity and radius:

$$\pi_f = f_{\text{d}}\mu^a u^b r^c,$$

where a, b and c are the desired indices that render π_f dimensionless. If the dimensions of the left and right sides of the equation are to be equal, then they form a linear system that have to be solved simultaneously. The solution results in the coefficients $a = b = c = -1$. Therefore, the first dimensionless quantity is equal to

$$\pi_f = \frac{f_{\text{d}}}{\mu u r}\,.$$

The second dimensionless quantity, noted π_{re}, is a combination of the density, diameter, velocity and viscosity. We write this as

$$\pi_{\text{re}} = \rho u^a r^b \mu^c\,.$$

In defining the dimensionless group, the exponent of any one of the quantities can be set equal to 1 without loss of generality. In the last equation, we have chosen to set the exponent of the density equal to 1, to bring it in accordance with the conventional definition of the Reynolds number, formally defined a little later. The dimensions of the quantities on the right side of such an equation are, after solving a similar system of equations, $a = b = 1$ and $c = -1$. Therefore, the dimensionless number

$$\pi_{\text{re}} = \frac{\rho u r}{\mu}\,.$$

The relationship between the two dimensionless quantities can finally be written as

$$\psi\left[\pi_f, \pi_{\text{re}}\right] = 0 \implies \pi_f = \frac{f_{\text{d}}}{\mu u r} = \psi\left[\pi_{\text{re}}\right],$$

where ψ is a function of the Reynolds number; *i.e.*, π_{re}.

In the last equation, the force has been non-dimensionalized by the *viscous force scale*, $\mu r u$. Instead of using the viscosity, radius and velocity to non-dimensionalize the force, we could have chosen to use the density, radius and velocity instead. This would have led to the dimensionless quantity $\pi_{fi} = f/\rho u^2 r^2$, where $\rho u^2 r^2$, the *inertial force scale*, is a suitable combination of density, velocity and radius with dimensions of force. It is possible to verify that the dimensionless forces scaled in these two different ways are related by

$$\pi_f = \pi_{\text{re}}\pi_{fi}\,.$$

The Reynolds number is then a ratio of the inertial and viscous force scales,

$$\pi_{\text{re}} = \frac{\rho u^2 r^2}{\mu r u}\,.$$

For this reason, the Reynolds number is often referred to as the balance between the viscous and inertial forces.

Further simplifications can be made in some limiting cases. When the group $\rho u r/\mu$ is very small, then the fluid flow is dominated by viscous effects, thus, the drag should not determine on the inertial force scale. Therefore, the drag has the form $\pi_f = \pi = \text{constant}$ or

$$f_{\text{d}} = \pi \mu u r\,.$$

The limitation of dimensional analysis is that the value of the constant cannot be determined, and more detailed calculations reveal that the exact value of the constant is 6π. This leads to *Stokes drag law* for the force on a sphere in the limit of small Reynolds number, $f_{\text{d}} = 6\pi\mu u r$.

The Reynolds number can be physically interpreted as the ratio of inertial and viscous forces or as the ratio of convection and diffusion. The latter interpretation is more useful, since it has analogies in mass and thermal transfer processes. It can be proven that the diffusion coefficient for momentum is the *kinematic viscosity*, $\nu = \mu/\rho$, where ρ is the mass density. It is possible to verify that the kinematic viscosity has the same dimensions as the mass diffusion coefficient; *i.e.*,

L^2/T. The Reynolds number can be written as $\pi_{\mathrm{re}} = ur/\nu$; *i.e.*, the ratio of convective transport of momentum, due to the fluid velocity, and diffusive transport, due to momentum diffusivity.

This type of analysis could be extended to more complicated problems. For instance, if the particle falling is not a sphere but a more complicated object, such as a spheroid, then there are two length scales, the major and minor axes of the spheroid, r_1 and r_2. In this case, the number of quantities increases to 6 and there are three dimensional groups. One of these could be assumed to be the ratio of the lengths (aspect ratio): r_1/r_2.

2. Dimensionless quantities

Dimensionless groups can be classified into three broad categories: the dimensionless fluxes, the ratios of convection and diffusion and the ratios of different types of diffusion. Before proceeding to define dimensionless quantities, we first define the diffusion coefficients for mass, momentum and energy, in order to provide a definite basis for the discussion. Here, we restrict ourselves to the macroscopic definition.

2.1. **Mass, momentum and energy diffusivities.** The fundamental constitutive relations [2] in transport processes are the Fick's law for mass diffusion, Fourier's law for heat conduction and Newton's law for viscosity. The respective diffusion coefficients can be defined as follows.

- When there is a concentration difference maintained across a slab of fluid, then there is transfer of mass from the surface at higher concentration to the surface at lower concentration. The mass flux (mass per unit area per unit time) is inversely proportional to the length and directly proportional to the difference in concentration or temperature across the material. If a concentration difference Δc, $\dim c = \mathsf{M}/\mathsf{L}^3$, is maintained between two ends of a slab of length l, the mass flux m'', $\dim m'' = \mathsf{M}/\mathsf{L}^2\mathsf{T}$, is given by Fick's law:

$$m'' = -\phi \frac{\Delta c}{l}\,,$$

  where ϕ is the diffusivity, $\dim \phi = \mathsf{L}^2/\mathsf{T}$. Here, the negative sign indicates that mass is transferred from the region of higher concentration to the region of lower concentration.

- For the transport of thermal energy, the energy flux is related to the temperature difference by Fourier's law. For a slab of material of length l with a temperature difference $\Delta \tau$ across the material, the energy flux e'' is given by

$$e'' = -k \frac{\Delta \tau}{l}\,,$$

  where k is the thermal conductivity, $\dim k = \mathsf{E}/\mathsf{LT\Theta}$, and the negative sign indicates that thermal energy is transferred from the region of higher to the region of lower temperature.

- The Newton's law of viscosity relates the shear stress τ (force per unit area at the wall) to the strain rate (change in velocity per unit length across the flow) for the simple shear flow of a fluid as shown in figure 1.1.2.

$$\tau_{xy} = \nu \frac{\Delta u_x}{l}.$$

  Note that there is no negative sign in Newton's law, in contrast to Fick's law and Fourier's law. This is due to the difference in convention with regard to the definition of stress in fluid mechanics and the definition of fluxes in transport

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[2] A constitutive relation is a relation between two physical quantities (especially kinetic quantities as related to kinematic quantities) that is specific to a material or substance, and approximates the response of that material to external stimuli, usually as applied fields or forces. They are combined with other equations governing physical laws to solve physical problems; *e.g.*, in fluid mechanics the fluid flow in a pipe, in solid state physics the response of a crystal to an electric field or, in structural analysis, the connection between applied stresses or forces to strains or deformations.

Some constitutive equations are simply phenomenological; others are derived from first principles. A common approximate constitutive equation frequently is expressed as a simple proportionality using a parameter taken to be a property of the material, such as electrical conductivity or a spring constant. However, it is often necessary to account for the directional dependence of the material, and the scalar parameter is generalized to a tensor. Constitutive relations are also modified to account for the rate of response of materials and their non-linear behavior.

phenomena. The shear stress τ_{xy} in Newton's law is defined as the force per unit area at a surface in the x direction whose outward unit normal is in the y direction. In contrast, the fluxes are defined as positive if they are directed into the volume. Therefore, the shear stress is actually the negative of the momentum flux. If the stress is defined to the the force per unit area acting at a surface whose inward unit normal is in the x direction, then this would introduce a negative sign in Newton's equation. However, it is conventional in fluid mechanics to define the stress with reference to the outward unit normal to the surface. As we will see later, this difference in convention will not affect the balance equations that are finally obtained for the rate of change of momentum.

In this course, we will adopt the convention of defining the stress τ_{xy} as the force per unit area in the x direction acting along a surface whose outward unit normal is in the y direction and use the last equation for Newton's law of viscosity.

The diffusion coefficients are the proportionality constants in the relationship between the flux of a quantity (mass, thermal energy, momentum) and the driving force. The flux of a quantity (mass, thermal energy, momentum) is the amount of that quantity transferred per unit area per unit time. The driving force for a quantity (mass, thermal energy, momentum) is the gradient (change per unit distance) in the density (quantity per unit volume) of that quantity. So the transport equations can be written in the general form

$$\begin{pmatrix} \text{transport of quantity} \\ \text{per unit area} \\ \text{per unit time} \end{pmatrix} = \begin{pmatrix} \text{diffusion} \\ \text{coefficient} \end{pmatrix} \frac{\begin{pmatrix} \text{change in density (per unit volume)} \\ \text{of the quantity} \\ \text{across the material} \end{pmatrix}}{\text{thickness of the material}}$$

From dimensional analysis of the above equation, see that the diffusion coefficients of all quantities have dimensions of L^2/T. These diffusion coefficients are defined from Fick's law, Fourier's law and Newton's law as follows.

(1) From Fick's law, the diffusion coefficient ϕ is the ratio of mass flux (mass transported per unit area per unit time) and the gradient in the concentration (mass per unit volume). Therefore, the mass diffusivity is just the diffusion coefficient ϕ.

(2) It is possible, on the other hand, to define a diffusion coefficient for thermal transfer as follows. The difference in temperature $\Delta\tau$ can be expressed in terms of the difference in the energy density between the two sides as $\Delta\tau = \Delta\epsilon/\rho c_v$, where $\Delta\epsilon$ is the thermal energy density (thermal energy per unit volume, $\dim\epsilon = \mathsf{E}/\mathsf{L}^3$) and c_v the specific thermal capacity, $\dim c_v = \mathsf{L}^2/\mathsf{T}^2\Theta$. With this, the equation for the thermal flux can be written as

$$e'' = \frac{k}{\rho c_v}\frac{\Delta\epsilon}{l}\,.$$

Note that the above equation has the same form as the mass flux equation, with a thermal diffusivity $\phi_h = k/\rho c_v$, $\dim\phi_h = \mathsf{L}^2/\mathsf{T}$.

(3) The *momentum diffusivity* is the relation between the momentum flux (rate of momentum transport per unit area per unit time) and the difference in the momentum density (momentum per unit volume). Consider the layer of fluid shown in figure 1.1.2. Since the momentum of a fluid parcel is the mass of that parcel multiplied by its velocity, the momentum density is the product of the mass density ρ and velocity u_x. Therefore, the equation for the flux, expressed in terms of the momentum density, is

$$\tau_{xy} = \nu\frac{\Delta(\rho u_x)}{l}\,,$$

where ν is the momentum diffusivity. For an incompressible fluid with constant density, the momentum diffusivity is $\nu = \mu/\rho$. The momentum diffusivity, ν, with $\dim\nu = \mathsf{L}^2/\mathsf{T}$, is also referred to as the *kinematic viscosity*.

Summarizing:

- mass transport: $m'' = -\phi\operatorname{grad}c$, where mass flux $\dim m'' = \mathsf{M}/\mathsf{L}^2\mathsf{T}$, mass diffusion coefficient $\dim\phi = \mathsf{L}^2/\mathsf{T}$ and concentration gradient $\dim\operatorname{grad}c = \mathsf{M}/L^4$.

Dimensionless quantity	Definition	Ratio
Reynolds number	$\pi_{\mathrm{re}} = \rho u l/\mu$	momentum convection to momentum diffusion
Prandtl number	$\pi_{\mathrm{pr}} = \nu/\phi_h$	momentum diffusion to thermal diffusion
Schmidt number	$\pi_{\mathrm{sc}} = \nu/\phi$	momentum diffusion to mass diffusion
Peclet number	$\pi_{\mathrm{pe}} = u l/\phi_h$	thermal convection to thermal diffusion

TABLE 1. Dimensionless quantities that are ratios of diffusivities. The Prandtl number $\pi_{\mathrm{pr}} = \nu/\phi_h = c_p\mu/k$ is the ratio of momentum and thermal diffusivity and the Schmidt number $\pi_{\mathrm{sc}} = \mu/\rho\phi = \nu/\phi$ the ratio of momentum and mass diffusivity.

- thermal energy transport: $e'' = -k/\rho c \operatorname{grad} \epsilon$, where thermal energy flux $\dim e'' = \mathsf{E}/\mathsf{L}^2\mathsf{T}$, thermal conductivity $\dim k = \mathsf{E}/\mathsf{L}\mathsf{T}\Theta$, mass density $\dim \rho = \mathsf{E}\mathsf{T}^2/\mathsf{L}^5$, specific thermal capacity $\dim c = \mathsf{L}^2/\mathsf{T}^2\Theta$ and energy density gradient $\dim \operatorname{grad} \epsilon = \mathsf{E}/\mathsf{L}^4$.
- momentum transport: $\tau = \nu \operatorname{grad} \rho u = \mu/\rho \operatorname{grad} \rho u$, where shear stress $\dim \tau = \mathsf{F}/\mathsf{L}^2$, kinematic viscosity $\dim \nu = \mu/\rho = \mathsf{L}^2/\mathsf{T}$, mass density $\dim \rho = \mathsf{F}\mathsf{T}^2/\mathsf{L}^4$, velocity $\dim u = \mathsf{L}/\mathsf{T}$.

The dimensionless quantities ratios of diffusivities are shown in table 1.

2.2. **Wording.** In the present document, the adjective *density* is used to express a quantity divided by volume; *e.g.*, energy density, $\dim \epsilon = \mathsf{E}/\mathsf{L}^3$, and the adjective *specific* to express a quantity divided by mass; *e.g.*, specific thermal capacity, $\dim c_v = \mathsf{L}^2/\mathsf{T}^2\Theta$.

2.3. **Ratio of convection and diffusion.** Convective transport takes place due to the mean flow of a fluid, even in the absence of a concentration difference. For example, if a fluid with concentration c travels with velocity u in a pipe, then the total amount of mass transported per unit time is cua_p, where a_p is the cross-sectional area of the tube. Therefore, the flux (mass transported by the fluid, per unit area perpendicular to the flow per unit time) is cu. Consequently, the ratio between the rate of transport due to convective and diffusive effects is ul/ϕ, where l is the length scale across which there is a change in the density of this quantity.

The dimensionless numbers which are ratios of convective and diffusive transport rates, seetable 1:

- the Reynolds number, $\pi_{\mathrm{re}} = \rho u l/\mu = ul/\nu$, the ratio of momentum convection and diffusion,
- the Peclet number for mass transfer, $\pi_{\mathrm{pe}} = ul/\phi$, the ratio of mass convection and diffusion, and
- the Peclet number for thermal transfer, $\pi_{\mathrm{pe}} = ul/\phi_h = \rho c_p ul/k$, where c_p is the specific thermal capacity at constant pressure.

2.4. **Dimensionless numbers in natural convection.** In natural convection, the driving force for convection is the body force caused by a variation in the density of the fluid, which is in turn caused by variation in temperature. In contrast to natural convection, the characteristic flow velocity is not known *a priori*, but has to be determined from the driving force due to the density difference. If we assume there is a balance between the driving force and the viscous stresses in the fluid, dimensional analysis can be used to infer that the characteristic velocity should scale as $u_c \approx fd/\mu$, where f is the driving force for convection per unit volume of fluid, d is the diameter of the body or the characteristic length and μ is the dynamic viscosity.

The driving force for convection, per unit volume of the fluid, is proportional to the product of the density variation $\Delta\rho$ and the acceleration due to gravity g. The density variation is is proportional to $\rho\beta\Delta\tau$, where $\Delta\tau$ is the variation in temperature and β is the coefficient of thermal expansion. Therefore, the force per unit area is proportional to $\rho g\beta\Delta\tau$. With this, the characteristic velocity for the flow is $u_c \approx \rho d^2 g\beta\Delta\tau/\mu$. The

Grashof number is the Reynolds number based upon this convection velocity,

$$\pi_{\mathrm{gr}} = \frac{\rho u_c d}{\mu} = \frac{\rho^2 d^3 g \beta \Delta \tau}{\mu^2} \, .$$

In defining the Grashof number, we used the momentum diffusivity and the body force to obtain the characteristic velocity scale. An alternative definition is the *Rayleigh number*, where the thermal diffusivity, $k/\rho c_p$, is used to determine the characteristic velocity. The characteristic velocity is then given by $u_c \approx f d^2 c_p / k$, where $f = \rho \beta \Delta \tau$ is the driving force for convection per unit volume of fluid. The Reynolds number based on this convection velocity and momentum diffusivity is the Rayleigh number,

$$\pi_{\mathrm{ra}} = \frac{\rho^2 c_p d^3 g \beta \Delta \tau}{\mu k} \, .$$

The *Rayleigh-Benard* instability of a fluid layer heated from below occurs when the Rayleigh number increases beyond a critical value.

2.5. **Other dimensionless groups.** There are two important dimensionless groups involving surface tension, which are the *Weber number* and the *capillary number*. The Weber number is the ratio of inertial and surface tension forces,

$$\pi_{\mathrm{we}} = \frac{\rho u^2 l}{\gamma} \, ,$$

while the capillary number is the ratio of viscous and surface tension forces,

$$\pi_{\mathrm{ca}} = \frac{\mu u}{\gamma} \, ,$$

where γ is the surface tension, $\dim \gamma = \mathsf{F}/\mathsf{L}$.

In problems involving free interfaces, if the Reynolds number is low, inertial forces are negligible compared to viscous forces, and the capillary number has to be determined in order to assess the ratio of viscous and surface tension forces. At high Reynolds number, it is appropriate to determine the Weber number in order to examine the ratio of inertial and surface tension forces. In addition to the Weber and capillary numbers, the *Bond number* is a dimensionless group appropriate for situations where a free interface is under the influence of a gravitational field. This dimensionless group is defined as the ratio of gravitational and surface tension forces,

$$\pi_{\mathrm{bo}} = \frac{\rho g l^2}{\gamma} \, .$$

2.6. **Dimensionless groups involving gravity.** The ratio of inertial and gravitational forces is given by the *Froud number*,

$$\pi_{\mathrm{fr}} = \frac{u^2}{gl} \, ,$$

In applications involving rotation of fluids, the Froud number is also the ratio of centrifugal and gravitational forces.

2.7. **Summary.** From the magnitudes of dimensionless quantities, one can immediately infer which effects are dominant and which are negligible. For instance, if the Reynolds number is small, then inertial effects are small compared to viscous effects. Thus, the effect of inertia can be neglected and fluid density is no longer an important parameter. However, it should be noted that though convective effects can be neglected with the Reynolds number or Peclet number is small, diffusive effects can not always be neglected even when these numbers are large, for reasons to do with the formation of momentum or thermal boundary layers near surfaces where these effects become important.

3. Diffusion

Transport of thermal energy, mass or momentum takes place by two mechanisms: convection and diffusion. Convection is the process by which material or thermal energy is transported due to the mean motion of the fluid in which it is carried. Diffusion, on the other hand, is the process by which material is transported by the thermal motion of the molecules within the fluid, even in the absence of any mean flow. The random thermal motion takes place on the microscopic length scale in the fluid, which is the molecular size in the liquid and the mean free path in a gas. Examples of convection and diffusion are as follows.

- A mixed flow reactor with an impeller, in which a reaction catalyzed by a solid catalyst takes place. The pipes at the inlet and outlet of the reactor transport material by convection into and out of the reactor. Within the reactor, transport takes place by convection due to the motion of the impeller, and the flow patterns generated therein. However, if we closely examine the surface of a catalyst, the fluid flow takes place tangential to the catalyst surface, and there is no flow perpendicular to the surface of the catalyst. Therefore, the transport of the reactant from the fluid to the solid surface, and the transport of product from the solid surface to the fluid, can take place only by diffusion.
- A shell and tube thermal exchanger, in which a hot fluid flows through the tube and a cold fluid flows on the shell side. The thermal energy is transported into the exchanger by convection by the fluid at the inlet of the shell side, and by convection by the fluid at the outlet on the tube side. However, the transport from the shell side to the tube side cannot take place by convection, since the fluid flow is tangential to the wall of the tube, and there is no convective transport perpendicular to the wall of the tube. The transport across the tube wall takes place due to diffusion in the fluids and the wall of the tube.
- Fluid flowing through a pipe which is pumped using a pump at the inlet. The action of the pump results in a pressure gradient down the tube, with a higher pressure at the inlet and a lower pressure at the outlet. The net flux of momentum (momentum transported per unit area per unit time) into the tube is the product of the pressure difference and the average velocity of the fluid. (There is a contribution to the flux due to the force exerted by the fluid velocity at the interface, but this contribution is equal at the inlet and outlet, and so there is no net flux due to this). The transport of momentum at the inlet is due to convection, and is absent when there is no fluid flow. The total rate of input of momentum into the tube due to the pump is balanced by the viscous (frictional) force exerted by the walls of the tube on the fluid. This frictional transfer at the wall cannot take place by convection, since there is no fluid flow perpendicular to the walls of the tube. Therefore, this takes place by the diffusion of momentum.

It can be seen thus that the convection is directional, and takes place only along the direction of flow. However, the random velocity fluctuations of the molecules that cause diffusion are isotropic, and therefore have no preferred direction. Therefore, diffusion takes place in the direction in which there is a gradient in the concentration, temperature or mean velocity. Transport takes place by a combination of convection and diffusion in the bulk flow, but can take place only diffusion at bounding surfaces, since there is no mean flow perpendicular to the surface. The mechanisms of mass, momentum and thermal diffusion are discussed in further detail in the following sections.

3.1. **Mass diffusion.**

3.1.1. *Mass diffusion in gases.* Diffusive transport takes place due to the random motion of the molecules, in the absence of any mean motion of the center of mass. This concept is easiest to understand by using a gas mixture in two bulbs separated by a tube. One of the bulbs contains the pure solvent A, while the other contains a mixture of A and a small amount of the solute B. It will be assumed, for simplicity, that A and B have equal molecular mass and diameter, and the initial pressures and temperatures in the two bulbs are equal. When the stop cork between the two is opened, there is no net transfer of

mass between the two bulbs, since the pressures and temperatures are equal. However, there will be a transfer of the solute B from one bulb to the other until the concentrations in the two bulbs are equal. Consider a surface across which there is a variation in the concentration. There is a constant transport of molecules across this surface due to the thermal motion of the molecules. The flux of molecules at the surface, n'', is defined as the number of molecules passing through the surface per unit area per unit time. If the solute concentration and temperature are constant, the total flux of molecules passing downward from above to below the surface is equal to the flux passing through in the upward direction. However, if there is a variation of concentration across the surface, then there is a net transport of solute molecules downward. This is because the molecules that travel downward through the surface are transported from a distance of the order of one mean free path above the surface, where the concentration is higher, whereas the molecules which travel upward are transported from a distance of the order of one mean free path below the surface, where the concentration is lower. The flux of molecules, which is the number of molecules transported downward through the surface per unit area per unit time is the number of particles per unit volume, η, times the average downward velocity of the particles. The *root mean square velocity* of the molecules in a gas can be estimated as

$$u_{\mathrm{rms}} = \sqrt{\frac{3k_{\mathrm{b}}\tau}{m}}\,,$$

where τ is the thermodynamic temperature, k_{b} the Boltzmann constant and m the mass of the molecule. The *mean velocity* is defined slightly differently, as the average of the magnitude of the velocity of all the particles. This turns out to be

$$u_{\mathrm{mean}} = \sqrt{\frac{8k_{\mathrm{b}}\tau}{\pi m}}\,.$$

The flux of molecules crossing a surface is from one side to the other is proportional to the mean molecular velocity and the number density of the molecules. The flux is given by

$$n'' = \frac{1}{4}\eta u_{\mathrm{mean}}\,.$$

The molecules reaching a plane have had their last collision, on average, a distance $2\lambda/3$ above the plane, where the mean free path, λ, is

$$\lambda = \frac{1}{\sqrt{2}\pi d^2 n}\,,$$

where d is the particle diameter and n the particle number.

The total flux of molecules is then

$$n''_{z-} = \frac{1}{4}u_{\mathrm{rms}}\left(\eta_0 + \frac{2}{3}\lambda\frac{\mathrm{d}\eta}{\mathrm{d}z}\bigg|_{z=0}\right)\,, \tag{3.1}$$

where η_0 is the particle density at the surface $z = 0$ and $(\eta_s - a^2\lambda(\mathrm{d}\eta/\mathrm{d}z)|z = 0)$ is the average concentration of the molecules traveling downward through the surface. The constant a^2 is a constant of $O\,[1]$, since the molecules that travel downward are transported from a location which is of the order of one mean free path λ above the surface. This constant can be evaluated exactly using kinetic theory of gases, but this is not necessary since we are only interested in obtaining the order of magnitude of the diffusion coefficient. In eq. (3.1), a Taylor series expansion has been used for the average density of the molecules that are transported through the surface, and this expansion has been truncated at the second term. This is a good approximation if the mean free path is small compared to the length over which the density varies.

The flux of molecules in the upward direction is

$$n''_{z+} = \frac{1}{4}u_{\mathrm{rms}}\left(\eta_0 - \frac{2}{3}\lambda\frac{\mathrm{d}\eta}{\mathrm{d}z}\bigg|_{z=0}\right)\,, \tag{3.2}$$

since the molecules are transported from a distance of the order of one mean free path below the surface $z = 0$. The total flux of molecules is given by

$$n''_z = n''_{z+} - n''_{z-} = \frac{1}{3} - \frac{\lambda}{d^2}\frac{\mathrm{d}\eta}{\mathrm{d}z}\bigg|_{z=0} = -\phi\frac{\mathrm{d}\eta}{\mathrm{d}z}\bigg|_{z=0}\,, \tag{3.3}$$

where ϕ, the diffusion coefficient, has dimensions of L^2/T. A more exact expression for the diffusion coefficient is obtained using the kinetic theory of gases, which provides the value of a, but the functional dependence of the flux on the temperature, molecular diameter and the concentration gradient is captured by the simple explanation leading to eq. (3.3). For a mixture of two components, with masses m_1 and m_2 and diameters d_1 and d_2, exact expressions for the diffusion coefficient can be obtained using methods from the kinetic theory of gases. For spherical molecules, the coefficient of diffusion is

$$\phi_{12} = \frac{3}{8nd_{12}^2} \left(\frac{k_{\mathrm{b}}\tau(m_1 + m_2)}{2\pi m_1 m_2} \right)^{1/2} , \qquad (3.4)$$

where $d_{12} = (d_1 + d_2)/2$. The coefficient of *self diffusion*, the diffusion of a molecule in a gas composed of molecules of the same type, can be obtained by setting $d_1 = d_2 = d$ and $m_1 = m_2 = m$ in the last equation

$$\phi_{11} = \frac{3}{8nd^2} \left(\frac{k_{\mathrm{b}}\tau}{\pi m} \right)^{1/2} .$$

The magnitude of the diffusion coefficient in a gas can be estimated as follows. The root mean square fluctuating velocity in a gas at $\tau = 300\,\mathrm{K}$ is $(3k_{\mathrm{b}}\tau/m)^{1/2}$, which is about $2000\,\mathrm{m/s}$ for hydrogen, and about $500\,\mathrm{m/s}$ for oxygen. The mean free path of the molecules in a gas, the distance that a gas molecule travels between collisions, is proportional to $(\eta d^2)^{-1}$, where η is the number of molecules per unit volume and d is the molecular diameter. The number of gas molecules per unit volume, from the ideal gas law, is $(p/k_{\mathrm{b}}\tau)$, where p is the pressure. For a gas at STP, $p = 1.013 \times 10^5\,\mathrm{N/m^2}$, $\tau = 300\,\mathrm{K}$ and $k_{\mathrm{b}} = 1.3087 \times 10^{-23}\,\mathrm{J/K}$, and the number of molecules per unit volume is $2.5 \times 10^{25}\,\mathrm{m^{-3}}$. The diameter of a hydrogen molecule is $1.372 \times 10^{-10}\,\mathrm{m}$, and therefore the mean free path of a hydrogen molecule at STP is approximately $2 \times 10^{-6}\,\mathrm{m}$, or $2\,\mathrm{microns}$. The diameter of larger molecules is also of the same order, though somewhat larger; *e.g.*, the diameter of a nitrogen molecule is $3.8 \times 10^{-10}\,\mathrm{m}$, and that of oxygen is $3.7 \times 10^{-10}\,\mathrm{m}$. Therefore, the mean free paths are correspondingly lower, and an upper limit on the mean free path of a gas at STP is about $2\,\mu\mathrm{m}$. The product of the mean free path and the u_{rms} is estimated as a constant times $4 \times 10^{-3}\,\mathrm{m^2/s}$ for hydrogen and about $2.5 \times 10^{-4}\,\mathrm{m^2/s}$ for nitrogen and oxygen. These are approximately in agreement with values reported in literature; for small molecules H_2 and He, Cussler reports the diffusion coefficient to be $1.132 \times 10^{-4}\,\mathrm{m^2/s}$, while for large molecules such as nitrogen and oxygen the diffusion coefficient is about 10 times less, $1.81 \times 10^{-5}\,\mathrm{m^2/s}$. These vary from the diffusion coefficient predicted by eq. (3.4) are in agreement with those reported in experiments to within about $2\,\%$.

It is useful to examine the assumptions that were used to derive the expression for the diffusion coefficient in eq. (3.3). The first assumption was that the mean free path is small compared to the length scale for diffusion, which is the distance between the two bulbs in this case, so that the expression for the concentration above the surface in eq. (3.2) can be truncated at the first term. The truncation of the Taylor series expansion for the concentration in equation eq. (3.2), valid if the length scale of the flow is large compared to the mean free path, is applicable for all applications at STP except those in microfluidics where the channel and tube sizes are of the order of microns.

3.1.2. *Mass diffusion in liquids.* The estimate of the diffusion coefficient for liquids calculated in a similar manner as in gases is not accurate. Since the mean molecular velocity in liquids and gases are about equal at the same temperature, whereas the mean free path is of the order of one molecular diameter, it would be expected that the diffusion coefficients in liquids is only about ten times less than that in gases. However, the diffusion coefficients of small molecules in liquids are about four orders of magnitude lower than that in gases. For example, the diffusion coefficient of nitrogen in water is $1.88 \times 10^{-9}\,\mathrm{m^2/s}$, while that of hydrogen in water is $4.5 \times 10^{-9}\,\mathrm{m^2/s}$. The diffusion coefficient of larger molecules, such as polymers, in water is smaller still. The diffusion coefficient of hemoglobin in water is $6.9 \times 10^{-11}\,\mathrm{m^2/s}$.

Equation 2.7 [equation for diffusion of gases] cannot be used for an accurate prediction of the diffusion coefficients in liquids because *cooperative motion* is necessary for the diffusion of molecules within a liquid. The molecules in a liquid are closely packed, and so the

translation of one molecules requires the cooperative motion of many other molecules. This is in contrast to a gas, where the molecules translate freely between successive collisions. An estimate for the diffusion coefficient can be obtained using the Stokes-Einstein equation for the diffusivity

$$\phi \sim \frac{k_{\mathrm{b}}\tau}{3\pi\mu d}, \tag{3.5}$$

where ϕ is the diffusivity coefficient, k_{b} Boltzmann constant, τ thermodynamic temperature, d the diameter of the molecule that is diffusing and μ the dynamic viscosity of the suspending fluid. This formula is strictly applicable only for colloidal particles in a fluid when the particle diameter is large compared to the diameter of the fluid, but is also used as a model equation for predicting the diffusivity of small molecules in a liquid. For nitrogen in water of viscosity $1 \times 10^{-3}\,\mathrm{kg/m\,s}$, this gives $\phi = 1.15 \times 10^{-9}\,\mathrm{m^2/s}$, whereas for hydrogen in water the diffusivity is $\phi = 3.4 \times 10^{-9}\,\mathrm{m^2/s}$. Though the order of magnitude of this prediction is in agreement with the experimentally measured diffusion coefficient, the numerical values are not exact. This is because the formula is strictly applicable only for large colloidal particles in a fluid and not for small molecules.

The diffusion coefficients in liquids and gases increase with temperature. In gases, the diffusion coefficient increases proportional to $\tau^{1/2}$, due to an increase in the root mean square velocity. Equation (3.5) indicates that the diffusion coefficient increases proportional to τ if the viscosity is a constant, due to an increase in the energy of the fluctuations. However, the viscosity of liquids decreases with temperature and so the diffusion coefficient increases faster than τ with an increase in the temperature.

3.1.3. *Diffusion in multicomponent systems.* So far, we have restricted attention to the diffusion of a solute in a solvent, and assumed that the solute concentration is small compared to that of the solvent. In this case, the motion of the solute does not cause a movement in the center of mass, and so there is no convective motion. However, when the solute and solvent concentrations are comparable, as well as in multicomponent systems, the motion of the solute could result in the motion of the center of mass. In this case, the constituents in the mixture have mean motion, which is the motion of the center of mass, as well as diffusive motion, which is motion relative to the center of mass.

3.2. **Momentum diffusion.** Using arguments similar to those used to estimate mass diffusivity in gases, the end result are the molecular definitions of dynamic and kinematic viscosities for gases:

$$\mu = \frac{5}{16d^2}\left(\frac{mk_{\mathrm{b}}\tau}{\pi}\right)^{1/2} \quad \text{and} \tag{3.6a}$$

$$\nu = \frac{5}{16nd^2}\left(\frac{k_{\mathrm{b}}\tau}{\pi m}\right)^{1/2}, \tag{3.6b}$$

where $\nu = \mu/\rho$ is the *kinematic viscosity* or the *momentum diffusivity*.

From eq. (3.4) and eq. (3.6), it can be seen that the self diffusivity ϕ_{11} and the kinematic viscosity ν are proportional to each other and the Schmidt number $\pi_{\mathrm{sc}} = \phi_{11}/\nu = 6/5$ for monoatomic gases of spherical molecules. In real gases, the Schmidt number varies between 1.32 and 1.4 for most polyatomic gases, but has a lower value between 1.25 and 1.3 for monoatomic gases. This discrepancy is because the actual pair potential between the gas molecules is not the hard sphere potential, but resembles the Lennard-Jones potential, which has an attractive component. Values between 1.32 and 1.36 are obtained for gases which interact by the Lennard-Jones potential. However, in all cases, the momentum and mass diffusivity in gases are of the same order of magnitude. The momentum diffusivity also increases with temperature, because the root mean square velocity increases as $\sqrt{\tau}$, whereas the mean free path is independent of temperature and depends only on the density. The momentum diffusivity decreases as the density is increased, because the mean free path decreases.

The momentum diffusivity for liquids turns out to be much higher than the mass diffusivity of liquids, because the transport of momentum does not require the physical motion of individual molecules, and is therefore not restricted by the collective rearrengement required for the translation of a molecule. Consequently, the momentum diffusivity in liquids

is only about one order of magnitude smaller than the mass diffusivity; for example, the kinematic viscosity of water is $1 \times 10^{-6}\,\mathrm{m^2/s}$ at $20\,^\circ\mathrm{C}$ and atmospheric pressure, whereas that for air is $1.5 \times 10^{-5}\,\mathrm{m^2/s}$ under the same conditions. Therefore, the Schmidt number for liquids of small molecules is about $10^{-3}\,\mathrm{m^2/s}$. The momentum diffusivity in liquids also decreases with an increase in temperature, in contrast to gases where it increases with an increase in pressure. This is due to the difference in the structure of gases and liquids. Since the molecules in a liquid are densely packed, neighboring molecules are located at the position corresponding to the potential energy minimum of the central molecule. In this case, the relative motion of the molecules is an activated process which has an energy barrier, and transport across this barrier is easier as the temperature is increased. This results in a lower stress requirement for a given strain rate, and consequently a lower kinematic viscosity.

3.3. **Thermal diffusion.** Thermal diffusion is the process of transfer of energy due to the random motion of molecules when there is a variation in the temperature in the system. In a gas, thermal diffusion takes place due to the physical motion of molecules across a surface in the gas when there is a temperature variation across the surface. In this case, the energy density ϵ is defined as the average energy per unit volume, in a manner analogous to the particle density, η, the mass of solute per unit volume. Consider a surface at $z = 0$ across which there is a variation in the temperature, and therefore a variation in ϵ. The flux of energy, which is the rate of transfer of energy per unit area downward through the surface, analogous to eq. (3.1), is given by

$$e''_{z-} = a_1^e u_{\mathrm{rms}} \left(\epsilon_0 + a_2^e \lambda \frac{\mathrm{d}\epsilon}{\mathrm{d}z} \right) ,$$

where a_1^e and a_2^e are $O\,[1]$ numbers. The average rate of transport of energy per unit area upward through the surface, analogous to eq. (3.2), is

$$e''_{z+} = a_1^e u_{\mathrm{rms}} \left(\epsilon_0 - a_2^e \lambda \frac{\mathrm{d}\epsilon}{\mathrm{d}z} \right) .$$

Using these, the total energy flux is

$$e''_z = -\phi \frac{\mathrm{d}\epsilon}{\mathrm{d}z} ,$$

where ϕ is the *thermal diffusivity*, with dimensions of L^2/T. The thermal conductivity is obtained by expressing the energy in terms of the temperature, $\epsilon = mnc_v\tau$, where c_v is the specific thermal at constant volume, defined as the energy per unit mass, to obtain

$$e''_z = -k \frac{\mathrm{d}\tau}{\mathrm{d}z} ,$$

where

$$k = 2a^e u_{\mathrm{rms}} \lambda mnc_v .$$

The thermal conductivity has units of $\mathsf{ML/T\Theta}$. A more exact calculation can be carried out using kinetic theory in order to remove the uncertainty in the value of a^e, and the result for a monoatomic gas of spherical molecules is

$$k = \frac{5}{2}c_v\mu \tag{3.7a}$$

$$= \frac{75}{64d^2} \left(\frac{k_{\mathrm{b}}^3 \tau}{\pi m} \right)^{3/2} . \tag{3.7b}$$

In deriving the above thermal conductivity, the value $c_v = 3k_{\mathrm{b}}/2m$ has been used. The diffusivity and thermal conductivity are related by

$$\phi = \frac{k}{nmc_v} = \frac{k}{\rho c_v} ,$$

where ρ is the mass density.

Equation (3.7b) for the thermal conductivity is in agreement with experimental results for monoatomic gases to within $1\,\%$ at STP. Equation (3.7b) is not applicable for diatomic and polyatomic gases, especially for gases of polar molecules, since there is an exchange between the translational and internal energy modes. The ratio of the momentum and

thermal diffusivity, $c_p \mu / k$, is known as the Prandtl number, π_{pr}. This ratio is predicted to be $(2/3)$ for monoatomic gases of spherical molecules, and experimentally observed values vary between 0.66 for unimolecular gases such as neon and argon, to a maximum of about 0.95 for water at boiling point at atmospheric pressure. For polyatomic molecules, there is a transfer of energy between the translational and internal modes, and a correlation of the type

$$\pi_{\mathrm{pr}} = \frac{c_p}{c_p + 1.25 r_{\mathrm{g}}}$$

is found to provide good predictions.

4. Unidirectional transport

In this chapter, we consider transport in which there is a variation in the mass, momentum and temperature fields in only one dimension. The analysis is considerably simplified in this case, since there is only one spatial coordinate to be considered. However, the examples solved here illustrate the basic principles of the solution of more complex problems in multiple dimensions, which involve shell balances to derive differential equations for the concentration, velocity and temperature fields, and then an integration procedure for determining the variations in the concentration, velocity and temperature.

4.1. **Solutions to the diffusion equation.**

4.1.1. *Unsteady transport into an infinite fluid.*
Mass transfer. Consider a flat surface in the xy plane located at $z = 0$ through which a solvent diffuses into the fluid. The plane surface is assumed to be of infinite extent in the xy plane, and the height of the fluid supported by the plane is also considered to be of infinite extent. Initially, the concentration of the solute in the solvent at the surface [3] is c_∞. At time $t = 0$, the solute concentration at the surface is instantaneously increased to c_0, and there is diffusion of the solute into the solvent. We would like to determine the variation of the concentration of the solute with time.

As the diffusion proceeds, there is transport of solute from the surface to the solvent, resulting in an increase in the concentration near the surface. However, the concentration far from the surface $z \to \infty$ remains unchanged at $c = c_\infty$. The conditions for the concentration field at the spatial boundaries and at the initial time are

$$c = \begin{cases} c_\infty & \text{for all } t \text{ as } z \to \infty; \\ c_0 & \text{for all } t > 0 \text{ at } z = 0; \\ c_\infty & \text{for all } z > 0 \text{ at } t = 0. \end{cases}$$

The solution is simplified by non-dimensionalizing (scaling) the concentration:

$$\bar{c} = \frac{c - c_\infty}{c_0 - c_\infty}.$$

Note that, as in thermal transport, the driving force is not bare c, but a change thereof, Δc. Using such a non-dim, the conditions for $\bar{c}$ become

$$\bar{c} = \begin{cases} 0 & \text{for all } t \text{ as } z \to \infty; \\ 1 & \text{for all } t > 0 \text{ at } \bar{c} = 0; \\ 0 & \text{for all } z > 0 \text{ at } t = 0. \end{cases}$$

Thermal transfer. The configuration consists of a flat surface in the xy plane of infinite extent and a fluid of thermal conductivity k and specific thermal capacity c_p in the half space $z > 0$. Initially, the temperature of the fluid and the surface is τ_∞. At time $t = 0$, the temperature of the surface is instantaneously increased to τ_0. Determine the temperature as a function of time.

As conduction proceeds, there is a transport of energy from the surface to the fluid, resulting in an increase in the temperature of the fluid. However, the temperature at a

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[3] c_∞ does not mean infinite concentration, but it refers to the concentration at a very long distance. This is analogous to the case of a hot body being cooled by a fluid stream. The body temperature can be denoted by τ_{b} and the fluid temperature constant at a long distance can be denoted by τ_∞.

large distance from the surface, $z \to \infty$, remains at $\tau = \tau_\infty$. Therefore, the conditions for the temperature at the spatial boundaries of the fluid and at initial time are

$$\tau = \begin{cases} \tau_\infty & \text{for all } t \text{ as } z \to \infty; \\ \tau_0 & \text{for all } t > 0 \text{ at } z = 0; \\ \tau_\infty & \text{for all } z > 0 \text{ at } t = 0 \,. \end{cases}$$

The solution is simplified by non-dimensionalizing (scaling) the temperature:

$$\bar{\tau} = \frac{\tau - \tau_\infty}{\tau_0 - \tau_\infty} \,.$$

The conditions for $\bar{c}$ become

$$\bar{\tau} = \begin{cases} 0 & \text{for all } t \text{ as } z \to \infty; \\ 1 & \text{for all } t > 0 \text{ at } z = 0; \\ 0 & \text{for all } z > 0 \text{ at } t = 0 \,. \end{cases}$$

Momentum transfer. The configuration consists of an infinite fluid in the $z > 0$ half space bounded by an infinite flat surface in the xz plane. The fluid and the surface are initially at rest. At time $t = 0$, the plane is instantaneously moved with a constant velocity u in the x direction. Determine the fluid velocity as a function of time.

As time proceeds, the momentum that is transported from the surface diffuses through the fluid, resulting in fluid motion. However, the fluid at a large distance from the surface $z \to \infty$ remains at rest. If u_x is the fluid velocity in the x direction, it is convenient to define a non-dimensional fluid velocity $\bar{u}_x = u_x/u$. The conditions for the non-dimensional fluid velocity at the spatial boundaries of the flow and at initial time are

$$\bar{u}_x = \begin{cases} 0 & \text{for all } t \text{ as } z \to \infty; \\ 1 & \text{for all } t > 0 \text{ at } z = 0; \\ 0 & \text{for all } z > 0 \text{ at } t = 0 \,. \end{cases}$$

Shell balance. In all three cases, mass, thermal and momentum transfer, the boundary and initial conditions are identical in form. Since the transport in all three cases involves diffusion in the direction perpendicular to the surface, and no variation along the surface, it is anticipated that the differential equation governing the transport will also be identical in form. The differential equation for the concentration field is first derived using a shell balance, and the analogous equations for heat and momentum transfer are provided.

Consider a non-moving shell of thickness Δz in the z coordinate and of thickness Δx and Δy in the xy plane. There is a transport of mass across the surfaces of the shell due to diffusion, which results in a change in the concentration in the shell. We consider the variation in the concentration within this control volume over a time interval Δt. Mass conservation requires that

$$\begin{pmatrix} \text{accumulation of mass} \\ \text{in the shell} \end{pmatrix} = \begin{pmatrix} \text{input of mass} \\ \text{into the shell} \end{pmatrix} - \begin{pmatrix} \text{output of mass} \\ \text{from the shell} \end{pmatrix}$$

The accumulation of mass in a time Δt is given by

$$\begin{pmatrix} \text{accumulation of mass} \\ \text{in the shell} \end{pmatrix} = \left(c\left[\xi, t + \Delta t\right] - c\left[\xi, t\right] \right) \Delta x \Delta y \Delta z \,.$$

The mass flux at the surface at z is given by

$$m_z'' = -\phi \frac{\partial c}{\partial z}\bigg|_z$$

and the mass entering the shell through the surface at z in a time interval Δt is given by the product of the mass flux, the area of transfer and the time interval Δt:

$$\begin{pmatrix} \text{input of mass} \\ \text{into the shell} \end{pmatrix} = -\Delta t \Delta x \Delta y \left(\phi \frac{\partial c}{\partial z}\bigg|_z \right) \,.$$

In a similar manner, the mass leaving the surface at $z + \Delta z$ is given by

$$\begin{pmatrix} \text{output of mass} \\ \text{from the shell} \end{pmatrix} = -\Delta t \Delta x \Delta y \left(\phi \frac{\partial c}{\partial z}\bigg|_{z+\Delta z} \right) \,.$$

Substituting the last equations in the mass balance equation and dividing by $\Delta t \Delta x \Delta y \Delta z$, we have

$$\frac{c\left[\xi, t+\Delta t\right] - c\left[\xi, t\right]}{\Delta t} = \frac{1}{\Delta z}\left(\phi \frac{\partial c}{\partial z}\bigg|_{z+\Delta z} - \phi \frac{\partial c}{\partial z}\bigg|_{z}\right).$$

The limits $\Delta t \to 0$ and $\Delta z \to 0$ are taken to obtain a partial differential equation for the concentration field:

$$\frac{\partial c}{\partial t} = \frac{\partial}{\partial z}\left(\phi \frac{\partial c}{\partial z}\right).$$

If the diffusion coefficient is independent of the spatial position, then the differential equation reduces to

$$\frac{\partial c}{\partial t} = \phi \frac{\partial^2 c}{\partial z^2} \implies \partial_t c = \phi \partial_{zz} c.$$

The last equation can be scaled by using $\bar{c}$:

$$\partial_t \bar{c} = \phi \partial_{zz} \bar{c}.$$

A similar shell balance procedure can be carried out for thermal transfer. The equation for the temperature field is

$$\frac{\partial \bar{\tau}}{\partial t} = \frac{\partial}{\partial z}\left(\phi \frac{\partial \bar{\tau}}{\partial z}\right) \implies \partial_t \bar{\tau} = \partial_z \left(\partial_z \bar{\tau}\right).$$

Though the final result for the momentum transfer process is exactly analogous to those of mass and thermal transport, the procedure is slightly different. We provide a brief outline of the calculation. First, note that there are now two directions in the problem. Since momentum is a vector, there is a direction associated with the momentum itself, which is the x direction. The second is the direction of diffusion, which is the z direction. The fundamental balance relation is

$$\begin{pmatrix} \text{rate of change of} \\ x \text{ momentum} \\ \text{in the shell} \end{pmatrix} = \begin{pmatrix} \text{sum of forces} \\ \text{in the } x \text{ direction} \end{pmatrix}.$$

The rate of change of momentum in the differential volume of thickness Δz about z in a time interval Δt is given by

$$\begin{pmatrix} \text{rate of change of} \\ x \text{ momentum} \\ \text{in the shell} \end{pmatrix} = \frac{\rho \Delta u_x \Delta x \Delta y \Delta z}{\Delta t}.$$

The forces acting on the two surfaces at z and $z + \Delta z$ are the products of the shear stress τ_{xz} and the surface area $\Delta x \Delta y$. It is important to keep track of the directions of the forces in this case, since the force is a vector. The shear stress τ_{xz} is defined as the force per unit area in the x direction acting at a surface whose outward unit normal is in the positive z direction. For the surface at $z + \Delta z$, the outward unit normal is in the $+z$ direction and, therefore, the force per unit area at this surface is $+\tau_{xz}|_{z+\Delta z}$. For the surface at z, the outward unit normal is in the $-z$ direction, and therefore the force per unit area at this surface is $-\tau_{xz}|_z$. Finally, the rate of change of momentum, which is the change in momentum per unit time, is given by $(\rho \Delta u_x)(s\Delta z)/\Delta t$. Therefore, the momentum balance equation is

$$s\Delta z \frac{\rho \Delta u_x}{\Delta t} = s\left(\tau_{xz}\bigg|_{z+\Delta z} - \tau_{xz}\bigg|_{z}\right).$$

Dividing through by $s\Delta z$, we obtain

$$\rho \frac{\Delta u_x}{\Delta t} = \frac{\tau_{xz}\bigg|_{z+\Delta z} - \tau_{xz}\bigg|_{z}}{\Delta z}.$$

Taking the limit $\Delta t \to 0$ and $\Delta z \to 0$, we obtain the partial differential equation

$$\rho \partial_t u_x = \partial_z \tau_{xz}.$$

The shear stress is given by the product of the viscosity and the gradient of the velocity

$$\tau_{xz} = \mu \lim_{\Delta z \to 0} \frac{\Delta u_x}{\Delta z} = \mu \frac{\partial u_x}{\partial z} \implies \tau_{xz} = \mu \partial_z u_x.$$

With this, the governing equation for the velocity field becomes

$$\rho \partial_t u_x = \partial_z \mu \partial_z u_x \,.$$

Note that the differential equation derived above has the same form as the concentration and energy diffusion equations, although it was derived from a force balance. This indicates that the diffusion process is the same for mass, momentum and energy. However, it should be noted that momentum could be transmitted by pressure forces in addition to viscous forces, and there is no analogue of pressure in mass and energy transport.

When the velocity u_x is scaled by u, the velocity of the bottom surface, the momentum equation becomes

$$\partial_t \bar{u}_x = \partial_z \nu \partial_z \bar{u}_x \,,$$

where $\nu = \mu/\rho$ is the momentum diffusivity (kinematic viscosity).

Solution. The conservation equations for mass, thermal energy and momentum are summarized as

$$\partial_t \bar{c} = \phi \partial_{zz} \bar{c} \,,$$
$$\partial_t \bar{\tau} = \phi \partial_{zz} \bar{\tau} \,,$$
$$\partial_t \bar{u}_x = \nu \partial_{zz} \bar{u}_x \,,$$

with boundary conditions:

$$\bar{c} = \bar{\tau} = \bar{u}_x = \begin{cases} 0 & \text{for all } t \text{ as } z \to \infty; \\ 1 & \text{for all } t > 0 \text{ at } z = 0; \\ 0 & \text{for all } z > 0 \text{ at } t = 0 \,. \end{cases}$$

Since such conservation equations are identical in form and the boundary conditions are also identical, then the same solution procedure can be used for all these and the solutions for the concentration, velocity and temperature fields, expressed in terms of the dimensionless variables $\bar{c}$, $\bar{\tau}$ and $\bar{u}_x$, turn out to be identical.

In order to solve the concentration equation with its boundary conditions, it is first important to realize that there no intrinsic length scale in the problem, because the fluid and the flat plate are of infinite extent. Since the concentration $\bar{c}$ is dimensionless, there are only three dimensional variables z, t and ϕ in the problem. These contain two dimensions, $\{\mathsf{L}, \mathsf{T}\}$, and it is possible to construct only one dimensionless number, $\pi = z/\phi t$. Therefore, just from dimensional analysis, it can be concluded that the concentration field does not vary independently with z and t, but only on the combination π. If this inference is correct, it should be possible to express the conservation equation in terms of the variable π alone. When z and t are expressed in terms of π, the concentration equation becomes

$$-\left(\frac{z}{2\phi^{1/2}t^{3/2}} \right) \frac{\partial \bar{c}}{\partial \pi} = \frac{\mathrm{d}}{\mathrm{d}t} \frac{\partial^2 \bar{c}}{\partial \pi^2} \,.$$

After multiplying throughout by t, the equation for the concentration field reduces to

$$\frac{\pi}{2} \frac{\partial \bar{c}}{\partial \pi} + \frac{\partial^2 \bar{c}}{\partial \pi^2} = 0 \implies \pi \partial_\pi \bar{c} + 2 \partial_{\pi\pi} \bar{c} = 0 \,.$$

The last equation validates the inference that the non-dimensionalized concentration field is only a function of π. It is also necessary to transform the boundary conditions into conditions for the π coordinate. The transformed boundary conditions are

$$\bar{c} = \begin{cases} 0 & \text{as } \pi \to \infty; \\ 1 & \text{at } \pi = 0; \\ 0 & \text{as } \pi \to \infty \,. \end{cases}$$

It is useful to note that the original conservation equation is a second order differential equation in z and a first order differential equation in t, so it requires two boundary conditions in the z coordinate and one initial condition. The conservation equation expressed in terms of π is a second order differential equation, which requires just two boundary conditions for π. The last equation shows that one of the boundary conditions for $z \to \infty$ and the initial condition $t = 0$ turn out to be identical conditions for $\pi \to \infty$ and, therefore, the transformation form $[z, t]$ produces no inconsistency in the boundary and initial conditions.

The equation $\pi\partial_\pi\bar{c} + 2\partial_{\pi\pi}\bar{c} = 0$ can be solved to obtain

$$\bar{c}\,[\pi] = \psi_1 + \psi_2 \int_\pi^\infty \mathrm{d}\pi' \, \exp\left[-\frac{\pi^2}{2}\right]\,.$$

The constants ψ_1 and ψ_2 are determined from the conditions $\bar{c} = 1$ at $\pi = 0$ and $\bar{c} = 0$ for $\pi = \infty$, to obtain

$$\bar{c}\,[\pi] = \sqrt{\frac{2}{\pi}} \int_\pi^\infty \mathrm{d}\pi' \, \exp\left[-\frac{\pi^2}{2}\right]\,,$$

where π is the geometrical constant.

From the solution, the last equation, it can be inferred that there is no intrinsic length scale in the system, but the length scale for the z coordinate is a function of time and proportional to $\sqrt{\phi t}$ at time t. Thus, the length scale over which diffusion has taken place increases proportional to $t^{1/2}$. Thus, this equation will be a solution for the concentration diffusion in a configuration bounded by two plates, so long as the distance between the two plates, say l, is large compared to $\sqrt{\phi t}$.

4.1.2. *Steady diffusion into a falling film.* This problem is a simplification of the actual diffusion in a falling film, which involves a combination of convection and diffusion. A thin film of fluid flows down a vertical surface. One side of the film is in contact with a gas which is soluble in the liquid, and as the liquid flows down, the gas is dissolved in the liquid. The concentration of gas in the liquid at the entrance is c_∞, while the concentration of gas at the liquid-gas interface is c_0. The difference in concentration between the initial concentration in the liquid and the concentration at the interface acts as a driving force for diffusion. The z coordinate is perpendicular to the gas-liquid interface, which is located at $z = 0$. We also assume that the penetration depth for the gas into the liquid (to be determined a little later) is small compared to the thickness of the liquid film, so that the boundary conditions in the z coordinate given by

$$\bar{c}\,[\pi] = \sqrt{\frac{2}{\pi}} \int_\pi^\infty \mathrm{d}\pi' \, \exp\left[-\frac{\pi^2}{2}\right]$$

are applicable. In addition, the boundary condition in the x coordinate is $c = c_\infty$ at $x = 0$.

4.1.3. *Diffusion in bounded channels.* Next we consider the problem of diffusion in a channel bounded by two walls separated by a distance l. Initially, the concentration of the fluid in the channel is equal to c_∞. At initial time, the concentration of the solute on the wall at $z = 0$ is instantaneously increased to c_0, while the concentration on the surface at $z = l$ remains equal to c_∞. The problem is to find the concentration field as a function of time. Similar problems can be formulated for thermal energy and momentum transfer.

The concentration field is first expressed in terms of the scaled concentration field $\bar{c}$ by

$$\bar{c} = \frac{c - c_\infty}{c_0 - c_\infty}\,.$$

The diffusion equation, obtained by a shell balance as before, is given by

$$\partial_t\bar{c} = \phi\partial_{zz}\bar{c}\,.$$

However, there is a modification in the boundary conditions:

$$\bar{c} = \begin{cases} 0 & \text{for all } t \text{ at } z = l; \\ 1 & \text{for all } t > 0 \text{ at } z = 0; \\ 0 & \text{for all } z > 0 \text{ at } t = 0\,. \end{cases}$$

In this case, it is not possible to effect a reduction to a similarity form, because there is an additional length scale l in the problem and so the z coordinate can be scaled by l. A scaled z coordinate is defined as $\bar{z} = z/l$ and the diffusion equation in terms of this coordinate is

$$\frac{\partial\bar{c}}{\partial t} = \frac{\phi}{l^2}\frac{\partial^2\bar{c}}{\partial\bar{z}^2}\,.$$

The above equation suggests that it is appropriate to define a scaled time coordinate $\bar{t} = \phi t/l^2$ and the conservation equation in terms of this scaled time coordinate is

$$\frac{\partial\bar{c}}{\partial\bar{t}} = \frac{\partial^2\bar{c}}{\partial\bar{z}^2} \implies \partial_{\bar{t}}\bar{c} = \partial_{\bar{z}\bar{z}}\bar{c}\,.$$

5. Conservation equations

Conservation equations are based on two principles: conservation laws and constitutive laws. The foundation of conservation laws are the mass conservation principle, the energy conservation principle and Newton's law for the conservation of momentum: the rate of change of momentum is equal to the sum of the applied forces.

There is a complication, however, when applying conservation laws to flow systems: fluids are transported with the mean flow, thus it's necessary to apply the principles in a reference frame moving with the fluid. Therefore, the time derivatives in the laws must be more carefully defined. There is a key concept to develop on a first instance: the *substantial derivative*.

5.1. **Cartesian coordinates.**

5.1.1. *Partial derivatives.* The partial time derivative of the concentration is the rate of change of concentration at a *fixed* location in space; *i.e.*, take a stationary, non-moving, control volume. Fixed the location of observation, determine then the change of concentration with time at this position. If the concentration at the position ξ at time t is $c[\xi, t]$ and the concentration at the position ξ at time $t + \Delta t$ is $c[\xi, t + \Delta t]$, then the partial derivative is written as

$$\frac{\partial c}{\partial t} = \partial_t c = \lim_{\Delta t \to 0} \frac{c[\xi, t + \Delta t] - c[\xi, t]}{\Delta t}.$$

Note that, since the position is fixed in space, then ξ is not a function of time.

5.1.2. *Substantial derivative.* Although the partial derivative is defined as the change in the value of the concentration at a point in the fluid, this does not reflect the change in the concentration in material volumes, because such volumes are convected with the flow. Therefore, the fluid volume which was located at ξ at time t would have moved to a new position $\xi + u\Delta t$ at time $t + \Delta t$, where u is the fluid velocity. The substantial derivative determines the change in concentration on material volumes moving with the fluid. If the fluid is moving in space, then the substantial derivative is defined as

$$\frac{\mathrm{d}c}{\mathrm{d}t} = \lim_{\Delta t \to 0} \frac{c[\xi + u\Delta t, t + \Delta t] - c[\xi, t]}{\Delta t} = \frac{\partial c}{\partial t} + \frac{\partial c}{\partial \xi^i} u^i = \partial_t c + u^i \partial_i c,$$

where Einstein summation convention was used.

The last equation can be written more compactly using the directional derivative notation:

$$\mathrm{d}_t c = \partial_t c + u^i \partial_i c = u \cdot \nabla c = \partial_t c + \nabla_u c.$$

where $\nabla_u c = u \cdot \nabla c$. Note that the time derivatives are different; *i.e.*, $\mathrm{d}_t c \neq \partial_t c$, that the last equation is written as a vectorial relationship, so it's independent of the underlying coordinate system, that the position is a function of t ($\xi[t]$) and that the scalar concentration field is a function of both position and time, $c = c[\xi[t], t]$.

5.1.3. *Conservation of mass.* The mass conservation equation simply states tha mass cannot be created or destroyed. Therefore, for any fluid volume,

$$\begin{pmatrix} \text{rate of mass} \\ \text{accumulation} \end{pmatrix} = \begin{pmatrix} \text{rate of mass} \\ \text{in} \end{pmatrix} - \begin{pmatrix} \text{rate of mass} \\ \text{out} \end{pmatrix}.$$

Consider now a control volume with size $\prod_{i=1}^{3} \Delta \xi^i$ and six faces. The rate of mass through the face at ξ^1 is $(\rho u^1)|_{\xi^1} \Delta \xi^2 \Delta \xi^3$, while the rate of mass out at $\xi^1 + \Delta \xi^1$ is $(\rho u^1)|_{\xi^1 + \Delta \xi^1} \Delta \xi^2 \Delta \xi^3$. Similar expressions can be written for the rates of mass flow through the other four faces. The total increase in mass for this volume is $\partial_t \rho \Delta \xi^1 \Delta \xi^2 \Delta \xi^3$. Therefore,

the mass conservation equation states that

$$\Delta\xi^1\Delta\xi^2\Delta\xi^3\frac{\partial\rho}{\partial t} = +\Delta\xi^2\Delta\xi^3\left(\left.\left(\rho u^1\right)\right|_{\xi^1} - \left.\left(\rho u^1\right)\right|_{\xi^1+\Delta\xi^1}\right)$$
$$+\Delta\xi^1\Delta\xi^3\left(\left.\left(\rho u^2\right)\right|_{\xi^2} - \left.\left(\rho u^2\right)\right|_{\xi^2+\Delta\xi^2}\right)$$
$$+\Delta\xi^1\Delta\xi^2\left(\left.\left(\rho u^3\right)\right|_{\xi^3} - \left.\left(\rho u^3\right)\right|_{\xi^3+\Delta\xi^3}\right).$$

Dividing by the volume $\prod_i\Delta\xi^i$ and taking the limit as these approach zero, we get

$$\partial_t\rho = -\partial_i\rho u^i.$$

The above equation can often be written using the substantial derivative

$$\partial_t\rho + u^i\partial_i\rho = -\rho\partial_i u^i.$$

The left side of the above equation is the substantial derivative, while the right side can be written as

$$\partial_t\rho = -\rho\left(\nabla\cdot u\right) = -\rho\operatorname{div}u,$$

where the dot product has the usual connotation, div is the divergence operator and the geometric derivative ∇ is defined as $\nabla = \gamma^i\partial_i$, where the elements of the frame $\{\xi^i\}$ are the unit vectors in the direction of the coordinate axes.

The above equation describes the change in density for a material element of fluid which is moving along with the mean flow. A special case is when the density does not change, so that $\partial_t\rho$ is identically zero. In this case, the continuity equation reduces to

$$\operatorname{div}u = \partial_i u^i = 0.$$

This is just the symmetric part of the rate of deformation tensor. As we had seen in the previous lecture, this symmetric part corresponds to volumetric compression or expansion. Therefore, if this is zero, it implies that there is no volumetric expansion or compression, and if mass is conserved then the density has to be a constant. Fluids which obey this condition are called *incompressible* fluids. Most fluids that we use in practical applications are incompressible fluids; in fact all liquids can be considered incompressible for practical purposes. Compressibility effects only become important in gases when the speed of the gas approaches the speed of sound, $332\,\mathrm{m/s}$.

5.1.4. *Diffusion equation for the concentration field.* The diffusion equation for the concentration field, c, can be determined in a manner similar to that for the density. However, in this case, the transport across the cubic faces takes place due to mean convection as well as due to the diffusion flux across the surfaces:

$$\partial_t c + \partial_i c u^i = -\left(\operatorname{div}m''\right).$$

This equation can also be written as

$$\partial_t c + \nabla\cdot cu = -\left(\operatorname{div}m''\right),$$

where the vector flux m'' is defined as $\gamma_i m''^i$.

The flux is expressed in terms of the concentration field as $m'' = \phi\operatorname{grad}c$. Using this, the equation for the concentration field is

$$\partial_t c + \nabla\cdot cu = \nabla\cdot\phi\nabla c.$$

If the diffusion coefficient is a constant, the equation for the concentration field becomes

$$\partial_t c + \nabla\cdot cu = \phi\nabla^2 c = \phi\operatorname{lap}c,$$

where $\nabla^2 = \operatorname{lap} = \partial_{ii}$ is the Laplace operator in Cartesian coordinates.

Using the definition of substantial derivative:

$$\mathrm{d}_t c = \phi\operatorname{lap}c,$$

The concentration equation assumes a slightly different form if it is expressed in terms of the mass fraction (mass per unit solution mass), instead of the concentration (mass per

Quantity	Symbol	Dimension
Thermal transfer rate	e'	E/T
Linear dimension of the body	l	L
Stream velocity	u	L/T
Temperature difference	τ	Θ
Volumetric thermal capacity of the liquid	c	E/L$^3\Theta$
Liquid thermal conductivity	k	E/LTΘ

TABLE 2. Relevant quantities and their dimensions for the calculation of the thermal transfer rate from a body to a fluid.

unit solution volume) of the component in a solution. The concentration is related to the mass fraction w by $c = \rho w$, so the equation for the mass fraction is

$$\partial_t \rho w + \nabla \cdot \rho w c = \phi \operatorname{lap} \rho w \,.$$

From this, if we subtract w times the mass conservation equation, we get thus

$$\rho \left(\partial_t w + u \cdot \nabla w \right) = \phi \operatorname{lap} \rho w$$

or, using the definition of substantial derivative,

$$\rho \mathrm{d}_t w = \phi \operatorname{lap} \rho w \,,$$

5.1.5. *Energy conservation equation.* The conservation equation for the energy density, ϵ, derived using procedures similar to that for the concentration equation, is

$$\partial_t \epsilon + \nabla \cdot \epsilon u = \nabla \cdot k \operatorname{grad} \tau \,,$$

where k and $k \operatorname{grad} \tau$ is the energy flux due to temperature gradients. The energy density is given by $\rho c_p \tau$, where τ is the thermodynamic temperature. With this, the energy equation becomes

$$\partial_t \rho c_p \tau + \nabla \cdot \rho c_p \tau u = \nabla \cdot k \operatorname{grad} \tau \,.$$

From this, we can subtract $c_p \tau$ times the mass conservation equation, to obtain

$$\rho c_p \left(\partial_t \tau + u \cdot \nabla \tau \right) = \nabla \cdot \phi \nabla \tau$$

or, using the definition of substantial derivative and assuming k to be constant,

$$\rho c_p \mathrm{d}_t \tau = \phi \operatorname{lap} \tau \,.$$

5.2. **Elements of vector calculus.** div, grad, curl and all that :).

5.3. **Diffusion equation in polar, cylindrical and spherical coordinates.** :(, super long without GA, GC and index notation :).

Note: since the derived equations are in vector form, they don't change. What changes is the form of the Laplacian :). Once this is found for the different coordinate systems, everything is downhill. One key piece in finding the Laplacian is to define tangent unit vectors as $\gamma_i = \partial_i \xi^i$ and to define normal unit vectors as $\gamma^i = \operatorname{grad} \xi$.

6. EXAMPLES

Some examples on the use of dimensional analysis and dimensionless quantities.

Example. A solid body, of definite geometric shape, is fixed in a stream of liquid and maintained at a definite temperature higher than the temperature of the liquid at points remote from the body. It's required to find the rate at which thermal energy is transferred from the body to the liquid.

Solution. The first step is to identify relevant transport properties and material properties; then, to choose a suitable dimensionally independent set, in the present case $\{E, L, T, \Theta\}$; and finally to express all the relevant quantities using the chosen set. The result of this process is shown in table 2.

The second step is to find out the number of dimensionless numbers, n, using the π-theorem. In the present case, $n = 6 - 4 = 2$.

Quantity	Symbol	Dimension
Thermal flux	e''	$\mathsf{H/TL}^2$
Pipe diameter	d	L
Pipe length	l	L
Average fluid velocity	u	$\mathsf{L/T}$
Fluid density	ρ	$\mathsf{M/L}^3$
Fluid viscosity	μ	$\mathsf{M/LT}$
Fluid specific thermal capacity	c_p	$\mathsf{H/M\Theta}$
Thermal conductivity	k	$\mathsf{H/LT\Theta}$
Temperature difference	$\Delta\tau$	Θ

TABLE 3. Relevant quantities and their dimensions for the thermal energy transfer to a fluid flowing in a pipe.

Then, form the first dimensionless quantity using the quantity being sought, e':

$$\pi_1 = \frac{e'}{lk\tau} \, .$$

By the same token, the second dimensionless quantity is found using the rest of the quantities that model the phenomenon:

$$\pi_2 = \frac{lcu}{k} \, .$$

Then, the form of the model equation is given by

$$\psi\left[\pi_1, \pi_2\right] = 0 \implies \pi_1 = f\left[\pi_2\right] \implies \frac{e'}{lk\tau} = \psi\left[\frac{lcu}{k}\right] \, .$$

[seek known dimensionless quantities]
Finally, the model can be written as

$$\frac{e'}{lk\tau} = \psi\left[\frac{lcu}{k}\right] \, . \hspace{4cm} \square$$

Example. A fluid flows through a pipe heated from the outside. The temperature of the wall of the pipe is higher than the average temperature of the fluid by a constant value $\Delta\tau$. The change in temperature of the fluid is due to the thermal transfer from the walls and not due to frictional heating generated by the flow. One would like to predict the rate of thermal transfer, per unit area of the wall of the pipe, so that the length of pipe required for the heat exchanger can be designed.

Solution. The first step is to collect the set of variables on which the thermal flux e'' may depend. This can depend on the thermal properties of the fluid, the conductivity k, the specific thermal capacity c_p, the difference in temperature between the fluid and the wall $\Delta\tau$, the flow properties of the fluid, the density ρ, dynamic viscosity μ, the average fluid velocity u, the diameter of the pipe d and the length of pipe l. The fundamental dimensions that we can classify these quantities into are $\{\mathsf{M}, \mathsf{L}, \mathsf{T}, \Theta\}$.

There are nine dimensionless groups and four dimensions in table 3, apparently necessitating five dimensionless groups. However, a further reduction is possible when *there is no interconversion between thermal energy (being transferred) and mechanical energy (driving the flow)*. In this case, it is possible to consider heat energy as a dimension H, because it is different from mechanical energy. There are now five dimensions, $\{\mathsf{H}, \mathsf{M}, \mathsf{L}, \mathsf{T}, \Theta\}$, and a total of nine dimensional quantities in table 3. Therefore, there are only four dimensionless groups.

Of the dimensionless groups, the easiest one to is the ratio l/d of the length and diameter of the pipe. The dimensionless group containing e'' is the *dependent* dimensionless quantity, which contains the dependent quantity, which has to be determined as a function of all the other *independent* quantities in the problem. For the independent variable e'', the relation is of the form

$$e'' d^a k^b \Delta\tau^c \mu^d \rho^e = \pi_1 \, .$$

The above relations can easily be solved to obtain $a = 1$, $b = c = -1$ and $d = e = 0$. Using these, the dimensionless group is

$$\pi_1 = \pi_{\mathrm{nu}} = \frac{e'' d}{k \Delta\tau} \, .$$

The previous dimensionless quantity is known as the *Nusselt number*. In thermal transfer at a boundary (surface) within a fluid, the Nusselt number is the ratio of convective to conductive

Quantity	Symbol	Dimension	Modified dimension
Mass flux	m''	M/L^2T	M_s/L^2T
Diffusion coefficient	ϕ	L^2/T	
Concentration difference	Δc	M/L^3	M_s/L^3
Particle diameter	d	L	
Particle velocity	u	L/T	
Fluid density	ρ	M/L^3	
Fluid viscosity	μ	M/LT	

TABLE 4. Relevant quantities and their dimensions for the mass transfer to a particle.

thermal transfer across (normal to) the boundary. In this context, convection includes both advection and conduction.

Of the two other dimensionless groups, one can easily be identified as the Reynolds number, $\pi_{\mathrm{re}} = \rho u d / \mu$, the ratio of inertia and viscosity for this case. The second dimensionless group contains the specific thermal energy capacity, c_p. Since c_p contains both the thermal energy and mass dimensions, the dimensionless quantities has to contain the thermal conductivity, k, as well as the (viscosity μ or density ρ). The dimensionless quantity constructed with the specific thermal energy, viscosity and conductivity is the Prandtl number,

$$\pi_{\mathrm{pr}} = \frac{c_p \mu}{k} \; .$$

Therefore, the general expression for the average thermal flux can be written as

$$\frac{e'' d}{k \Delta \tau} = \psi \left[\frac{l}{d}, \frac{\rho u d}{\mu}, \frac{c_p \mu}{k} \right]$$

or, more compactly, as

$$\pi_{\mathrm{nu}} = \psi \left[\frac{l}{d}, \pi_{\mathrm{re}}, \pi_{\mathrm{pr}} \right] \; .$$

Dimensional analysis has certainly simplified the problem, since it is much easier to deal with relationships between four dimensionless quantities, rather than with nine dimensional quantities. However, it is not possible to obtain further simplification using dimensional analysis. There are two possible ways to further simplify the problem. One is to do further analytic calculations that incorporate the details of the thermal and mass transfer processes. The other is to perform experiments and then to obtain empirical correlations between the parameters. In the latter case, it is sufficient to consider the variation in the thermal flux for variations in the dimensionless quantities alone and it is not necessary to examine variations in individual quantities.

Example. Consider a stirred tank reactor for heterogeneous catalysis, where the reactants and products are in solution and the catalyst is in the form of solid particles. The dissolved reactant R diffuses to the surface of the suspended catalyst particle, reacts at the surface and the product diffuses back into the fluid. It is necessary to determine the average flux of the reactant to the surface, given the difference in concentration $\Delta c = c_\infty - c_s$, where c_∞ is the concentration in the bulk and c_s is the surface concentration. There is also relative motion of characteristic velocity u between the catalyst particle and the fluid, due to stirring.

Solution. The different dimensional quantities of relevance are presented in table 4.

The choice of dimensional quantities requires further discussion. It is clear that the average mass flux depends on the bulk concentration, the diffusion coefficient and the particle diameter. However, it is also necessary to include the fluid density, viscosity and the particle velocity relative to the fluid for the following reason. When the particle moves relative to the fluid, the generated flow pattern alters the distribution of the solute around the particles and thereby modifies the diffusion flux at the particle surface. The flow pattern, in turn, depends on the fluid viscosity, density and the flow velocity, and, therefore, the average mass flux could also depend on these.

In table 4, there are seven dimensional quantities and three dimensions. On this basis, we would expect that there are four dimensionless quantities. However, a further simplification can be made by distinguishing between the mass dimension in the mass transport (the solute mass) and that in the flow dynamics (the mass of the total fluid). The flux and the diffusion coefficient contain the mass of the solute, whereas the mass of the fluid (solute plus solvent) appears in the density and fluid viscosity. If the solute concentration does not affect the fluid density and viscosity, we

can make a distinction between the mass dimension for the solute, M_s, from the mass dimension for the fluid, M. In the modified dimensions shown in table 4, the mass flux and the diffusion coefficient depend on the solute mass M_s, while the density and viscosity depend on the fluid mass M. There are now four dimensions, $\{M, M_s, L, T\}$, and therefore there are only three dimensionless quantities.

The first dimensionless group can be constructed by non-dimensionalizing the flux by the diffusion coefficient, the concentration difference and the particle diameter:

$$\pi_1 = m''(\Delta c)^a \phi^b d^c,$$

The indices a, b and c are determined from dimensional consistency to provide the dimensionless flux, called the Sherwood number,

$$\pi_{\mathrm{sh}} = \frac{m'' d}{\phi \Delta c}.$$

Two other dimensionless groups can be defined. One of the dimensionless numbers is the Reynolds number, $\pi_{\mathrm{re}} = \rho u d / \mu$, the ratio of fluid inertia and viscosity. The second dimensionless group can be defined in two ways. One possible definition is the Schmidt number, $\pi_{\mathrm{sc}} = \mu / \rho \phi$, the dimensionless combination of the diffusivity, viscosity and density. The alternate dimensionless group is the Peclet number, $\pi_{\mathrm{pe}} = u d / \phi$, constructed from the flow velocity, diameter and the mass diffusivity. If we use the Reynolds and Schmidt numbers, then the dimensionless flux can be expressed as

$$\pi_1 = \frac{m'' d}{\phi \Delta c} = \psi \left[\frac{\rho u d}{\mu}, \frac{\mu}{\rho \phi} \right]$$

or, equivalently,

$$\pi_{\mathrm{sh}} = \psi \left[\pi_{\mathrm{re}}, \pi_{\mathrm{pe}} \right]. \qquad \qquad \square$$

Example. In designing new processes, it is not sufficient to study the the process on the laboratory scale, but to also study the exact industrial set up on a small scale before building a larger scale industrial apparatus. Dimensional analysis plays a very important role in industrial scale up. Scaling up cannot be done by multiplying all parameters by a given factor, but the dimensionless groups have to be kept a constant while scaling up. This will be illustrated using the example of a stirred tank reactor. In this, the fluid is stirred using an impeller of a certain shape, and the impeller is to be designed so that optimum mixing is achieved for minimum power.

Solution. For a given impeller shape, it is necessary to estimate the power consumption for stirring at a given frequency f. The power consumption will, in general, depend on the shape and dimension of the impeller, as well as the vessel, as well as other details such as baffles, etc. If we keep the relative ratios of the lengths of the impeller, vessel, baffles, etc., a constant, then there is only one length scale in the problem, which we will consider the impeller diameter d. In addition, the power can also depend on the density of the fluid, ρ, the fluid viscosity μ and the frequency of rotation f. An additional dependence arises on the acceleration due to gravity g. This is because sometimes during stirring, the interface of the fluid raises at the edges and lowers in the middle. This upward motion due to centrifugal forces is balanced by a downward force due to gravity and so gravity could also be an important factor. This is because it is important to ensure that the dimensions of the interface (curvature, extent of depression at the center) are also in the same proportion as the impeller diameter. When considering the interface, the surface tension (normally denoted by the symbol γ) is also a relevant parameter. The surface tension has dimensions of force/length of energy/area; *i.e.*, M/T^2. The relevant parameters with their dimensional dependencies are shown in table 5.

The dimensionless variables derived above have the following physical interpretations. The *power number*, $\pi_{\mathrm{po}} = p / f^3 d^5 \rho$, is the dimensionless quantity that involves the dependent variable, the power, which has to be determined as a function of all the other independent variables. This gives the ratio of the power required to the work done by centrifugal forces. On the other hand, the *Reynolds number*, $\pi_{\mathrm{re}} = \rho d^2 f / \mu$, is the ratio of centrifugal forces and viscous forces, or the ratio of convection and diffusion. The dimensionless group $f^2 d / g$ is the *Froude number*, which gives the ratio of centrifugal and gravitational forces. The dimensionless group $\rho f d^3 / \gamma$ is the *Weber number*, which is the ratio of centrifugal and surface tension forces.

Since there are seven variables and three dimensions, it is possible to create four dimensionless groups. Let us assume these four contain p, μ, g and γ expressed in terms of the other variables. Then, the four groups are $(p / f^3 d^5 \rho)$, $(f d^2 \rho / \mu)$, $(f^2 d / g)$ and $(\rho f^2 d^3 / \gamma)$. Therefore, the expression

Quantity	Symbol	Dimension
Power	p	$\mathsf{ML}^2/\mathsf{T}^3$
Frequency	f	$1/\mathsf{T}$
Diameter	d	L
Density	ρ	M/L^3
Viscosity	μ	M/LT
Gravity	g	L/T^2
Surface tension	γ	M/T^2

TABLE 5. Relevant quantities and their dimensions for the calculation of the power required for the impeller in a reactor.

for the power has to have the form:

$$\frac{p}{f^3 d^5 \rho} = \psi \left[\frac{f d^2 \rho}{\mu}, \frac{f^2 d}{g}, \frac{\rho f^2 d^3}{\gamma} \right].$$

It is instructive to determine the order of magnitudes of the different dimensionless quantities in the problem. The density of the liquid is usually of the order of $10^3 kg/m^3$, the viscosity of a very viscous fluid such as a polymer melt could be as high as 1kg/m.s and the surface tension of a liquid-gas interface is, at maximum, $0\,1kg/s^2$. If the frequency is of the order of $1\,rev/s\,to\,10\,rev/s$, the Froude number $f^2 d/g \sim 0.1\,to\,10$, indicating that both centrifugal and gravitational forces are important in the present problem. The Weber number $\rho f^2 d^3/\gamma \sim 104\,to\,106$, which is large, indicating that the surface tension effects are small when compared to inertial effects. Therefore, the effect of surface tension can be neglected in the present application. The Reynolds number $\rho d^2 f \mu \sim 103\,to\,104$, which is large. Therefore, it might naively be expected that viscous effects can be neglected in comparison to inertial effects. However, as it can be seen using analysis of boundary layers, diffusion *cannot* be neglected, because it is diffusive transport which is responsible for the transport of mass, momentum and energy at the bounding surfaces of the fluid. With the neglect of surface tension effects, the last relation reduces to

$$\frac{p}{f^3 d^5 \rho} = \psi \left[\frac{f d^2 \rho}{\mu}, \frac{f^2 d}{g} \right].$$

In a scale up,

the dimensionless numbers have to be kept a constant.

For example, we are interested in designing a reactor with an impeller diameter of $1m$ with a revolution of $10rev/s$ and the fluid in the reactor is water with density $1000kg/m^3$ and viscosity $10^{-3}kg/m.s$. In order to determine the performance, we design a smaller reactor with an impeller of size $10cm$. What is the fluid that should be used and what is the speed at which the reactor should operate? The speed of rotation can be determined from the consideration that the Froude number has to be a constant. If quantities for the big reactor are denoted with the subscript b and those for the small reactor are denoted by the subscript s, then for the Froude number to be a constant, we require

$$f_{\mathrm{b}}^2 d_{\mathrm{b}} = f_{\mathrm{s}}^2 d_{\mathrm{s}}.$$

Substituting the dimensions and the frequency of the big reactor, we get the impeller speed of the small reactor as $316rev/s$. The choice of fluid to be used in the small reactor is determined by the condition that the Reynolds number has to be a constant:

$$\frac{\rho_{\mathrm{b}} f_{\mathrm{b}} d_{\mathrm{b}}^2}{\mu_{\mathrm{b}}} = \frac{\rho_{\mathrm{s}} f_{\mathrm{s}} d_{\mathrm{s}}^2}{\mu_{\mathrm{s}}}.$$

Relating the frequency and diameters of the two reactors, we get

$$\frac{\rho_{\mathrm{s}}}{\mu_{\mathrm{s}}} = 31.6 \frac{\rho_{\mathrm{b}}}{\mu_{\mathrm{b}}}.$$

Finally since the Reynolds number and the Froude number are kept a constant between the two configurations, the Power number is also a constant

$$\frac{p_{\mathrm{b}}}{f_{\mathrm{b}}^3 d_{\mathrm{b}}^5 \rho_{\mathrm{b}}} = \frac{p_{\mathrm{s}}}{f_{\mathrm{s}}^3 d_{\mathrm{s}}^5 \rho_{\mathrm{s}}}.$$

Therefore, the ratio of the power required in the two configurations is

$$\frac{p_{\mathrm{b}}}{p_{\mathrm{s}}} = 3160 \frac{\rho_{\mathrm{b}}}{\rho_{\mathrm{s}}}.$$

Quantity	Symbol	Dimension
Elastic constant	κ	$\mathsf{F/L}$
Oscillation time	t	T
Volume of box	v	L^3
Density of liquid	ρ	$\mathsf{FT}^2/\mathsf{L}^4$
Acceleration of gravity	g	$\mathsf{L/T}^2$

TABLE 6. Relevant quantities and their dimensions for the calculation of the time of oscillation of a box attached to a spring.

Quantity	Symbol	Dimension
Pressure exerted by gas	p	$\mathsf{M/LT}$
Mass of the atom	m	M
Number of atoms per unit volume	n	$1/\mathsf{L}^3$
Absolute temperature	τ	Θ
Gas constant per atom	r_{g}	$\mathsf{ML}^2/\mathsf{T}^2\Theta$

TABLE 7. Relevant quantities and their dimensions for the calculation of the pressure exerted by an ideal gas in a box.

From the power requirement of the small reactor, the power estimate for the big reactor can be obtained using the above relation.

Example. Consider an elastic pendulum made by attaching a massless spring of elastic constant κ a box of volume v filled with a liquid of density ρ. The mass of the liquid is acted upon by gravity. We are required to find an expression for the time of oscillation.

Solution. A list of the quantities and their dimensions in the $\{\mathsf{F},\mathsf{L},\mathsf{T}\}$ system is presented in table 6.

In table 6, it can be seen that $n = 5 - 3 = 2$, thus π quantities must be constructed. However, one may notice that the volume of the box times the density of the liquid provides the mass of the liquid. This observation reduces the number of quantities from 2 to 1, where the mass of the system has the dimensions $\dim m = \mathsf{FT}^2/\mathsf{L}$. With this new set, one can write the only dimensionless quantity modeling the phenomenon

$$\pi = \frac{t}{\sqrt{m/\kappa}}\,.$$

Using this quantity, the model equation becomes

$$\psi\left[\pi\right] = 0\,,$$

where π is the zero of the function ψ. As function of the original quantities, density and volume, the model becomes

$$t = \pi\sqrt{\frac{v\rho}{\kappa}}\,,$$

where the value of the dimensionless quantity, π, must be experimentally determined.

Example. Let's apply the principles of dimensional analysis to a problem of kinetic theory of gases: to find the pressure exerted by a perfect gas.

Solution. The atoms of the gas in kinetic theory are considered as perfect spheres, completely elastic, and of negligible dimension compared with their distance apart. The only constant with dimensions required in determining the behavior of each atom is therefore its mass. The behavior of the aggregate of atoms as also characterized by the density of the gas or the number of atoms per unit volume. The problem domain is mechanics and the pressure exerted by the gas is to be found by computing the change of momentum per unit time and per unit area of the atoms striking the walls of the enclosure. The mechanics system of units is thus indicated. But, in addition to the ordinary mechanical features, there is the element of temperature to be considered. How does temperature enter in writing down the equations of motion of the system? The answer is through the gas constant, which gives the average kinetic energy of each atom as a function of the temperature. The analysis of the problem is summarized in table 7.

There are $n = 5 - 4 = 1$ dimensionless quantity to construct:

$$\pi = \frac{p}{nr_{\mathrm{g}}\tau}\,.$$

Note that, in the model, the pressure exerted by the gas is independent on the mass of the individual atoms.

7. ENERGY TRANSPORT

People goes to high place, water flows to low place

— JUNPING SHI,
PARTIAL DIFFERENTIAL EQUATIONS AND MATHEMATICAL BIOLOGY

All streams flow to the sea because it is lower than they are. Humility gives it its power.

— LAO TZU,
TAO TE CHING

The flame that burns twice as bright burns half as long.

— LAO TZU,
TAO TE CHING

Be careful with notation:

Caution. We use the prime notation (Lagrange's notation for derivatives) to express time rate changes; *e.g.*, when expressing a body internal energy time rate change: i', or, equivalently, $i' = \partial_t i$. Note that $\dim i' = \mathsf{E}/\mathsf{T}$.

Under the same dimensional basis, we also use the prime notation to express energy flows; *e.g.*, when expressing thermal flow, *aka* thermal power, e'; since $\dim e' = \mathsf{E}/\mathsf{T}$. The same applies for other flows, like work change rate, *aka* mechanical power, w'.

On the other hand, however, in order to preserve undecorated variables and similarly looking equations, we use an analogous notation for fluxes: the double prime notation; *e.g.*, when expressing thermal energy flux: e''. Note that now $\dim e'' = \mathsf{E}/\mathsf{L}^2\mathsf{T}$, which is *not* the second derivative of thermal energy with respect to time; *i.e.*, $e'' \neq \ddot{e} = \mathrm{d}_t\mathrm{d}_t e$.

Therefore, in the case of any doubt, use the physicist's best allies: mathematical interpretation, physical reasoning and dimensional analysis.

7.1. **Relation of thermal energy transfer and thermodynamics.**

7.1.1. *Theory.* Consider a body of mass m and volume v being heated by an inflow of *thermal energy*, *aka thermal flow* or *thermal power*, e'. Due to heating, the body expands and performs *work* onto the surroundings at a rate w'. While both processes take place, on the other hand, the body *internal energy* i changes, or accumulates, at a rate i' given by the *energy conservation principle*:

$$i' = e' - w',$$

where the IUPAC sign convention for thermodynamics was used to find the signs for the different terms.

The body internal energy is related to the body *thermodynamic temperature* θ via the phenomenological expression

$$i = cm\tau,$$

where c is a property of the body material called *specific thermal capacity* [4], defined as the capacity that a body has to store or release thermal energy, $\dim c = \mathsf{E}/\mathsf{M}\Theta$, and τ is the body thermodynamic temperature.

If $p\,\mathrm{d}v$ is the only work that occurs, then,

$$e' = pv' + i'.$$

---

[4] This property is called in literature *specific energy capacity*.

This last equation has two well-known special cases: when the body is allowed to expand freely, *constant pressure process*, and when expansion is constrained, *constant volume process*:

$$e' = \begin{cases} mc_v\tau', & \text{for constant volume processes; } i.e.,\ \mathrm{d}v = 0, \\ mc_p\tau', & \text{for constant pressure processes; } i.e.,\ \mathrm{d}p = 0, \end{cases}$$

where c_v is the *specific thermal capacity at constant volume* and c_p the *specific thermal capacity at constant pressure*.

When the body is made of an incompressible substance, then, for any pressure variation, $\mathrm{d}v = 0$ and thus the two specific capacities are equal:

$$c_v = c_p = c\,.$$

This approximation works well for solids and liquids. With this estimate, the energy conservation equation becomes

$$e' = i' = mc\tau'\,.$$

The work now is to solve the last equation to predict e. Finding the solution, however, is not possible at this stage, for i is not known *a priori*, so some principles must be added to complete the problem formulation. These principles are called *transport laws* or *constitutive equations* and are *not* a part of thermostatics. They include Fourier's law of thermal conduction, Newton's law of cooling and Stephan-Boltzmann's law of thermal radiation. Moreover, constitutive equations express physical quantities, in this case the internal energy i and thermal energy e, in terms of *state variables*, in this case temperature τ.

7.1.2. *Technical notes.* Some technical notes on energy transfer theory.

Technical note. The mathematical treatment of physical phenomena of systems composed of many particles depends on the size of the system; *i.e.*, on the number of particles composing it. To better describe such a dependence, we rely on the concepts of microscopic and macroscopic systems. Microscopic systems can be mathematically treated by statistical mechanics, while macroscopic systems by energy transfer theory.

Consider a system to be composed of n particles. A system is called *macroscopic* if

$$\frac{1}{\sqrt{n}} \ll 1\,,$$

which means that statistical arguments can be applied to reasonable accuracy. For instance, if we wish to keep the statistical error below one percent then a macroscopic system would have to contain more than about ten thousand particles. Any system containing less than this number of particles would be regarded as *microscopic*, and, hence, statistical arguments could not be applied to such a system without unacceptable error. Statistical quantum mechanics is required to analyze such systems.

Thermal energy transfer is based on the macroscopic description of physical phenomena; it is thus an approximation to the microscopic description of phenomena ultimately given by statistical quantum mechanics. However, thermal energy transfer can be approximated by classical statistical mechanics. This approximation is valid when the number of particles in the system.

Technical note. Thermal flow is also called *thermal energy transfer rate*.

Technical note. IUPAC sign convention: All net energy transfers *to* the system are positive. All net transfers *from* the system are negative. A useful mnemonic is the wording '+accumulation = +inflow - outflow + release - storage'.

Note. Statistical mechanics provides a microscopic explanation of *temperature*, based on macroscopic systems' being composed of many particles, such as molecules and ions of various species, the particles of a species being all alike. It explains macroscopic phenomena in terms of the mechanics of the molecules and ions, and statistical assessments of their joint adventures. In the statistical thermodynamic approach, by the *equipartition theorem* each classical degree of freedom that the particle has will have an average energy of $k_\mathrm{b}\tau/2$, where k_b is Boltzmann's constant. The *translational motion* of the particle has three degrees of freedom, one in every direction of space, so that, except at very low temperatures where quantum effects predominate, the average translational energy of a particle in an system with temperature τ will be $3k_\mathrm{b}\tau/2$.

On the molecular level, temperature is the result of the motion of the particles that constitute the material. Moving particles carry kinetic energy. Temperature increases as this motion and the

kinetic energy increase. The motion may be the translational motion of particles or the energy of the particle due to molecular vibration or the excitation of an electron energy level.

In other words, since every degree of freedom that a particle has carries energy e that equals $k_\mathrm{b}\tau/2$ and since k_b is a *universal constant*, then energy is proportional to temperature: $e \propto \tau$. Therefore, one is entitled to think on temperature as energy, energy in "disguise".

Dim. Analysis. When analyzing thermal energy transfer, the most suitable *dimensional system* is the $ELT\Theta$ system – a *dimensionally independent system*. Within this framework, the dimensions of energy transfer, *aka* heat, of work and of internal energy are $\dim e = \dim w = \dim i = \mathsf{E}$ and of energy flow, *aka* thermal power or thermal flow, of work rate, *aka* mechanical power, and of internal energy change rate, *aka* accumulation, are $\dim e' = \dim w' = \dim i' = \mathsf{E}/\mathsf{T}$.

Technical note. In giving the dimensions of the specific heat capacity c as $\mathsf{E}/\mathsf{M}\Theta$, we are abusing of the $ELT\Theta$ system by adding mass, M, to it. This addition extends the dimensionally *independent* $ELT\Theta$ system to the dimensionally *dependent*, redundant, $EMLT\Theta$ system. We do so consciously, so to stress physics instead of mathematical purity; for, in the "pure" $ELT\Theta$ system, the dimensions of mass are $\mathsf{ET}^2/\mathsf{L}^2$ and then the dimensions of the c are $\mathsf{L}^2/\mathsf{T}^2\Theta$; disguising therefore its physical meaning. In other words, we prefer to interpret specific heat capacity as the capacity that a body has to store energy at a given temperature per unit mass or $\dim c = \mathsf{E}/\mathsf{M}\Theta$, rather than the less informative $\mathsf{L}^2/\mathsf{T}^2\Theta$.

7.2. Modes of energy transfer.
Thermal energy is transferred inside a body or among bodies by three means:

  (1) thermal (heat) conduction;
  (2) thermal (heat) convection and
  (3) thermal radiation.

7.2.1. *Thermal conduction.*
Consider a body, say a rod, being heated up to temperature τ_1 at one end while simultaneously being cooled down to τ_2 at the other end. Consider also the body to be thermally isolated everywhere but not at the ends. Then, it can be observed that, driven by the temperature difference, $\Delta\tau = \tau_1 - \tau_2$, the thermal flow happens from the hot end to the cold one. Since such a flow happens through the body surface, it is useful to define physical quantity, *thermal flux*, to better express the energy flow and surface relation.

Thermal flux, e'', is thus defined as thermal flow per unit area, $\dim e'' = E/L^2T$. Then, *thermal conduction*, often called heat conduction, through a body is based on experimental observation: *Fourier's law*.

Fourier's law states that

> the local thermal flux resulting from thermal conduction is proportional to the magnitude of the temperature gradient and opposite to it in sign. Mathematically,
> $$e'' = -k\,\mathrm{grad}\,\tau\,.$$
> The minus sign accounts for the second law of thermostatics: thermal flow happens in the direction of *falling* temperature.

The proportionality "constant" in Fourier's law, k, is a definite positive number describing a substance thermal property, *thermal conductivity*, $\dim k = E/TL\Theta$. Thermal conductivity, rather than a constant, is a coefficient, because its value depends on temperature, pressure and, in mixtures, on the composition. It is a scalar as long as the material is *isotropic*, which means that the ability of the material to conduct thermal energy depends on position within the material, but for a given position not on the direction.
Thermal conductivity values: Because of how molecules are arranged, solids will have generally higher thermal conductivity values than gases. Thus, the process of thermal energy transfer is more efficient in solids than in gases.

In a gas, k is proportional to the molecular speed and molar specific heat and inversely proportional to the cross-sectional area of molecules.

The values for k are experimentally found and presented in references as tables or figures.

Example. The front of a slab of lead ($k = 35\,\mathrm{W/m\,K}$) is kept at $110\,^\circ\mathrm{C}$ and the back is kept at $50\,^\circ\mathrm{C}$. If the area of the slab is $0.4\,\mathrm{m}^2$ and it is $0.03\,\mathrm{m}$ thick, then compute the thermal energy flux and the thermal energy transfer rate.

Solution. Use Fourier's law to find the energy flux:

$$e'' = -k\operatorname{grad}\tau \sim -k\Delta\tau/\Delta x = -(35)((110-50)+273.15)/(0.03) = 70\,\mathrm{kW/m}^2\,.$$

The thermal energy transfer rate is thus

$$e' = e''s = (70)(0.4) = 28\,\mathrm{kW}\,. \qquad\qquad\qquad\qquad\qquad\qquad \Box$$

7.2.2. *Thermal convection.* Consider a typical convective cooling situation: cool gas flows past a warm body. The fluid immediately adjacent to the body forms a thin slowed-down region called *boundary layer*. Thermal energy is conducted into this layer, which sweeps it away and, farther downstream, mixes it into the stream. We call such a process of carrying thermal energy away from a body surface by a moving fluid *convection*. Isaac Newton considered the convective process and suggested that the cooling would be such that

$$\dot{\tau}_{\text{body}} \propto \tau_{\text{body}} - \tau_{\text{fluid}}\,,$$

wherein τ_{fluid} is the temperature of the incoming fluid. This statement suggests that energy is flowing from the body. But if energy is constantly replenished, then the body temperature need not change. Therefore, with $e' = mc\dot{\tau}$, we get

$$e' \propto \tau_{\text{body}} - \tau_{\text{fluid}} \implies e'' = \bar{f}\left(\tau_{\text{body}} - \tau_{\text{fluid}}\right)\,,$$

where $e'' = e'/s$, s is the surface area of the body and $\bar{f}$ is the *film coefficient* or *heat transfer coefficient*. The bar over $\bar{f}$ indicates that's an *average* over the surface of the body. Without the bar, f denotes the *local* value of the film coefficient at a point on the surface. The dimensions of both coefficients are $\dim f = \dim \bar{f} = E/TL^2\Theta$.

It turns out that Newton oversimplified the process description, when he made his conjecture. Thermal convection is complicated and $\bar{f}$ can depend on the temperature difference $\tau_{\text{body}} - \tau_{\text{fluid}} = \Delta\tau$:

- f is really independent of $\Delta\tau$ when the fluid is forced past a body and $\Delta\tau$ is not too large. This is called *forced convection*.
- when fluid buoys up from a hot body or down from a cold one, f varies as some weak power of $\Delta\tau$ – typically as $\Delta\tau^{1/4}$ or $\Delta\tau^{1/3}$. This is called *free* or *natural convection*. If the body is hot enough to boil a liquid surrounding it, then $\bar{f}$ will typically vary as $\Delta\tau^2$.

Typical values of the film coefficient are presented in equations, tables or figures. However, they should be judiciously applied in actual designs.

Lumped-capacity solution – heat equation. The problem now is to predict the transient cooling of a convectively cooled object. Apply the familiar filst law statement to have

$$e' = i' \implies -\bar{f}s\left(\tau - \tau_{\text{fluid}}\right) = \mathrm{d}_t\left(\rho cv\left(\tau - \tau_{\text{ref}}\right)\right)\,,$$

where s and v are the surface area and volume of the body, τ the temperature of the body, $\tau = \tau\,[t]$, and τ_{ref} is an arbitrary temperature at which the internal energy i is defined to equal zero.

The last equation can be solved by separating the variables τ and t. After solving the equation, after applying the initial condition $\tau\,[t=0] = \tau_{\text{i}}$, wherein τ_{i} the body initial temperature, and after rearranging terms, one has

$$\frac{\tau - \tau_{\text{fluid}}}{\tau_{\text{i}} - \tau_{\text{fluid}}} = \exp\left[-t/\tau\right]\,.$$

Note that all the physical parameters in the problem have now been "lumped" into the *time constant* τ. This time constant represents the time required for a body to cool to $1/e$ or 35% of its initial temperature difference above (or below) τ_{fluid}. The ratio t/τ can also be interpreted as

$$\frac{t}{\tau} = \frac{\bar{f}st}{\rho cv} = \frac{\text{capacity for convection from surface}}{\text{thermal capacity of the body}}\,.$$

Note that the thermal conductivity of the body is missing from the last equations. The reason is that we have assumed that the body temperature is nearly uniform and thus means that internal conduction is unimportant. If $L/k\bar{f} \ll 1$, then the body temperature τ is almost constant within the body at any time. Therefore,

$$\frac{\bar{f}L}{k} \ll 1 \implies \tau\left[\xi, t\right] \sim \tau\left[t\right] \sim \tau_{\text{surface}}$$

and the thermal conductivity k becomes irrelevant to the cooling process. This condition must be satisfied if the lumped solution is to be accurate.

We call the group $\bar{f}L/k = \pi_{\text{bi}}$ *Biot number*. If π_{bi} were large, then the situation would be reversed in this case, $\pi_{\text{bi}} \ll 1$, and then the convection process offers little resistance to the thermal transfer (conduction). We could solve the *thermal diffusion equation*, *aka* heat diffusion equation:

$$\alpha\partial_{xx}\tau = \partial_t\tau\,,$$

object to the simple boundary condition $\tau\left[\xi, t\right] = \tau_{\text{fluid}}$, when $x = L$ to determine the temperature in the body and its rate of cooling, in this case.

Biot number will be therefore the basis for determining what sort of problem we have to solve.

7.2.3. *Thermal radiation.* When thermal energy is applied to a body, it generates motion of the charged particles in the body matter. Then, the body radiates electromagnetic energy – *thermal radiation*. Equivalently, this means that all matter with temperature greater than the absolute zero emits thermal radiation, or, in other words, thermal radiation can be seen as the conversion of thermal energy into electromagnetic energy. Examples of thermal radiation are the visible light and infrared light emitted by an incandescent light bulb, the infrared radiation emitted by animals and detectable with an infrared camera.

The thermal radiation of real bodies is modeled after a hypothetical radiative body called a *black-body*. If a radiation-emitting object meets the physical characteristics of a black body in thermodynamic equilibrium, then the radiation is called *black-body radiation*. There are three laws that describe the physical properties of black-bodies: Planck's law describes the *spectrum* of black-body radiation, which depends only on the object's temperature; Wien's displacement law determines the most likely *frequency of the emitted radiation* and, finally, Stefan-Boltzmann law gives the black-body *radiant emissivity*.

Thermal transfer by thermal radiation: All bodies constantly emit energy by a process of electromagnetic radiation. The intensity of such energy flux depends upon the body temperature. Most of the thermal energy that reaches you when you sit in front of a fire is radiant energy. Radiant energy warms you when you walk under the sun.

Objects cooler than the fire or the sun emit much less energy, because the energy emission varies as the fourth power of absolute temperature. Very often, the emission of energy, or radiant energy transfer, from cooler bodies can be neglected in comparison with convection and conduction. (Approximate solutions and order of magnitude physics can be helpful here!) But energy transfer processes that occur at high temperatures, or with conduction or convection suppressed by evacuated insulators, usually involve a significant fraction of radiation.

The electromagnetic spectrum: Thermal radiation occurs in a range of the electromagnetic spectrum of energy emission. Accordingly, it inhabits the same wavelike properties as light or radio waves. Each quantum of radiant energy has a wavelength λ and a frequency μ associated with it.

The full electromagnetic spectrum includes an enormous range of energy-bearing waves, of which thermal energy is only a small part.

Tables show the various forms over a range of wavelengths that spams 17 orders of magnitude. Thermal radiation, whose main component is usually the spectrum of infrared radiation, passes through a three-order-of-magnitude window in λ or μ. This window ranges $0.1\,\mu\text{m}$ to $1000\,\mu\text{m}$, with a geometric mean of $10\,\mu\text{m}$.

Black-bodies: The model for the perfect thermal radiator is the so-called *black-body*. This is a body that absorbs all energy that reaches it and reflects nothing. The term is a bit confusing, since they *emit* energy. Thus, under infrared vision, a black-body would glow

with "color" appropriate to its temperature. Perfect radiators are "black" in the sense that they absorb all visible light (and all other radiation) that reaches them.

To model a black-body, a *Hohlraum* is used. Whet are the important features of a thermally black-body? First consider a distinction between thermal (heat) radiation and infrared radiation. *Infrared radiation* refers to a particular range of wavelengths, while thermal radiation refers to the whole range of radiant energy flowing from one body to another. Suppose that a radiant thermal flux e'' falls upon a translucent plate that's not black. A fraction α of the total incident energy, called the *absorptance*, is absorbed by the body; a fraction ρ, called the *reflectance*, is reflected by the body and a fraction τ, called the *transmittance*, passes through. Thus,

$$1 = \alpha + \rho + \tau\,.$$

This relation can also be written for the energy carried by each wavelength in the distribution of wavelengths that makes up thermal radiant energy from a source at any temperature.

$$1 = \alpha_\lambda + \rho_\lambda + \tau_\lambda\,.$$

All radiant energy incident on a black-body is absorbed, so that $\alpha_{\mathrm{b}} = \alpha_{\lambda_{\mathrm{b}}} = 1$ and $\rho_{\mathrm{b}} = \tau_{\mathrm{b}} = 0$. Furthermore, the energy emitted by a black-body reaches a theoretical maximum given by Stefan-Boltzmann law.

Stefan-Boltzmann law: The energy flux radiating from a body is designated by $e''[t]$, $\dim e'' = E/L^2T$. The symbol $\check{e}_{\lambda_{\mathrm{body}}}[\lambda, \tau]$ designates the distribution function of radiative flux in λ, or the *monochromatic emission power*:

$$\check{e}_{\lambda_{\mathrm{body}}}[\lambda, \tau] = \mathrm{d}_t e''[\lambda, \tau] \qquad \text{or} \qquad e''[\lambda, \tau] = \int_0^\lambda \check{e}_{\lambda_{\mathrm{body}}}[\lambda, \tau]\,\mathrm{d}\lambda\,.$$

Thus,

$$e''[\tau] = e''[\infty, \tau] = \int_0^\infty \check{e}_{\lambda_{\mathrm{body}}}[\lambda, \tau]\,\mathrm{d}\lambda\,.$$

The dependence of $e''[\tau]$ on temperature τ for a black-body, e''_{bb}, was found experimentally by Stefan and proved theoretically by Boltzmann. Stefan-Boltzmann law states that

$$e''_{\mathrm{bb}}[\tau] = \sigma_{\mathrm{sb}}\tau^4\,,$$

where Stefan-Boltzmann constant $\sigma_{\mathrm{sb}} = 5.670\,373(21) \times 10^{-8}\,\mathrm{W/m^2\,K^4}$. In terms of other fundamental constants:

$$\sigma_{\mathrm{sb}} = \frac{2\pi^5}{15}\frac{k_{\mathrm{b}}^4}{h_{\mathrm{p}}^3 c_0^2} = \frac{2\pi^5}{15}\frac{r_{\mathrm{g}}^4}{h_{\mathrm{p}}^3 c_0^2 n_{\mathrm{a}}^2}\,,$$

where k_{b} is Boltzmann constant, h_{p} Planck constant, c_0 speed of light in vacuum, r_{g} ideal gas constant and n_{a} Avogadro's number.

[a lot missing!]

7.3. **A look ahead.** To solve actual problems, three tasks must be completed:

(1) thermal energy (heat) diffusion equation must be solved object to appropriate boundary and initial conditions;
(2) the film (convective thermal transfer) coefficient must be determined if convection is relevant and
(3) the factor F_{1-2} must be determined to calculate radiative thermal energy transfer.

Appendix A. Energy continuity equation

A.1. **Derivation.** Consider a body being heated from one side while being cooled from the other, opposite, side. Consider also that no work is performed. Experience shows that the body internal energy varies with time t and position ξ due to the external energy difference; *i.e.*, external energy flowing through the body external surface gets temporally and spatially distributed within the body. To model such a distribution, we will make use of the energy conservation principle.

Let $i = i[t, \xi]$ be the internal energy density field of a non-moving control volume dv inside the body of volume v. Then, the internal energy in the whole body is $\int_v i \, dv$. Therefore, the body internal energy changes, accumulates, at a rate

$$d_t \int_v i \, dv = \int_v \partial_t i \, dv = \int_v i' \, dv \,.$$

On the other hand, let ∂v be the body outer surface, boundary, and, accordingly, let $n \, ds$ be the directed control surface. Then, the thermal energy flowing *out* of the control surface is $-e'' \cdot n \, ds$. And, thus, the total thermal energy flowing out of the body through ∂v equals

$$-\int_{\partial v} e'' \cdot n \, ds = -\int_v \nabla \cdot e'' \, dv = -\int_v \operatorname{div} e'' \, dv \,.$$

By the energy conservation principle, the internal energy change rate and the thermal flow must balance one another:

$$\int_v i' \, dv = -\int_v \operatorname{div} e'' \, dv \,.$$

The last equation must be equal regardless of any control volume choice:

$$i' + \operatorname{div} e'' = 0 \,.$$

The next step is to relate the internal energy density with the thermal flux. This relation comes from two phenomenological laws, *aka constitutive equations*:

(1) As mentioned in the above sections, a body internal energy is related to the body temperature τ by

$$i = \rho c \tau \,,$$

where ρ and c are two body (material) properties, *mass density*, mass per unit volume, and *specific heat capacity*, the capacity that the body material has to store energy per unit mass and per unit temperature. Thus,

$$i' = (\rho c \tau)' = \partial_t (\rho c \tau) = \partial_t \rho c \tau \,.$$

(2) Fourier's law of thermal energy conduction states that the thermal energy flux is proportional to the temperature gradient:

$$e'' = -k \operatorname{grad} \tau \,.$$

The minus sign in this equation accounts for the second law of thermodynamics: thermal energy flows in the direction of falling temperature. The constant of proportionality k is a body (material) property, *thermal conductivity*, $\dim k = E/LT\Theta$. It is dependent on both the temperature and pressure – in mixtures also on the composition.

Using the empirical laws, find that

$$\partial_t \rho c \tau = \operatorname{div} k \operatorname{grad} \tau \,.$$

Consider, finally, the body to be composed of an homogeneous, isotropic material. Then, the mass density, the specific heat capacity and the thermal conductivity are constant. Therefore, write the last equation as

$$\partial_t \tau = \alpha \operatorname{lap} \tau \qquad \text{or as} \qquad \tau' = \alpha \operatorname{lap} \tau \,,$$

where α is the *thermal diffusivity*, $\dim \alpha = L^2/T$, and lap Laplace operator. Refer to the last equation as the *thermal transfer equation*, the *thermal diffusion equation*, or, more commonly, as *heat equation*.

Note the definition of thermal diffusivity: $\alpha = k/\rho c$; *i.e.*, thermal diffusivity is the ratio of thermal energy conduction, $\dim k = E/LT\Theta$, to the volumetric thermal capacity, $\dim \rho c = E/L^3\Theta$. Thus, in a sense, thermal diffusivity is the measure of thermal inertia. In a substance with high thermal diffusivity, thermal energy moves rapidly through it because the substance conducts energy quickly relative to its volumetric thermal capacity or "thermal bulk".

A.2. **Technical notes.** Some explanations on the maths involved during the derivation.

Technical note. It is assumed that, during the thermal energy transfer, the body material is not affected by it; *i.e.*, the body material does not undergo thermal decomposition.

Math note. For modeling the phenomenon, energy density was assumed to be a smooth scalar field and the body to be bounded by a smooth outer surface.

Notation. The symbol d_t defined by $d_t \doteq d/dt$ denotes the *ordinary* derivative with respect to time and $\partial_t \doteq \partial/\partial t$ denotes the *partial* derivative with respect to time.

Math note. In going from the surface integral to the volume integral,

$$-\int_{\partial v} e'' \cdot n \, ds = -\int_v \nabla \cdot e'' \, dv = -\int_v \operatorname{div} e'' \, dv \,,$$

the divergence theorem was used.

Dim. Analysis. The accumulation in the body must balance energy outflow:

$$\int_v i' \, dv = \int_v \partial_t i \, dv = -\int_v \operatorname{div} e'' \, dv \,.$$

This equation satisfies a fundamental physics law: the energy conservation principle. It also satisfies another fundamental physics principle: dimensional homogeneity principle for physics law.

The dimensions of the terms in the left-hand-side, LHS, of the last equation are $\dim \partial_t = 1/T$, $\dim i = E/L^3$, *i.e.*, internal energy *density*, $\dim dv = L^3$. Then, the whole LHS integral has dimensions of energy change rate, or energy flow, E/T.

The dimensions of the terms in the right-hand-side, RHS, are $\dim \operatorname{div} = \dim \nabla \cdot = 1/L$, $\dim e'' = E/L^2 T$, $\dim dv = L^3$. Then, the whole RHS integral has dimensions of energy flow, E/T.

Since the LHS and the RHS of the equation have the same dimensions, thus, the principle of dimensional homogeneity is satisfied.

Math note. During the derivation, we went from

$$\int_v \left(i' + \operatorname{div} e'' \right) dv = 0 \qquad \text{to} \qquad i' + \operatorname{div} e'' = 0 \,;$$

or, in other words, we made the integrand to vanish. To explain this "math move", making the integrand equal to zero, we need to analyze how the derivation was done, mathematically – the math framework behind the deduction.

To find the energy distribution inside our given body, we have followed Riemann's ideas on integration. He would have said:

> To find the energy distribution within the body, follow the process:
> - first, divide the body volume v into n smaller control volumes dv_i, where i runs from 1 to n. Note that the number and sizes of the control volumes are up to you. There is neither a fixed number nor a fixed size. In fact, they not even need be all of the same size! Nevertheless, do make sure that n is large enough to cover the whole body volume.
> - Then, find the energy distribution in each control volume and
> - finally, find the total energy distribution inside of the whole of the body by adding the energy distribution of the n control volumes together by means of integration.
>
> Note that the result has to be *independent* on the number of control volumes and on their sizes.
>
> To explain this better. Say, for instance, that you take n control volumes of equal size dv_1 and, say, I take m smaller control volumes of size dv_2; or, $n < m$ since $dv_1 > dv_2$. Say both choices cover the whole body. Then, you calculate the energy distribution of your control volumes and so do I. To find the total energy distribution, you next add the energy distribution of every of your control volumes and so do I. Finally, we compare results. Good maths requires both results, your total energy distribution and mine, be the same!

This explanation implies, mathematically, the vanishing integrand.

Notation. Another common form of writing the heat equation is by using the geometric derivative: $\partial_t \tau = \alpha \nabla^2 \tau$.

Technical note. As it stands, the heat equation, $\tau' = \alpha \operatorname{lap} \tau$, is written in vector notation; thus, it is valid in *any* coordinate system. However, once a particular coordinate system is selected, then,

the appropriate form of Laplace operator must be found. For instance, in a Cartesian coordinate system, $[x, y, z]$, the heat equation becomes

$$\tau' = \partial_t \tau = \alpha \partial_k \partial_l g^{kl} \tau \qquad \text{or} \qquad \tau_{,t} = \alpha \tau_{,\xi\xi} = \alpha \left(\tau_{,xx} + \tau_{,yy} + \tau_{,zz} \right),$$

The second equation follows from two facts of Cartesian coordinate systems: the metric g does not depend on position, thus $\partial_k \partial_l g^{kl} \tau = g^{kl} \partial_k \partial_l \tau$ and $g = \mathrm{diag}\,[1, 1, 1]$.

For non-Cartesian coordinate systems, however, g does depends on position, so $\partial_k \partial_l g^{kl} \tau \neq g^{kl} \partial_k \partial_l \tau$ and therefore the derivatives of the metric with respect to the coordinates and the metric coefficients g^{kl} must be found.

Notation. Consider a smooth scalar field $\phi = \phi\,[x, y, z]$. Then, the comma derivative notation is defined as

$$\phi_{,x} = \frac{\partial \phi}{\partial x}, \quad \phi_{,y} = \frac{\partial \phi}{\partial y}, \quad \phi_{,z} = \frac{\partial \phi}{\partial z}, \quad \phi_{,xy} = \frac{\partial}{\partial x}\frac{\partial}{\partial y}\phi \quad \text{and so on}.$$

Geometry. Remember that, in vector calculus, divergence is an operator that measures the magnitude of a vector field's source or sink at a given point, in terms of a signed scalar. Or, more technically, the divergence represents the volume density of the outward flux of a vector field from an infinitesimal volume around a given point.

Then, recall the equation:

$$i' = -\operatorname{div} e''.$$

This equation models the phenomenon of a body being heated up from one side while being cooled down from another side or the phenomenon of a body releasing energy from its center while it cools down. Take the second phenomenon. The LHS of the model equation represents the rate at which a body internal energy changes with respect to time: the rate at which energy is released from the center to the outer portions of the body and finally to the environment surrounding the body.

The RHS, on the other hand, because of the divergence, represents how the central energy diffuses from the center throughout the body to the environment. It has a minus sign because energy is being dissipated instead of being accumulated.

The equality holds, physically, because energy is conserved: if it is being released and not accumulated within the body, energy has no other place to go but to its surrounding environment.

Geometry. Recall that Laplace operator $\operatorname{lap} f\,[\xi]$ of a function f at a point ξ, up to a constant depending on the dimension, is the rate at which the average value of f, over spheres centered at ξ, deviates from $f\,[\xi]$ as the radius of the sphere grows; *i.e.*, Laplace operator of a function represents the difference between the value of the function at a point and the average of the values at surrounding points. Another way of looking at Laplace operator is by writing it in a Cartesian coordinate system $[x, y, z]$:

$$\operatorname{lap} = \nabla^2 = \partial_{xx} + \partial_{yy} + \partial_{zz}.$$

See that, then, this operator finds the *change in the change* of the function (if you make a graph, the change in the slope) in all directions from the point of interest. That may not seem very interesting, until you consider that acceleration is the change in the change of position with time or that the maxima and minima of functions (peaks and valleys) are regions in which the slope changes significantly.

Now, recall the thermal diffusion equation:

$$\tau' = -\alpha \operatorname{lap} \tau.$$

This equation models the phenomenon of a body being heated up from one side while being cooled down from another side or the phenomenon of a body releasing energy from its center while it cools down. Take the second phenomenon. The LHS of the model equation represents the rate at which a body temperature changes with respect to time: the rate at which temperature diffuses from the center to the outer portions of the body and finally to the environment surrounding the body. In an analogous way as internal energy in the $i' = -\operatorname{div} e''$ equation. Something unsurprising, since energy and temperature are related via the equipartition theorem.

The RHS, on the other hand, because of Laplace operator, represents how the central temperature diverges from the center to the surrounding points. It has a minus sign because temperature is being dissipated instead of being gathered. The coefficient α, thermal diffusion, is a body material property that acts as both a dimensional conversion factor between temporal temperature changes and spatial temperature changes ($\dim \tau' = \Theta/T$ and $\dim \operatorname{lap} \tau = \Theta/L^2$) or as representing how a material diffuses or infuses temperature (internal energy). Thermal conductors diffuse (infuse) temperature (internal energy) at a greater rate than thermal insulators.

A.3. **Another derivation.** [John H. Lienhard IV, John H. Lienhard V, a heat transfer book] In this reference, the energy continuity equation is called heat diffusion equation, *aka* heat conduction equation in other sources.

A.3.1. *Objective.* We must now develop some ideas that will be needed for the design of thermal (heat) exchangers. The most important of these is the notion of an overall *thermal energy transfer coefficient*, *aka* heat transfer coefficient. This is a measure of the general resistance of a thermal (heat) exchanger to the flow of energy (heat), and usually it must be built up from analyses of component resistances. Although we shall count radiation among these resistances, this overall energy transfer coefficient is most often dominated by *convection and conduction.*

We need to know values of the film coefficient $\bar{f}$ to handle convection. Calculating $\bar{f}$ becomes sufficiently complex that we defer it to later chapters. For the moment, we shall take the appropriate value of $\bar{f}$ as known information and concentrate upon its use in the overall heat transfer coefficient.

The thermal (heat) conduction component also becomes more complex than the planar analyses we did in earlier chapters. But its calculation is within our present scope. Therefore we devote this section to deriving the full thermal conduction equation, *aka* heat conduction or heat diffusion equation, solving it in some fairly straightforward cases, and using our results in the overall coefficient. We undertake that task next.

Consider the general temperature distribution in a three-dimensional body as depicted in Fig. 2.1 (a body being heated by a candle). For some reason, say heating from one side, the temperature of the body varies with time and space. This field $\tau = \tau\,[\xi, t] = \tau\,[x, y, z, t]$, defines instantaneous *isothermal surfaces*, τ_1, τ_2 and so on.

We next consider a very important vector associated with the scalar, τ. The vector that has both the magnitude and direction of the maximum increase of temperature at each point is called the *temperature gradient*, $\mathrm{grad}\,\tau$:

$$\mathrm{grad}\,\tau = \nabla\tau = \gamma^i \partial_i \tau = \hat{x}\partial_x \tau + \hat{y}\partial_y \tau + \hat{z}\partial_z \tau \,.$$

A.3.2. *Fourier's law.* "Experience" – that is, physical observation – suggests two things about the thermal flow that results from temperature nonuniformities in a body. These are:

(1) e'' and $\mathrm{grad}\,\tau$ are exactly opposite one another in direction [5]:

$$\frac{e''}{|e''|} \propto -\frac{\nabla\tau}{|\nabla\tau|}$$

and

(2) the magnitude of the thermal flux is directly proportional to the temperature gradient:

$$|e''| \propto |\nabla\tau| \,.$$

Notice that the thermal flux is now written as a quantity that has a specified direction as well as a specified magnitude. Fourier's law summarizes this physical experience succinctly as

$$e'' = -k\nabla\tau = -k\,\mathrm{grad}\,\tau \,.$$

The coefficient k – the thermal conductivity – also depends on position and temperature in the most general case:

$$k = k\,[\xi, \tau\,[\xi, t]] \,.$$

Fortunately, most materials (though not all of them) are very nearly *homogeneous.* Thus we can usually write $k = k\,[\tau]$. The assumption that we really want to make is that k is constant. Whether or not that is legitimate must be determined in each case. As is apparent from Fig. 2.2 and Fig. 2.3, k almost always varies with temperature. It always rises with τ in gases at low pressures, but it may rise or fall in metals or liquids. The problem is that of assessing whether or not k is approximately constant in the range of interest. We could safely take k to be a constant for iron between $0\,^\circ\mathrm{C}$ to $40\,^\circ\mathrm{C}$ (see Fig.

_____

[5] This is a consequence of the second law of thermostatics: thermal energy flows in the direction of falling temperature.

2.2), but we would incur error between $-100\,^\circ\text{C}$ to $800\,^\circ\text{C}$. Thus, if $\Delta\tau$ is not large, one can still make a reasonably accurate approximation using a constant average value of k.

We must now write the thermal energy conduction equation in three dimensions. We begin with the energy conservation principle – thermal energy flow equals energy accumulation within the body:

$$e' = i' \,.$$

This time we apply the last equation to a three-dimensional control volume, as shown in Fig. 2.4.1. The control volume is a finite region of a conducting body, which we set aside for analysis. The surface is denoted as s and the volume and the region as v; both are at rest. An element of the surface, $\mathrm{d}s$, is identified and two vectors are shown on $\mathrm{d}s$: one is the unit normal vector, $\hat{n}$ (with $|\hat{n}| = 1$), and the other is the thermal energy flux vector, $e'' = -k\,\mathrm{grad}\,\tau = -k\nabla\tau$, at that point on the surface.

We also allow the possibility that a volumetric thermal energy release flow equal to r', $\dim r' = E/TL^3$, is distributed through the region. This might be the result of chemical or nuclear reaction, of electrical resistance heating (Joule heating), of external radiation into the region or of still other causes.

With reference to Fig. 2.4, we can write the thermal energy flow conducted *out* of $\mathrm{d}s$, in dimensions of E/T, as

$$(-k\nabla\tau) \cdot (\hat{n}\,\mathrm{d}s) \,.$$

The thermal energy released (or accumulated) within the region v must be added to the total energy flow into s to get the overall rate of thermal energy addition to v:

$$e' = -\int_s (-k\nabla\tau) \cdot (\hat{n}\,\mathrm{d}s) + \int_v r'\,\mathrm{d}v \,.$$

The rate of energy increase (accumulation) of the region v is

$$i' = \int_v (\partial_t \rho c \tau)\,\mathrm{d}v \,,$$

where the derivative of τ is in partial form because τ is a function of both position, ξ, and time, t.

Finally, we combine e' and i' using the energy conservation principle. After rearranging the terms, we obtain

$$\int_s (-k\nabla\tau) \cdot (\hat{n}\,\mathrm{d}s) = \int_v \left(\partial_t \rho c \tau + r' \right)\,\mathrm{d}v \,.$$

To get the left-hand side into a convenient form, we introduce Gauss's theorem, which converts a surface integral into a volume integral. This reduces the last equation into

$$\int_v \left(\nabla \cdot k\nabla\tau - \partial_t \rho c \tau + r' \right)\,\mathrm{d}v \,.$$

Next, since the region v is arbitrary, the integrand must vanish identically. We therefore get the *thermal energy diffusion equation* in three dimensions:

$$\nabla \cdot k\nabla\tau + r' = \partial_t \rho c \tau \,.$$

The limitations on this equation are:

- Incompressible medium. (This was implied when no expansion work term was included.)
- No convection. (The medium cannot undergo any relative motion. However, it can be a liquid or gas as long as it sits still.)

If the variation of k with τ is small and if the medium is homogeneous, then k and ρc can be factored out of the last equation to get:

$$\nabla^2 \tau + \frac{1}{k} r' = \frac{1}{\alpha} \partial_t \tau \,,$$

where $\alpha = k/\rho c$ is the body thermal diffusivity. In a sense, thermal diffusivity is the measure of thermal inertia. In a substance with high thermal diffusivity, thermal energy moves rapidly through it because the substance conducts energy quickly relative to its volumetric thermal capacity or "thermal bulk".

Geometry. As seen in the thermal energy diffusion equation, *aka* heat equation, when there are no volumetric thermal energy releases, *i.e.*, $r' = 0$, then we have

$$\tau_{,t} = \alpha \tau_{,\xi\xi} \,.$$

Here thermal diffusivity can be geometrically interpreted as the ratio of the time derivative of temperature to its *curvature*, quantifying thus the rate at which temperature concavity is "smoothed out".

Technical note. Notice the reactive term r'/k. It has the dimensions of

$$\dim \frac{r'}{k} = \frac{E/TL^3}{E/TL\Theta} = \frac{\text{flow of chemical energy release}}{\text{thermal energy conduction}} \,.$$

Thus, if thermal conduction is high, then thermal energy coming from the reaction flows quickly through the body, being then released to the environment. Otherwise, then thermal energy coming from the reaction is stored within the body, this, in turns, enhances the reaction rate, since $r = f[\tau]$.

A.4. **Yet another derivation.** [Evans M. Harrell II and James V. Herod, Linear Methods of Applied Mathematics. `http://www.mathphysics.com/pde/HEderiv.html`]

Newton articulated some principles of thermal flow through solids, but it was Fourier who created the correct systematic theory. Inside a solid there is no convective transfer of thermal energy and little radiative transfer, so temperature changes only by conduction, as the energy we now recognize as molecular kinetic energy flows from hotter regions to cooler regions.

(1) The first basic principle of thermal energy is that

the thermal energy contained in a material (internal energy) is proportional to the temperature, the density of the material and a physical characteristic of the material called the *specific thermal capacity*. In mathematical terms,

$$i = \int_v \rho c \tau \, [t, \xi] \, \mathrm{d}v \,.$$

(2) For the other principles of thermal transfer, let us do some experiments with the following materials: a hot stove, some iron rods of different, relatively short lengths and various widths and various ceramic rods of different lengths and widths. Since these will be thought experiments only, it will be safe to use a finger as the probe. Putting your finger right on the stove will convince you that the energy transfer is proportional to the difference in temperature between your finger and the stove. Using, if necessary, a different, undamaged finger, you will also find that the rate of thermal transfer is inversely proportional to the length of an iron rod intervening between your finger to the stove (fixing the cross-sectional area). In other words, the rate of thermal flow from one region to another is proportional to the temperature gradient between the two regions. You will probably also agree that the rate of thermal flow will be proportional to the area of the contact; for example, a short pin with one end on a hot stove and the other touching your hand is preferable to putting the palm of your hand on a frying pan. Finally, a ceramic material on the stove being usually more pleasant to the touch than hot iron, we see that the rate of thermal transfer depends on the material, as measured with a physical constant known as the *thermal conductivity*. The second basic principle is thus that

the thermal transfer (thermal flow, thermal power) through the boundary of a region is proportional to the thermal conductivity, to the gradient of the temperature across the region and to the area of contact, so if the boundary of the region v is written as ∂v, with outward normal vector n, then

$$e' = \int_{\partial v} k n \cdot \mathrm{grad} \, \tau \, [t, \xi] \, \mathrm{d}s \,.$$

If we differentiate the internal energy equation with respect to time, applying the differentiation under the integral sign, and apply divergence theorem to the thermal transfer integral, then we find that

$$\int_v \partial_t \rho c \tau \, [t, \xi] \, \mathrm{d}v = \int_v \mathrm{div} \, k \, \mathrm{grad} \, \tau \, [t, \xi] \, \mathrm{d}v \, .$$

Since the region v can be an arbitrary piece of the material under study, the integrands must be equal at almost every point. If the material under study is made out of an homogeneous, isotropic substance and if temperature gradients are not so big, then ρ, c and k are independent of the position ξ. Thus, we obtain the thermal diffusion equation

$$\partial_t \tau \, [t, \xi] = \alpha \, \mathrm{lap} \, \tau \, [t, \xi] \, ,$$

where $\alpha = k/\rho c$ is called *thermal diffusivity*. Ordinary substances have values of α ranging from about $5 \, \mathrm{cm}^2/\mathrm{g}$ to $9000 \, \mathrm{cm}^2/\mathrm{g}$.

The one-dimensional thermal diffusion equation in Cartesian coordinates

$$\tau_{,t} = \alpha \tau_{,xx}$$

would apply, for instance, to the case of a long, thin metal rod wrapped with insulation, since the temperature of any cross-section will be constant, due to the rapid equilibration to be expected over short distances.

A.5. **Solutions to the thermal diffusion equation.** We are now in position to calculate the temperature distribution or thermal flux in bodies with the help of the heat diffusion equation. In every case, we first calculate $\tau \, [\xi, t]$. Then, if we want the thermal flux as well, we differentiate τ to get e'' from Fourier's law.

The thermal diffusion equation is a partial differential equation (p.d.e.) and the task of solving it may seem difficult, but we can actually do a lot with fairly elementary mathematical tools. For one thing, in one-dimensional steady-state situations the heat diffusion equation becomes an ordinary differential equation (o.d.e.); for another, the equation is linear and therefore not too formidable, in any case. Our procedure can be laid out, step by step:

(1) Play with geometrical analysis – make sketches, pics and drawings, physical analysis, dimensional analysis and approximate methods. Guess the solution beforehand. Even if you are proven wrong by the formal analysis, guessimations enhance physical intuition!

   Note. In the analysis of thermal transfer, the dimensionaly independent system $\{E, L, T, \Theta\}$ is generally the most adequate. However, the SI system, based on $\{M, L, T, \Theta\}$, should not be overlooked.

(2) Pick the coordinate scheme (coordinate system) that best fits the problem and identify the independent variables that determine τ.

(3) Write the appropriate d.e., starting with one of the forms of the thermal diffusion equation.

   Note. Non-dimensionalization of the d.e. prior to obtain its solution provides a deeper physical understanding of the phenomenon regardless if it results in an "easier" equation to solve. Use and interpret physically the resulting non-dim. equation as well as any characteristic physical quantities and dimensionless numbers.

   Remark. If non-dimensionalization is considered, then do not forget to include all of the physical quantities: quantities that appear in the diffusion equation, in the initial conditions and in the boundary conditions.

(4) Obtain the general solution of the d.e. (This is usually the easiest step.)

(5) Write the "side conditions" on the d.e. – the initial and boundary conditions. This is the trickiest part and the one that most seriously tests our physical or "practical" understanding any heat conduction problem. Normally, we have to make two specifications of temperature on each position coordinate and one on the time coordinate to get rid of the constants of integration in the general solution.

   Warning. Very Important: Never, never introduce inaccessible information in a boundary or initial condition. Always stop and ask yourself, "Would I have access to a numerical

value of the temperature (or other data) that I specify at a given position or time?" If the answer is no, then your result will be useless.

(6) Substitute the general solution in the boundary and initial conditions and solve for the constants. This process gets very complicated in the transient and multidimensional cases. Numerical methods are often needed to solve the problem.

(7) Put the calculated constants back in the general solution to get the particular solution to the problem.

Note. Non-dimensionalization of the solution can also be helpful at this stage. Not only, non-dim. reduces the number of physical quantities to analyze, so does become useful when plotting equations.

(8) Play with the solution – look it over– see what it has to tell you. Make any checks you can think of to be sure it is correct. Again dimensional analysis is the first tool to apply! Approximate methods and the use of characteristic quantities are also valuable.

(9) If the temperature field is now correctly established, we can, if we wish, calculate the thermal flux at any point in the body by substituting $\tau\left[\xi, t\right]$ back into Fourier's law.

A.6. **Examples.** Some examples on using the proposed method for solving the thermal diffusion equation.

Example. A large, thin concrete slab of thickness l is "setting". Setting is an exothermic process that releases r', $\dim r' = E/TL^3$, unit $r' = \mathrm{W/m^3}$. The outside surfaces are kept at the ambient temperature, so $\tau_\mathrm{w} = \tau_\infty$. What is the maximum internal temperature?

Guess. Thermal energy is being released from the slab center to its walls. If its assumed that the center temperature is greater than the wall (ambient) temperature, then temperature attains its maximum at the center and decreases to ambient temperature. Additionally, since the outer surfaces are kept at constant temperature, then the process is to be steady, but ranging spatially throughout the slab thickness. If one measures the spatially variation as x, then the slab temperature must satisfy $\tau = \tau\left[x\right]$.

Another important point is given by the symmetry of the problem. The center temperature is maximum at the center, $l/2$, and minimum at the walls, $x = 0$ and $x = l$, with a smooth decay. This gives a room to think about the temperature distribution inside the slab as a parabola with its vertex at τ_max and with its directrix greater than the horizontal line formed by the wall temperatures, τ_w, at $x = 0$ and $x = l$.

Dim. Analysis. Place a Cartesian coordinate axis that runs from one wall to the other covering the slab thickness; let x measure distances within the thickness: $0 \leq x \leq l$. Since temperature distribution is independent on time (steady process), then $\tau = \tau\left[x\right]$ and thus x is the independent quantity and τ the dependent quantity. Finally, the slab geometry provides two parameters, x and l, and the slab material, concrete, provides the thermal property, k, thermal conductivity.

Choose the set $\{E, L, T, \Theta\}$ as the dimensionally independent set of dimensions. Within this system, the quantities dimensions are:

$$\dim x = \dim l = L\,, \quad \dim \tau = \dim \tau_\mathrm{w} = \Theta\,, \quad \dim r' = E/TL^3 \quad \text{and} \quad \dim k = E/LT\Theta\,.$$

According to Buckingham's theorem, the model can be described by $6 - 4 = 2$ dimensionless quantities. The first dimensionless quantity, π_1, must include, as an advice, the sought quantity, τ. Form this group by [6]

$$\pi_1 = \frac{k\left(\tau - \tau_\mathrm{w}\right)}{r'l^2} = \frac{\text{conduction energy flow gradient}}{\text{released energy flow gradient}} = \frac{\text{conduction gradient}}{\text{``production'' gradient}}\,.$$

The second dimensionless quantity, π_2, can be formed by the geometrical parameters:

$$\pi_2 = x/l\,.$$

Then, according to the dimensionally homogeneity principle for physics laws, the model can be written as

$$f\left[\pi_1, \pi_2\right] = 0 \implies \pi_1 = f\left[\pi_1, \pi_2\right] \implies k\left(\tau - \tau_\mathrm{w}\right)/r'l^2 = f\left[x/l\right]\,.$$

The last equation is the final result of dimensional analysis. The actual form of the function f has to be determined by experiment or by analytic considerations.

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[6] A dimensionless quantity that includes τ is readily available: τ/τ_w. However, in thermal transfer, temperature differences are more important than temperatures alone, since differences are the driving force behind the transfer.

Approx. Solution. After dimensional analysis was carried out, we arrived to

$$k \left(\tau - \tau_{\mathrm{w}} \right) / r' l^2 = f \left[x/l \right] .$$

When guessing the solution, on the other hand, we established that a parabola can express the temperature dependence on the thickness distance. Accordingly, the function f can be then hypothesize to satisfy

$$k \left(\tau - \tau_{\mathrm{w}} \right) / r' l^2 = a \left(x/l \right)^2 + b \left(x/l \right) + c ,$$

where the coefficients $\{ a, b, c \}$ must be determined.

These coefficients can be calculated using the theorem that states that three points uniquely determine a parabola. These points are

$$\begin{cases} \left[x/l = 0, k \left(\tau - \tau_{\mathrm{w}} \right) / r' l^2 = 0 \right] , \\ \left[x/l = 1/2, k \left(\tau - \tau_{\mathrm{w}} \right) / r' l^2 = \pi \right] , \\ \left[x/l = 1, k \left(\tau - \tau_{\mathrm{w}} \right) / r' l^2 = 0 \right] , \end{cases}$$

where π is an unknown dimensionless quantity that, geometrically, shows the parabola height, its distance from the horizontal line formed by the x-axis to the parabola vertex and, physically, the maximum value of temperature, $\tau_{\max} = \tau \left[1/2 \right]$, attained at $x/l = 1/2$, or,

$$\pi = k \left(\tau_{\max} - \tau_{\mathrm{w}} \right) / r' l^2 .$$

Using the points in the hypothetical equation for f, one finds that

$$a = -4\pi , \quad b = 4\pi \quad \text{and} \quad c = 0 ,$$

and, thus, one arrives at

$$\frac{k \left(\tau - \tau_{\mathrm{w}} \right)}{r' l^2} = 4\pi \frac{x}{l} \left(1 - \left(\frac{x}{l} \right) \right) .$$

Doing honest physics (*i.e.*, solving the differential equation), one finds that $4\pi = 1/2$ or $\pi = 1/8$, thus the model becomes

$$\frac{k \left(\tau - \tau_{\mathrm{w}} \right)}{r' l^2} = \frac{1}{2} \frac{x}{l} \left(1 - \left(\frac{x}{l} \right) \right)$$

and, finally, the maximum temperature, $\tau_{\max}$, is attained at

$$\pi = \frac{k \left(\tau_{\max} - \tau_{\mathrm{w}} \right)}{r' l^2} = \frac{1}{8} . \qquad \qquad \Box$$

Solution. This solution is based in the general procedure to solve the thermal diffusion equation.

Choose a Cartesian coordinate system with ξ varying only in one-dimension, so that

$$0 \leq x \leq l \qquad \text{and} \qquad \tau = \tau \left[x \right] .$$

Write the model equation for a one-dimensional, steady state case:

$$\tau_{,xx} = -r'/k .$$

Obtain the general solution to the model equation by integration to have

$$\tau = -\frac{r'}{k} x^2 + c_1 x + c_2 ,$$

where c_1 and c_2 are integration constants.

Apply, next, the boundary conditions

$$\tau \left[x = 0 \right] = \tau_{\mathrm{w}} \qquad \text{and} \qquad \tau \left[x = l \right] = \tau_{\mathrm{w}} .$$

Substitute the boundary conditions into the general solution to have

$$c_1 = \frac{r' l}{2k} \qquad \text{and} \qquad c_2 = \tau_{\mathrm{w}} .$$

Replace the values of the constants into the general solution to find the particular solution

$$\tau = -\frac{1}{2} \frac{r'}{k} x^2 + \frac{1}{2} \frac{r'}{k} x + \tau_{\mathrm{w}} ,$$

which can be written in the dimensionless form:

$$\frac{k \left(\tau - \tau_{\mathrm{w}} \right)}{r' l^2} = \frac{1}{2} \frac{x}{l} \left(1 - \left(\frac{x}{l} \right) \right) .$$

Finally, as a verifying step, note that the resulting temperature distribution is parabolic and, as expected, symmetrical. It satisfies the boundary conditions at the wall and maximizes in the center. By nondimensionalizing the result, a simple curve can represent all situations. That is highly desirable when the calculations are not simple, as they are here. (Even here τ actually depends on five different quantities and its solution is a single curve on a two-coordinate graph.)$\Box$

Appendix B. Coordinate systems and index notation

B.1. **Cartesian coordinate system.** Consider a region $\mathcal{V}$ to be a part of an n dimensional Euclidean space, $\mathcal{E}^n$. Consider, next, a Cartesian coordinate system; *i.e.*, a coordinate system equipped with a frame $\{\gamma_k\}$ whose elements satisfy

$$\gamma_k \cdot \gamma_l = g_{kl} = [k = l]_{\text{Iv}} \,.$$

If frame elements satisfy the last equation, then they are *orthogonal* to each other and *normal* (have unit length); thus, the frame $\{\gamma_k\}$ is said to be *othornormal*.

Express now the position of any point ξ in $\mathcal{V}$ as an n-tuple

$$\xi = \left[\xi^1, \ldots, \xi^n\right] \,,$$

or as a linear combination of the frame elements

$$\xi = \xi^k \gamma_k \,,$$

where the elements of $\{\xi^k\}$ are called the *components of ξ onto the $\{\gamma_k\}$ frame*. (Einstein summation convention in force!)

To find the components of ξ on $\{\gamma_k\}$, apply

$$\xi^k = \xi \cdot \gamma_k \,.$$

B.1.1. *Reciprocal Cartesian coordinate system.* Consider now a reciprocal Cartesian coordinate system $\{\gamma^k\}$ whose elements are the inverse [7] of the $\{\gamma_k\}$ elements:

$$\gamma^k = \gamma_k{}^{-1} = \gamma_k \,,$$

since the frame elements are orthonormal; *viz.*, $\gamma_k{}^{-1} = \gamma_k/\gamma_k^2$, but $\gamma_k^2 = 1$.

B.1.2. *Geometric derivative, gradient, divergence, Laplacian.* Define the geometric derivative (operator) ∇ by its components as [8]

$$\nabla = \gamma^k \partial_k \,.$$

This means, treat the geometric derivative as another vector.

Consider a scalar field $\phi = \phi\left[\xi\right]$. Then, define the gradient of ϕ by

$$\operatorname{grad}\phi = \nabla\phi = \gamma^k \partial_k \phi \,.$$

Consider next a vector field $\psi = \psi\left[\xi\right]$. Then, define the divergence of ψ by

$$\operatorname{div}\psi = \nabla \cdot \psi = \gamma^k \partial_k \cdot \gamma^l \psi_l = \partial_k g^{kl} \psi_l \,,$$

where $g^{kl} = \gamma^k \cdot \gamma^l$.

Finally, define Laplace operator on a scalar field ϕ by

$$\operatorname{lap}\phi = \operatorname{div}\operatorname{grad}\phi = \nabla \cdot \nabla\phi = \gamma^k \partial_k \cdot \gamma^l \partial_l \phi = \partial_k \partial_l g^{kl}\phi \,.$$

B.2. **Alternative coordinate systems.** Consider next another, alternative, coordinate system $\{\gamma_{k'}\}$, related to the Cartesian coordinate by

$$\xi^k = f\left[\xi^{k'}\right] \,.$$

It is possible now to express the Cartesian frame $\{\gamma_k\}$ in the alternative coordinate system by using the *tangent vectors* $\{\gamma_{k'}\}$ *defined* by [9]

$$\gamma_{k'} = \partial_{k'}\xi \,.$$

These tangent vectors need *not* be orthogonal nor normal.

---

[7] The square of a vector a is defined as $a^2 = aa$, which, by axiom, $a^2 \in \mathcal{E}^1$. The inverse of a nonzero vector a is then defined as $a^{-1} = a/a^2$.

[8] In traditional notation,

$$\nabla = \gamma^k \frac{\partial}{\partial \xi^k} = \hat{x}\frac{\partial}{\partial x} + \hat{y}\frac{\partial}{\partial y} + \hat{z}\frac{\partial}{\partial z} \,.$$

[9] In traditional notation:

$$\gamma_{k'} = \partial_{k'}\xi = \frac{\partial \xi}{\partial \xi^{k'}} \,.$$

Onto this alternative frame $\{\gamma_{k'}\}$, any point position ξ can be expressed as a linear combination of the alternative frame elements:

$$\xi = \xi^{k'} \gamma_{k'} \,,$$

where $\xi^{k'} = \xi \cdot \gamma_{k'}$.

The metric coefficients for the alternative frame are found by

$$g_{k'l'} = \gamma_{k'} \cdot \gamma_{l'} \,.$$

B.3. Examples. Examples of this section:

Example. In Cartesian coordinates, a particle position is given by $\xi = [x, y]$, where x and y are the coordinates of the particle. Express the position in polar coordinates.

Solution. Polar coordinates, ρ and φ, are defined by

$$x = \rho \cos [\varphi] \qquad \text{and} \qquad y = \rho \sin [\varphi] \,,$$

where $\rho^2 = x^2 + y^2$ and $\varphi = \arctan 2 \, [y, x]$, see `https://en.wikipedia.org/wiki/Polar_coordinates#Converting_between_polar_and_Cartesian_coordinates`.

Then, ξ can be written as

$$\xi = [x, y] = \rho \, [\cos [\varphi], \sin [\varphi]] \,.$$

The tangent vectors are thus

$$\gamma_\rho = \frac{\partial \xi}{\partial \rho} = [\cos [\varphi], \sin [\varphi]] \implies \hat{\gamma}_\rho = \frac{\gamma_\rho}{|\gamma_\rho|} = [\cos [\varphi], \sin [\varphi]]$$

in the ρ direction and

$$\gamma_\varphi = \frac{\partial \xi}{\partial \varphi} = \rho \, [-\sin [\varphi], \cos [\varphi]] \implies \hat{\gamma}_\varphi = \frac{\gamma_\varphi}{|\gamma_\varphi|} = \frac{\gamma_\varphi}{\rho} = [-\sin [\varphi], \cos [\varphi]]$$

in the φ direction.

In Cartesian coordinates, unit vectors are constant in direction and in magnitude. However, in polar coordinates, neither unit vector is constant.

With the unit tangent vectors, ξ can be written as

$$\xi = [x, y] = [\rho \cos [\varphi], \rho \sin [\varphi]] = \rho \, [\cos [\varphi], \sin [\varphi]] = \rho \hat{\gamma}_\rho \,. \qquad \square$$

Example. Express a particle velocity in polar coordinates.

Solution. Since the particle position in polar coordinates can be written as $\xi = \rho \hat{\gamma}_\rho$, the particle velocity, $\dot{\xi}$, can be calculated by calculating the change of the particle position

$$\mathrm{d}\xi = \mathrm{d} \left(\rho \hat{\gamma}_\rho \right) = \mathrm{d}\rho \hat{\gamma}_\rho + \rho \mathrm{d}\hat{\gamma}_\rho \,.$$

The change of $\hat{\gamma}_\rho$ is given by

$$\mathrm{d}\hat{\gamma}_\rho = [-\sin [\varphi] \, \mathrm{d}\varphi, \cos [\varphi] \, \mathrm{d}\varphi] = \mathrm{d}\varphi \, [-\sin [\varphi], \cos [\varphi]] = \mathrm{d}\varphi \hat{\gamma}_\varphi \,.$$

Thus, the change of the particle position becomes

$$\mathrm{d}\xi = \mathrm{d} \left(\rho \hat{\gamma}_\rho \right) = \mathrm{d}\rho \hat{\gamma}_\rho + \rho \mathrm{d}\varphi \hat{\gamma}_\varphi \,.$$

Finally, the change of the particle position per unit time, *i.e.*, velocity, is

$$\dot{\xi} = \frac{\mathrm{d}\xi}{\mathrm{d}t} = \frac{\mathrm{d}\rho}{\mathrm{d}t} \hat{\gamma}_\rho + \rho \frac{\mathrm{d}\varphi}{\mathrm{d}t} \hat{\gamma}_\varphi = \dot{\rho} \hat{\gamma}_\rho + \rho \dot{\varphi} \hat{\gamma}_\varphi \,,$$

where $\dot{\rho}$ is the *radial velocity*, rate at which ρ changes magnitude or stretches' and $\rho\dot{\varphi}$ the *circumferential velocity*, rate at which ρ changes direction or swings.

Appendix C. Notation

C.1. Maths.

C.1.1. *Sets.*

- set: set A, $\mathcal{A}$.
- n-dim set: nset nA, $\mathcal{A}^n$.
- n-dim. Euclidean space: espace n, $\mathcal{E}^n$.
- region: region A, $\mathcal{A}$.
- elements of a set. elset(a,b,c), $\{a, b, c\}$.
- tulpe. tuple(a,b,c), $[a, b, c]$.

C.1.2. *Functions.*
- function value at: vat x, $[x]$.
- order of: orderof, O.

C.1.3. *Geometric objects.*
- boundary: bound, ∂.
- area: area, a.
- surface: surf, s.
- volume: vol, v.
- diameter: diam, d.
- length: length, l.
- radius: radius, r.

C.1.4. *Geometric algebra.*
- magnitude: magn u, $|u|$.
- inner product: iprod, $a \cdot b$.
- outer product: oprod, $a \wedge b$.
- inverse: inv a, a^{-1}.
- unit vector: uvec a, $\hat{a}$.
- unit frame basis vector: ufbvec a, $\hat{\gamma}_a$.

C.1.5. *Geometric calculus.*
- geometric derivative: gder, ∇.
- Laplace operator (derivative): lder, ∇^2.
- directional derivative: dirdev ab, $\nabla_a b$.
- divergence: div, div.
- gradient: grad, grad.
- Laplace operator: lap, lap.

C.1.6. *Calculus.*
- differential operator: dx, d.
- difference operator: Dx, Δ.

C.1.7. *Derivatives.*
- dot derivative: dt a, $\dot{a}$.
- dot dot derivative: ddt a, $\ddot{a}$.
- expanded ordinary derivative: xod at, $\dfrac{\mathrm{d}a}{\mathrm{d}t}$.
- expanded partial derivative: xpd at, $\dfrac{\partial a}{\partial t}$.
- n expanded partial derivative: nxpd at2, $\dfrac{\partial^2 a}{\partial t^2}$.
- indexed ordinary derivative: iod t, d_t.
- indexed partial derivative: ipd t, ∂_t.
- indexed geometric derivative: igder k, ∂_k.
- comma derivative: cder Tt, $T_{,t}$.

C.1.8. *Index notation.*
- basis vector: bvec, γ.
- frame (basis) element: fbvec 1, γ_1.
- reciprocal frame (basis) element: rbvec 1, γ^1.
- frame: frm k, $\{\gamma_k\}$.
- reciprocal frame: rfrm k, $\{\gamma^k\}$.
- metric: met, g.
- metric in frame: fmet 12, g_{12}.
- metric in reciprocal frame: rmet 12, g^{12}.
- up indexed partial derivative: upipd 1, ∂^1.
- down indexed partial derivative: dnipd 1, ∂_1.
- frame (contravariant) components: fvec pos 1, ξ^1.
- reciprocal frame (covariant) components: rvec pos 1, ξ_1.

C.1.9. *Matrices.*
- diagonal: diag, diag.
- signature: sig, sig.

C.1.10. *Brackets.*
- Iverson brackets: iverson k, $[k]_{\text{Iv}}$.

C.2. **Physics.**

C.2.1. *Mechanics.*
- position: pos, ξ.
- pressure: press, p.
- velocity: vel, u.
- acceleration due to gravity: grav, g.
- force: force, f.
- drag (force): drag, *drag*.
- buoyancy (force): buoy, f_{b}.
- shear stress: shear, τ.
- surface tension: surftens, γ.
- frequency: freq, f.
- power: power, p.
- spring constant: kspring, κ.
- energy: energy, e.
- kinetic energy: ken, e_{kin}.
- potential energy: pen, e_{pot}.

C.2.2. *Energy transport.*
- time change rate: rate a, a'.
- flow: flow q, q'.
- flux: flux q, q''.
- thermal energy (heat): then, e.
- thermal energy density: thendens, ϵ.
- mechanical work: work, w.
- internal energy: ien, i.
- accumulation (*e.g.*, internal energy): accu ien, i'.
- thermodynamic temperature: temp, τ.
- specific heat capacity: kshcap, c.
- thermal diffusivity: kthdiff, α.
- thermal conductivity: kthcond, k.
- coefficient of thermal expansion: kthexp, β.
- local film (heat transfer) coefficient (thermal convection): kthconv, f.
- global (average) film coefficient: kavthconv, $\bar{f}$.
- time constant (conduction-convection lumped solution): ktime, τ.
- thermal radiation absorbance: absorb, α.
- thermal radiation reflectance: reflect, ρ.
- thermal radiation transmittance: transm, τ.
- body energy flux distribution function: dbflux, $\breve{e}_{\lambda_{\text{body}}}$.
- black-body energy flux: bbflux, e''_{bb}.
- black-body energy flux distribution function: dbbflux, $\breve{e}_{\lambda_{\text{bb}}}$.

C.2.3. *Mass transport.*
- n (number of) particles: npart, n.
- number of particles density: npartdens, η.
- mass: mass, m.
- mass density: dens, ρ.
- chemical reaction thermal energy: chthen, r.
- mass concentration: conc, c.
- mass fraction: mfrac, w.
- mass diffusion coefficient: kdiff, ϕ.

- mean free path: mfpath, λ.

C.2.4. *Momentum transport.*
- dynamic viscosity: dynvis, μ.
- kinematic viscosity: kinvis, ν.

C.2.5. *Waves.*
- wavelength: wlen, λ.
- wave frequency: wfreq, μ.

C.2.6. *Physical constants.*
- Boltzmann constant: kboltz, k_{b}.
- Stefan-Boltzmann constant: kstef, σ_{sb}.
- Planck constant: kplanck, h_{p}.
- speed of light in vacuum: klight, c_0.
- ideal gas constant: kgas, r_{g}.
- Avogadro's number: kavog, n_{a}.

C.3. **Dimensional analysis.**
- units of a physical quantity: unit q, unit q.
- dimension of a physical quantity: dim q, dim q.
- physical dimension: phdim L, L.
- physical dimension of temperature: phdimtemp, Θ.
- dimensionless quantity: kdim, π.
- characteristic physical quantity: chpq, u_c.
- scaled physical quantity: scpq, $\bar{u}$.
- dimensionless function: dimfunc, ψ.
- Biot number: kbiot, π_{bi}.
- Reynolds number: kreynolds, π_{re}.
- Prandtl number: kprandtl, π_{pr}.
- Schmidt number: kschmidt, π_{sc}.
- Peclet number: kpeclet, π_{pe}.
- Grashof number: kgrashof, π_{gr}.
- Rayleigh number: krayleigh, π_{ra}.
- Weber number: kweber, π_{we}.
- Capillar number: kcapillar, π_{ca}.
- Bond number: kbond, π_{bo}.
- Froud number: kfroud, π_{fr}.
- Nusselt number: knusselt, π_{nu}.
- Sherwood number: ksherwood, π_{sh}.
- power number: kpower, π_{po}.