

FUNDAMENTALS OF TRANSPORT PHENOMENA IN COMBUSTION

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Contents

1. Dimensional Analysis and Mathematical Modeling
 - 1.1. Units, Dimensions, Similarity
 - 1.2. Dimensionless Numbers
 - 1.3. Dimensional Analysis
 - 1.4. Equation of Continuity, Motion and Energy
2. Transport Phenomena
 - 2.1. Laws
3. Fluid Flow
 - 3.1. Definitions
 - 3.2. Newton's Law of Momentum Transport
 - 3.2.1. Poiseuille's Law
 - 3.2.2. Dynamic and Kinematic Viscosity
4. Heat Transfer
 - 4.1. Mechanisms
 - 4.2. Heat Conduction
 - 4.2.1. Fourier's Law - Thermal Conductivity
 - 4.2.2. Heat Capacity
 - 4.2.3. Thermal Diffusivity
 - 4.3. Heat Transfer
 - 4.4. Empirical Correlations
 - 4.5. Heat Convection at a Surface
 - 4.6. Heat Radiation
5. Mass Transfer
 - 5.1. Molecular Diffusion
 - 5.1.1. Diffusion – Fick's Law
 - 5.1.2. Kinetic Theory
 - 5.1.3. Rate of Diffusion
 - 5.1.4. Kinetic theory of gases
 - 5.1.5. Schmidt Number
 - 5.2. Conclusions
 - 5.3. Transport at Interfaces
 - 5.3.1. Gas/Liquid Interface
 - 5.3.2. Gas/Solid Interface

- 5.4. Surface Tension
- 5.5. Chemical Reaction Kinetics
- 6. Prediction methods for Physical Properties
 - 6.1. Corresponding States
 - 6.2. Similarity of the Three Transport Phenomena
 - 6.3. Dynamic Viscosity - Thermal Conductivity
- 7. Conclusions
- Acknowledgement
- Glossary
- Bibliography
- Biographical Sketches

Summary

In this chapter combustion rates, whether in diffusion flames or furnaces, are analyzed on the basis of fluid dynamics, heat and mass transfer, and chemical kinetics. In what follows, these phenomena are tackled individually. An approach considering them simultaneously is presented in *Combustion Research and Computer Fluid Dynamics*.

1. Dimensional Analysis and Mathematical Modeling

Physical models are empirically studied starting from a hope that the small model will behave approximately as the real system to be studied. The real system is too large for real, full-scale study. Moreover, it is physically or materially impossible to vary all variables as widely as desired. Physical models, however, will never entirely mimic reality, for dimensional analysis shows that it is either impossible or impractical to produce identical values for all relevant dimensionless numbers. Geometric, kinematic, dynamic, thermal, and kinetic similarities are impossible to be realized simultaneously, so it is impossible to simulate a large combustion system at a different scale.

Mathematical modeling derives from the need to treat the qualities and properties of a system in an abstract, purely mathematical fashion. Simplified cases may be amenable to an analytical approach; more complete ones are analyzed integrating basic equations of conservation and rates. Until few decades ago computing capacity was limiting, but at present computer programs tackle even the most complex systems (see *Combustion Research and Computer Fluid Dynamics*).

1.1. Units, Dimensions, Similarity

Units play an essential role in science and technology, and most physical and chemical laws are based on a careful analysis of experimental data. Units have an arbitrary aspect: length may be expressed in micrometer (fine dust), feet (a human dimension), or astronomical values, such as light-years. Still, the same laws, principles or formulas often apply at extremely different scales!

The **dimensions** of physical quantities are related to the units needed to express it. In mechanics, every dimension can be expressed in terms of length, time, and mass or alternatively in another combination, e.g. in terms of force, length and mass. For

instance, the dimension of a force is (mass, m) x (length, L) x (time, θ)⁻². Heat is linked to work by Joule's experiment, in which work ($m L^2 \theta^{-2}$), more exactly potential energy, was converted into heat H .

Similarity is a quality of geometrically analogous systems, described by the same mathematical equations and boundary conditions. Similarity makes it possible to study aerodynamic effects in wind tunnels or hydraulic systems on models. Non-dimensional quantities are a logical option in similar systems. In this approach any quantity is related to a 'typical' quantity in the system, serving as unity: selecting a 'typical' length, time, mass, etc. allows rendering these quantities dimensionless, by considering their ratio to the 'typical' representative in each system. In mechanics, once three dimensions are chosen, all others are fixed: selecting a typical length, L and velocity, v defines the typical time, θ as L/v .

1.2. Dimensionless Numbers

Dimensionless numbers are of paramount importance in studying geometrically and physically analogous systems, in modeling, design and experimental research. Dimensional analysis allows impressive savings in deriving rate data, since it suffices experimentally varying dimensionless combinations of variables, rather than testing the specific effect of each variable individually.

For the purposes of the experimenter, different systems, sharing the same dimensionless numbers, are equivalent. According to the Buckingham π -theorem of dimensional analysis, the functional dependence between a certain number n of variables can be reduced by the number k of independent dimensions occurring in those variables, to give a set of $p = n - k$ independent, dimensionless numbers. A ratio of two quantities showing similar dimensions, however, remains undetected:

- for fluid flow through a pipe, the ratio of Diameter D to the length L relates the entrance effects, as long as a boundary layer is not yet fully developed;
- in heat transfer at the wall of a pipe the ratio of the average viscosity μ to that at the wall, μ_w , also appears in numerous empirical correlations.

Such a supplemental effect or a lacking entity will appear spontaneously, as empirical data will show larger spread than the experimental error accounts for.

1.3. Dimensional Analysis

In its most primitive form, dimensional analysis is used to correct algebraic derivations, since in any expression only quantities of the same dimension can be added or subtracted. In any equation its two sides must share the same dimensions. Furthermore, arguments to exponential, trigonometric and logarithmic functions must be dimensionless numbers.

Dimensional analysis is applied in physics, chemistry, and engineering to simplify a problem by reducing the number of independent variables (π -theorem) to the smallest possible number. Systems, which share the same geometry, equations, boundary conditions, and values for the dimensionless parameters are called similar and do not

need separate study.

For example, to derive the time, θ required by a pendulum to fulfill its movement, the length L , the mass, m stretching the wire, and the acceleration of gravity, g , are relevant. For simplicity, the angle is neglected. Since the pendulum law is unknown, an empirical power law is proposed as a guess:

$$\theta = L^\alpha m^\beta g^\gamma \quad (1)$$

At both sides the dimensions must be identical, i.e.

$$[\theta] = [L]^\alpha [M]^\beta [L\theta^{-2}]^\gamma \quad (2)$$

leading to one condition for each dimension:

$$\text{for } \theta \quad 1 = -2\gamma \quad \text{so that } \gamma = -\frac{1}{2} \quad (3)$$

$$\text{for } L \quad 0 = \alpha + \gamma \quad \text{so that } \alpha = \frac{1}{2} \quad (4)$$

$$\text{for } M \quad 0 = \beta \quad (5)$$

$$\text{and} \quad \theta = L^{\frac{1}{2}} g^{-\frac{1}{2}} \quad (6)$$

Surprisingly, the pendulum period does not depend on m !
It is easily confirmed experimentally that:

$$\theta = 2\pi L^{\frac{1}{2}} g^{-\frac{1}{2}} \quad (7)$$

If a moving fluid meets an object, it exerts a force on the object, according to a complicated law of **fluid dynamics**. The variables are: speed, density and viscosity of fluid, size of the body, and force. Using the π -theorem, one can reduce these five physical variables to two dimensionless parameters: drag coefficient C_D and Reynolds number, Re .

The same derivation can be applied to the flow of a fluid in a pipe. When establishing the flow conditions at which laminar flow turns turbulent, four parameters should simultaneously be considered: internal diameter D_i , viscosity μ , density ρ , and average fluid velocity v . However, there is no need to vary four parameters separately, since the dimensionless combination $Re = D_i \rho v / \mu$, is a sufficient substitute. As in the case of the pendulum, proposing a power law and identifying dimensions at both sides of the equation, the law is easily derived as:

$$dp/dx = v^\alpha \mu^\beta \rho^\gamma D_i^\delta = v^{2-\beta} \mu^\beta \rho^{1-\beta} D_i^{1-\beta} = v^2 \rho^{-1} D_i^{-1} (v \rho D_i \mu^{-1})^{-\beta} \quad (8)$$

The quantity between brackets is the (dimensionless) Reynolds Number.

1.4. Equation of Continuity, Motion and Energy

In fluid mechanics integrating fundamental equations (of continuity, motion, and energy) is a route for solving almost all problems, at least on paper. These equations can best be studied using the basic treatise by Bird et al. Writing the Navier-Stokes equation in terms of impulse yields a series of terms, related to:

- A. Substance-determined inertia.
- B. Convective Inertia.
- C. Gravity.
- D. Pressure Forces.
- E. Viscous Forces.

When the various variables in these equations are reduced to their dimensionless form, dividing each quantity by its 'typical' quantity within the same system, then the resulting (now dimensionless) equation has still some (dimensionless) coefficients left. These appear as the Number of Reynolds ' Re ' (Ratio B/E), or Froude ' Fr ' (Ratio B/C). Similarity implies equality of all coefficients of these equations, which leads to the two conditions:

$$\begin{aligned} Re_1 &= Re_2 \\ Fr_1 &= Fr_2 \end{aligned} \tag{9}$$

In other cases more dimensionless may be required, e.g. the Strouhal Number (Ratio A/B) or the Euler Number Eu (Ratio D/B).

Similarly, the equation of energy is composed of terms describing:

- A. Substance-determined energy transport.
- B. Convective energy transport.
- C. Conductive energy transport.
- D. Chemical energy liberated.

This leads to the following Dimensionless Numbers:

Strouhal Number Str (Ratio A/B).

Peclet Number Pe (Ratio B/C) = $Re \cdot Pr$

Damköhler Number III Dam III (Ratio D/B).

Fourier Number Fo (Ratio C/A)

Damköhler Number IV Dam IV (Ratio D/C).

The Thring Number Th (Ratio B/C_{Radiant}) is important in furnaces.

Finally, the equation describing mass diffusion is composed of terms:

- A. Substance-determined mass transport.
- B. Convection mass transport.

- C. Diffusion mass transport.
- D. Chemical mass converted.

This leads to the following Dimensionless Numbers:

Strouhal Number: Str (Ratio A/B).

Peclet' Number (Ratio B/C): $Pe = Pe \cdot Le = Re \cdot Sc$

Damköhler Number Dam_{II} (Ratio D/C).

2. Transport Phenomena

2.1. Laws

Transport Phenomena relate to the tendency of temperature, concentration, and velocity to strive towards uniform values. They are a generic group of processes, by which a quantity (matter, heat, momentum, or electrons) is transferred from regions of high concentration, temperature, fluid velocity, or electric potential, to those regions where this quantity is lower. The same type of empirical equation controls these processes:

- Matter diffusion (Fick's Law),
- Conduction, or thermal diffusion (Fourier's Law),
- Viscosity, or momentum diffusion (Newton's Law),
- Diffusion of electrons in an electrical field (Ohm's Law).

These processes are pre-eminent in engineering, both where taking place at high (heat or mass transfer controlled chemical operations) or low rates (e.g. insulators). These distinct rate Laws were empirically developed, e.g. Ohm's Law:

$$I = A i = \frac{\Delta V}{R} = A \frac{\Delta V}{(\rho \cdot L)} = \varepsilon A \frac{dV}{dz} \quad (10)$$

and define the relationships between:

- flow rate I ,
- driving force ΔV ,
- flux I , a flow rate I per unit cross-section A ,
- resistance R , and
- Resistivity ρ or, inversely, Conductivity ε .

The above Laws define important physical properties empirically: diffusivity, thermal conductivity, viscosity, electrical conductivity. As in electric circuits, resistances R are additive, when a series of such resistances R_i are overcome sequentially. If they occur in parallel, $1/R_i$ is an additive quantity:

$$\text{Resistances in series: } R = \sum R_i \quad (11)$$

$$\text{Resistances in parallel: } \frac{1}{R} = \sum \frac{1}{R_i} \quad (12)$$

The generic diffusion equation is time-dependent, i.e. it also applies to non-steady-state situations.

Although rate laws are similar, there are also notable differences between the underlying phenomena:

- Momentum transfer and mass transfer entail material transport. Heat transfer is immaterial, since only internal energy is exchanged.
- Heat conductivity involves a single material. Diffusion involves distinct molecules, e.g. P diffusing in A. Moreover A and P can be monitored in both mass and molar concentrations.
- Heat moves through walls, while momentum and diffusion are halted. This gives rise to different boundary conditions.

3. Fluid Flow

3.1. Definitions

Fluid dynamics is the study of gases and liquids in motion. Gases are compressible, varying in volume in response to a change in pressure; liquids remain incompressible.

Fluids flow steadily and predictably at low velocity; its flow regime is streamline, viscous or **laminar**. Streamlines show the direction of flow. Rate and shear distribution are calculated relatively simply from the basic equations and Newton's Law. At high rates, flow varies erratically in a regime of **turbulent flow**, reached after either an abrupt (flow in tubes) or more gradual transition (see *Mechanical and Cyclonic Collectors*). Fluid flow is stationary, or transient, rotational (swirling), or non-rotational, with straight streamlines.

The **equation of continuity** formulates a simple mass balance, over entire stream tubes or elementary volumes in Cartesian, cylindrical, or spherical coordinates. For fluid flow in a tube of variable cross-section, the mass flow rate is the same everywhere in the tube. Generally, density is constant and so are volumetric flow rates.

In gravity flow (e.g. hydroelectric power), potential energy (elevation) is transformed into kinetic energy (speed). Gases mostly move by increasing the pressure at the inlet of a system, most commonly by means of fans, blowers, or compressors. Overpressure creates a net force $F = A (p_2 - p_1)$ and also an acceleration of the fluid.

For fluids that are incompressible, non-viscous and in steady fluid flow, Bernoulli's equation relates the energy associated with pressure, velocity, and height of a fluid at one point to the same parameters at a second, downstream point. Their sum remains constant: since the fluid is non-viscous, no mechanical energy is degraded to thermal energy.

The equation requires appropriate empirical correction factors accounting for the inevitable head losses. When a fluid moves through a duct, friction with the wall and local impediments create losses, computed as an equivalent length of duct L , or in terms of the kinetic term $0.5 \rho v^2$. These corrections allow computing how much of the original energy is still available. Since friction losses depend on fluid velocity, and fluid velocity on available head a trial and error procedure is required to establish the flow.

Friction factors are plotted as a function of Reynolds number and roughness of the tube: smooth tubes create less loss than when asperities disturb the flow. Local losses occur in constrictions, valves, elbows, etc.

A **boundary layer** is defined as the space adjacent to a surface in which flow rates are reduced by friction from the surface. It is much thinner in fully developed turbulent flow, than in laminar flow.

3.2. Newton's Law of Momentum Transport

All fluids exhibit viscosity (internal friction) transforming kinetic in thermal energy (i.e., degrading work to heat). Viscosity tends to equalize differences in fluid momentum and velocity: fast moving fluid is retarded by slower moving fluid, and by solid walls (boundary effects). From a transport point of view, viscosity is conductivity rather than resistance, since it is the diffusion factor for momentum, as transported from fluid regions with high momentum (or fluid velocity) to others with lower levels of motion.

Consider a viscous fluid, separating two parallel plates with area A and mutual distance d . One plate is retained in its original position, while the other one is moving at a slow speed v . Commonly, the force F required to keep the second plate moving and the first one immobile is proportional to the area A and also to v , and inversely proportional to d , giving the relationship:

$$\frac{F}{A} = \mu \frac{v}{d} \quad (13)$$

Newton's Law defines dynamic viscosity μ as an empirical factor of proportionality between shear stress F/A and v/d and a material constant for a given fluid. Any fluid in which these quantities are proportional is indeed called Newtonian.

3.2.1. Poiseuille's Law

Consider a long capillary tube. A pressure difference Δp is maintained to keep fluid flowing, and the resulting flow rate is proportional to Δp and inversely proportional to the viscosity μ . Poiseuille's Law gives this volumetric fluid flow Q as:

$$Q = \pi \cdot r^4 \cdot \Delta p / 8 \mu L . \quad (14)$$

with r the pipe radius, L its length.

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Bibliography

Bird R.B., Stewart W.E., and Lightfoot E.N. (1968). *Transport Phenomena*, New York: John Wiley [Basic book for self-study in the fields of momentum, heat, and mass transfer]

Benson, S.W. (1968). *Thermochemical Kinetics*, New York: Wiley.

Chapman S. (1991). *The Mathematical Theory of Non-Uniform Gases: An Account of the Kinetic Theory of Viscosity, Thermal Combustion and Diffusion in Gases*, Cambridge, UK: Cambridge Univ Press [Book on the kinetic theory of gases, as related to transport properties]

Günther R. (1974). *Verbrennung und Feuerungen*. Berlin – Heidelberg – New York: Springer Verlag. [Book on combustion, flames, free jets, and their interactions in furnaces]

Hirschfelder J.O., Curtiss C.F., and Bird R.B. (1964). *Molecular Theory of Gases and Liquids*, New York: Wiley. (1964) [Book on fluids structure and interaction]

Reid R.C., Prausnitz J.M., Polling B.E. (1987). *The Properties of Gases and Liquids*, 4th ed., Appendix A, New York: McGraw-Hill. [Treatise comparing physical properties with correlations estimating them]

Ullmann's Encyclopedia of Industrial Chemistry (1990). 6th ed., Florida, US: VCH. [Numerous interesting discussions and data, including dimensional analysis and correlations related to transfer phenomena]

Wikipedia, <http://www.wikipedia.org/wiki> and <http://en.wikipedia.org/wiki/SI> [Comprehensive encyclopedia explaining numerous themes of physics, chemistry and other sciences]

Biographical Sketches

Alfons Buekens was born in Aalst, Belgium; he obtained his M.Sc. (1964) and his Ph.D (1967) at Ghent University (RUG) and received the K.V.I.V.-Award (1965), the Robert De Keyser Award (Belgian Shell Co., 1968), the Körber Foundation Award (1988) and the Coca Cola Foundation Award (1989). Dr. Buekens was full professor at the Vrije Universiteit Brussel (VUB), since 2002 emeritus. He lectured in Ankara, Cochabamba, Delft, Essen, Sofia, Surabaya, and was in 2002 and 2003 Invited Professor at the Tohoku University of Sendai.

Since 1976 he acted as an Environmental Consultant for the European Union, for UNIDO and WHO and as an Advisor to Forschungszentrum Karlsruhe, T.N.O. and VITO. For 25 years, he advised the major industrial Belgian Bank and conducted more than 600 audits of enterprise.

Main activities are in thermal and catalytic processes, waste management, and flue gas cleaning, with emphasis on heavy metals, dioxins, and other semi-volatiles. He coordinated diverse national and international research projects (Acronyms Cycleplast, Upcycle, and Minidip). Dr. Buekens is author of one book, edited several books and a Technical Encyclopedia and authored more than 90 scientific publications in refereed journals and more than 150 presentations at international congresses. He is a member of Editorial Boards for different journals and book series.

He played a role in the foundation of the Flemish Waste Management Authority O.V.A.M., of a hazardous waste enterprise INDAVER, and the Environmental Protection Agency B.I.M./I.B.G.E. He was principal ministerial advisor in Brussels for matters regarding Environment, Housing, and Classified

Enterprise (1989). Since 1970 he has been a Member of the Board of the Belgian Consumer Association and of Conreur, grouping more than a million members in Belgium, Italy, Portugal, and Spain.

He is licensed expert for conducting Environmental Impact Assessments (Air, Water, Soil) and Safety Studies regarding large accidents (Seveso Directive).

Sylwia Oleszek-Kudlak, born and educated in Poland, received her M.Sc. (1999) in Chemical Engineering from Wroclaw University of Technology. From 2000 she started work as a research assistant at the Institute of Environmental Engineering of the Polish Academy of Sciences in Poland. From 2001 she is Ph.D. student at the Tohoku University of Sendai in Japan (Scholarship of Ministry of Education, Science, Sports and Culture, Government of Japan (Monbukagakusho)). Her research interest is in the area of physical-chemical properties for organic compounds of environmental concern.