1 Introduction

Through and through the world is infested with quantity: To talk sense is to talk quantities. It is no use saying the nation is large . . . How large?

It is no use saying the radium is scarce . . . How scarce?

You cannot evade quantity. You may fly to poetry and music, and quantity and number will face you in your rhythms and your octaves.[1]

1.1 MOTIVATION FOR USING SCALING ANALYSIS

This book is directed to a broad spectrum of readers since modeling transport and reaction processes is common to many fields of pure and applied science. The book should be useful to educators who are seeking effective pedagogical tools for introducing their students to an ever-expanding body of knowledge in the field of transport phenomena and reactor design. It should also be of value to engineers and scientists who need to apply and develop mathematical models for transport and reaction processes. It will be helpful to students who are seeking ways to better understand the broad range of subjects encompassed by transport and reaction processes.

As defined in this book, the subject of scaling analysis, deals with a systematic method for nondimensionalizing a system of describing equations for transport or reaction processes. The resulting dimensionless system of equations represents the minimum parametric representation of the process. By this we mean that the solution for any quantity that can be obtained from these equations will be at most a function of the dimensionless independent variables and the dimensionless groups generated by the scaling process. For example, scaling a heat-conduction process will lead to a set of dimensionless equations whose solution for the dimensionless temperature will be a function of the dimensionless spatial and temporal

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[1] Alfred North Whitehead (1861–1947), in *The World of Mathematics*, J. R. Newman, ed., Simon & Schuster, New York, 1956.

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independent variables and dimensionless parameters such as the Prandtl number ($C_p\mu/k$, in which μ is the shear viscosity, C_p the heat capacity, and k the thermal conductivity). Quantities that are obtained by evaluating the solution to the dimensionless equations at fixed values of the spatial and temporal variables or by integrating a dimensionless dependent variable over the spatial or temporal domain will be functions of a reduced set of dimensionless spatial or temporal variables and the relevant dimensionless groups. In some cases the dimensionless dependent variable of interest might be a function of only the dimensionless groups. For example, in a steady-state heat-conduction process, the dimensionless heat-transfer coefficient (Nusselt number) will be a function of the relevant dimensionless groups, such as the Prandtl number and geometric aspect ratios. This minimum parametric representation of a transport or reaction process is useful since it identifies the dimensionless variables and groups that can be used to correlate data from either laboratory or numerical experiments (i.e., computer simulations). The resulting dimensionless groups can also be used for scale-up or scale-down analyses by invoking the principles of geometric and dynamic similarity.

There is no unique set of dimensionless dependent and independent variables and associated dimensionless groups for a system of equations describing a transport or reaction process. For any system of describing equations, one set of dimensionless dependent and independent variables and corresponding dimensionless groups can always be obtained from any other set. However, one can scale a system of describing equations in a unique way to ensure that the relevant dependent and independent variables and their derivatives are bounded of order one. By this we mean that the magnitude of the particular dimensionless variable or its derivative is bounded between zero and more-or-less 1. For those familiar with formal ordering arguments, we are bounding our variables to be *little oh* of 1 [i.e., $\circ(1)$] as opposed to *big oh* of 1 [i.e., $\bigcirc(1)$], which means that the quantity is essentially 1. Note that by *of order one* we do not mean exactly 1. In $\circ(1)$ scaling, one can say, for example, that $0.8 \cong 1$ or $3 \cong 1$; that is, the quantity is well within an order of magnitude of 1. In this book this special application of scaling that leads to unique dimensionless variables and groups is referred to as $\circ(1)$ *scaling*.

The nondimensionalization associated with $\circ(1)$ scaling is indeed unique. However, arriving at this unique scaling often involves a process of trial and error. That is, one has to assume that a particular transport or reaction process is dominated by some mechanism(s) (e.g., heat conduction in a particular direction for a multidimensional heat-transfer process) and then has to nondimensionalize the describing equations by comparing the other terms to the one that embodies this mechanism. After obtaining a system of dimensionless describing equations, one evaluates the resulting dimensionless groups for the relevant geometric and physical parameters of interest. If all the dimensionless groups are bounded of order one [i.e., $\circ(1)$], the original assumption as to the controlling mechanism(s) was correct. However, if any of the dimensionless groups is much larger than 1, it can indicate that the scaling was not correct for the geometric and physical parameters of interest or that there is a region of influence or boundary layer in which a temporal or spatial derivative becomes very large. In either case one has to repeat the scaling analysis with a different set of assumptions as to the controlling mechanism(s). The possibility also exists that proper scaling will yield a dimensionless group that is much larger than 1, which multiplies some grouping that involves the difference between two dimensionless quantities each of which is bounded of $\circ(1)$. In this case the large dimensionless group implies that the grouping it multiplies is much less than 1. We will see that scaling analysis is forgiving in that, when done correctly, all terms in the relevant equations will be bounded of order one; that is, the product of any dimensionless group and the grouping of dimensionless dependent and/or independent variables that it multiplies is $\circ(1)$.

The utility of $\circ(1)$ scaling is that when all the relevant dependent and independent variables and their derivatives are bounded of order one in the resulting dimensionless describing equations, one can assess the importance of various terms on the basis of the values of the dimensionless groups that multiply them. If all the dimensionless dependent variables and their derivatives and the independent variables are bounded of $\circ(1)$, the dimensionless groups should also be bounded between 0 and 1. Hence, if a dimensionless group is of order 0.01 or less, the term that it multiplies can be ignored in developing a model for the particular transport or reaction process while incurring only a very small ($\sim 1\%$) error. Hence, by using $\circ(1)$ scaling, one can appropriately simplify the describing equations for a transport or reaction process. For example, the equations of motion can be nondimensionalized appropriately using $\circ(1)$ scaling to determine the condition required to neglect the inertia terms; that is, a very small Reynolds number, which is the familiar creeping-flow approximation.

The trial-and-error process involved in arriving at the proper $\circ(1)$ scaling is of particular value in designing experiments. In the absence of solving model equations, $\circ(1)$ scaling permits determining the values of the geometric and process parameters that are required to achieve certain experimental conditions. For example, $\circ(1)$ scaling permits determining the adsorbent bed properties required to ensure that an adsorption process is controlled by equilibrium considerations rather than intraparticle diffusion.

Scaling analysis is also useful for developing perturbation expansion solutions to the describing equations. Scaling will identify dimensionless parameters whose limiting values (i.e., very large or very small) permit making certain approximations in solving the describing equations. For example, when the Reynolds number is very small, one can develop an analytical solution for the flow around a sphere falling at its terminal velocity in a Newtonian fluid with constant physical properties; the result is the familiar Stokes flow solution for creeping flow over a sphere. However, one can account for the neglected inertia terms in the equations of motion by considering a perturbation expansion solution to the describing equations in terms of the small Reynolds number. The zeroth-order term in this perturbation expansion corresponds to the Stokes solution for creeping flow. The first-order term that accounts for some effects of the inertia terms was first worked out by Proudman and Pearson.[2] Perturbation solutions that are well behaved in the limit

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[2] I. Proudman and J. R. A. Pearson, *J. Fluid Mech.*, **2**, 237 (1957).

of the perturbation parameter becoming very small or very large are referred to as *regular perturbation expansions*. Perturbation expansions that are not well behaved in the limit of a perturbation parameter becoming very small or very large are referred to as *singular perturbation expansions*. An example of the latter is very high Reynolds number flows. If one tries to solve the equations of motion in the limit of very large Reynolds numbers by attempting a perturbation expansion in the (small) reciprocal Reynolds number, one cannot properly account for the neglected viscous terms. This is a direct consequence of the reduction in the order of the describing equations when one develops the zeroth-order solution in the reciprocal Reynolds number. To solve singular perturbation expansion problems, one needs to use the method of multiple scales, whereby different scales are used in the inner region, the outer region, and the overlap region between them. Scaling analysis is an invaluable tool for determining when perturbation solutions are possible and in determining the proper scales for the various regions. This book complements classical references on perturbation expansion methods.[3,4]

For the same reason that scaling analysis is useful in determining the scales and expansion parameters in perturbation analyses, it is useful in assessing potential problems that can occur in solving a system of describing equations numerically. That is, when certain dimensionless groups become very small or very large, problems can be encountered in solving the resulting system of describing equations numerically. For example, when the Reynolds number becomes very large, the viscous effects will be confined to a very thin region in the vicinity of the solid boundaries. If one uses a coarse mesh or does not employ a numerical routine with a remeshing capability, the numerical routine will not provide sufficient resolution in the vicinity of the solid boundaries and thereby either will not run or will provide erroneous results. Scaling analysis can be used to identify these *boundary-layer regions* so that a proper numerical method can be employed to solve the problem.

Scaling analysis is particularly useful to an educator who is faced with explaining seemingly unrelated topics such as creeping flows, boundary-layer flows, film theory, and penetration theory. Topics such as these often are developed in textbooks in a rather intuitive manner. Scaling analysis provides a systematic way to arrive at these model approximations that eliminates guesswork; that is, scaling analysis provides an invaluable pedagogical tool for teachers. Disparate topics in transport and reaction processes can be presented in a unified and integrated manner. For example, a *region of influence* in scaling provides a means for presenting a unified approach to boundary-layer theory in fluid dynamics, penetration theory in heat and mass transfer, and the wall region for confined porous media.

Scaling analysis also provides a very effective learning tool for students. Textbooks on transport and reaction processes generally justify simplifying assumptions leading to the creeping-flow, boundary-layer, penetration theory, and plug-flow reactor equations and others through ad hoc arguments rather than by a systematic approach such as that provided by scaling analysis. Hence, a student might

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[3] M. Van Dyke, *Perturbation Methods in Fluid Mechanics*, Parabolic Press, Stanford, CA, 1975.

[4] A. H. Nayfeh, *Perturbation Methods*, Wiley, New York, 1973.

not see the interrelationship between the various approximations made in describing transport and reaction processes, such as the analogy between boundary-layer theory in fluid dynamics and penetration theory in heat or mass transfer. Moreover, the ad hoc approach to simplifying the equations describing transport and reaction processes does not provide students with a basis for simplifying more complex problems not described in textbooks.

1.2 ORGANIZATION OF THE BOOK

Scaling analysis is used by many pure and applied scientists at least in some form; for example, in dimensional analysis. Many textbooks use order-of-magnitude arguments to simplify the describing equations for transport and reaction processes. However, what is lacking is a systematic treatment of scaling analysis that can be used reliably without the need for the intuition that is either an inherent talent or has been learned through years of practical experience. Hence, in Chapter 2 we present scaling analysis in general terms as a series of steps to be followed. We distinguish between the steps used in scaling for the purpose of dimensional analysis, which leads to nonunique dimensionless groups, and those to be followed for the special case of $\circ(1)$ scaling, which leads to a unique minimum parametric representation.

Since this is intended to serve as both a reference book and as a textbook for a course in mathematical modeling, the subject matter covered by Chapters 3 through 5 is organized according to the conventional topics in transport phenomena: fluid dynamics, heat transfer, and mass transfer. The rationale for this organization is that one needs to know how to scale the fluid dynamics to handle scaling of convective heat and mass transfer. The latter is a necessary precursor to treating the special topic of mass transfer with chemical reaction, which is covered in Chapter 6.

Chapter 7 is an integrating chapter in which we consider the application of scaling to process design, which can involve coupled fluid flow, heat and mass transfer, and chemical reactions. In particular, we illustrate how scaling can be used to assess a new process or to design experiments (e.g., the sizing of equipment) to ensure that desired conditions are met.

We presume that the reader has a basic knowledge of transport and reaction processes; the book is not intended to replace textbooks that treat these subjects in depth. A basic knowledge of the language of continuum mechanics (i.e., vector and tensor mathematics) is assumed. However, the appendices summarize useful background material relevant to modeling transport and reaction processes. Since there is no general agreement in the literature on the sign convention in the constitutive equations or surface forces in the equations of motion, the appendices include a brief review of the sign convection used in the book. The appendices also summarize the forms of the continuity, equations of motion for both conventional fluid flow and flow through porous media, and energy- and species-balance equations in generalized vector–tensor notation as well as in rectangular, cylindrical, and spherical coordinates. Useful integral relationships for scalars, vectors, and tensors are also included in the appendices.

The format in Chapters 3 through 5 is designed to illustrate the application of scaling analysis by means of problems drawn from fluid dynamics, heat transfer, and mass transfer. These problems are organized to illustrate how scaling can be used to develop basic concepts such as creeping flows, boundary-layer theory, film theory, and penetration theory. The format is to begin by indicating what the problem is supposed to demonstrate. For example, analysis of an impulsively oscillated plate is presented to illustrate both how to handle time scaling and to show what is meant by a region of influence. Several problems are illustrated in detail, followed by a comparable number of example problems that are outlined in less detail.

Chapter 6 is organized somewhat differently since it considers problems in mass transfer with chemical reaction that require scaling analysis on both the micro- and macroscales: for example, on the scale of a small adsorbent particle and on the much larger scale of the contacting device that contains these particles. Hence, after introducing the concepts of micro- and macroscaling, the problems in this chapter focus on the use of scaling to identify the various reaction regimes that can be encountered in mass transfer with chemical reaction.

Whereas scaling analysis is used in Chapters 3 through 6 to justify classical approximations made in fluid dynamics, heat and mass transfer, and mass transfer with chemical reaction, in Chapter 7 we use scaling analysis to design and assess novel technologies. The four examples considered in this chapter are considerably more complex since they involve coupled transport and in some cases chemical reaction as well. These examples were chosen because scaling analysis contributed significantly to the process design and technology development.

Chapters 3 through 7 end with a summary that emphasizes the principles of scaling analysis that were illustrated in the worked problems. Unworked practice problems included at the end of each chapter explore in more detail the examples considered in the chapter and apply scaling analysis to related problems.