A Course in

TRANSPORT PHENOMENA

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BACKGROUND AND OBJECTIVES

AN INTEGRATED fundamental approach is taken in teaching Transport Phenomena (ChE 620) at Purdue. The course is offered in the Spring Semester and is normally preceeded by a course in Advanced Chemical Engineering Calculations (ChE 527). ChE 620 is the only Transport course for the terminal Master's student but leads to the specialized courses on Heat Transfer (ChE 622), Mass Transfer (ChE 624) and Fluid Mechanics (ChE 635) which are offered in the second year for those who have qualified for the Doctoral program. As a rule, our graduate students have had some undergraduate experience with Transport in the sense of Bird, Stewart and Lightfoot (BSL). New mathematical techniques (linear algebra, partial differential equations, cartesian tensors, etc.) are introduced in ChE 527, where experience in Transport is furthered by frequent in-class illustrations and homework assignments. I consider that the most important objective of ChE 620 is to provide a strong and simple conceptual basis on which all previous transport experience and any future additions to it may be arranged in well-organized structures that provide, in their totality, a perspective of Transport Phenomena. To meet this objective I particularly look for continuity of course coverage and emphasize the economy of the subject rather than its detail. The more detailed description of this course provided in this article should better illustrate these points.

"Suggested" and "assigned" readings are given on a regular weekly basis. These are designed to exercise, and even strain, the self-study habits of the individual. Simultaneously, complete lists of standard references on a variety of topics are established for easy future reference. However, a cautious approach is taken with respect to periodical literature. A "select" accumulation of recent research results is compiled in a library file for easy access. Time limits this specific activity to a minimum, but it is considered an important factor in engaging the student in "Scholarly Activity," which, after all, is one of the primary purposes of any graduate course. Some discussion of recent research results of the Instructor, whenever pertinent, serve well for this purpose since they convey a natural enthusiasm and know-how.

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Dr. Theofanous' research interests are in the field of transport phenomena. He is active in fundamental research (turbulent and multiphase systems), as well as in application oriented work including problems from the environmental (river reaeration), biomedical (mucociliary transport) and nuclear (coolant dynamics and safety of LMFBR) fields.

The course meets twice a week for an equivalent of three credit hours. Note-taking during lectures is eliminated through the use of detailed handouts on most lecture material. In class, emphasis is placed on ideas and their complete and *logical* evolution rather than mere enumeration of results. This approach is probably not too efficient in terms of class coverage but the handout notes compensate for the defect. A total of about 45 homework problems, which help build up the student's confidence in problem solving, are assigned and carry about 35% of the total grade. Student cooperation is encouraged for their solution. A detailed solution for each homework problem is provided via handouts. A two-hour final examination is given at the end of the semester and carries another 35% of the course grade. Frequent 15-20 minute quizzes motivate the student to keep abreast with assigned material since they account for the remaining 30% of the final grade.

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COURSE OUTLINE

THE COURSE BEGINS with a brief, but general introduction which states the basic problem of Transport of Heat, Mass or Momentum in a continuum. An overview of the concepts of densities, fluxes, equations of change and constitutive equations is given and exemplified in terms of simple physical situations which are well-known to the student. The role of initial and boundary conditions and some standard difficulties associated with the solution of the resulting mathematical problems, together with the need for intelligent simplifications, are briefly mentioned. Within this introduction, we discuss in some detail the basic structure of the course and the role and aims of each part. Finally, the introduction is completed with an effort to motivate the more casual observers in the class. Some "exciting" transport problems are posed and some "interesting" solutions are discussed. The choice of topics is arbitrary and naturally biased by my recent research activities. Taylor-Proudman colums, cavitation and pressure signals, mucociliary transport in the mammalian lung, surface tension driven flows in alveolar clearance, and transfer at free turbulent interfaces are some recent topics utilized. The course is formally separated into two parts. Part A, occupying roughly half of the semester, is concerned with the general formulation of Transport Phenomena. Part B undertakes an organized approach to applications of the general theory.

A. FORMULATION

Our aim is to formulate the equations of change for a general multi-component continuum and to consider briefly the various approaches of constitutive theory. The mathematical machinery and, in general, the level of abstraction required for this part of the course cause some difficulties to all but the best-prepared students. However, properly paced lectures and detailed handout notes alleviate most of the problems. Further comfort and a sense of security are provided by the sections on shell balances, equations of change, constitutive equations and macroscopic balances of BSL, which are evenly distributed as self-study assignments during the period occupied by this part of the course. A large number of homework problems chosen primarily to enhance the physical feel of a variety of transport situations is assigned in this period. But development of mathematical skills is also sought to the greatest possible extent.

1. Equations of change

We start with discussion and examples of scalar, vector, and dyadic fields. The tensorial character is discussed in physical terms of zero, first and second order tensors. The *entity* nature of tensors is thus emphasized and its relation to the collection of its components is exemplified. Vector (dyadic) notation is adopted throughout for the inherent conceptual clarity it conveys. Components are not introduced until just before the part of the course dealing with applications. The basic vector differential invariants are then introduced in terms of their coordinate-free representations. General control volumes are introduced, and a number of important operations and theorems (Green-Gauss, Reynold's Transport Theorem) are discussed and interpreted physically. The basic "conservation principles" are first discussed for the conceptually easier case of a collection of discrete particles, and the continuum *ideas* are then obtained in the limit. Cauchy's equation of motion, mass continuity, and total energy and, in addition, the equations of change of kinetic energy and vorticity are derived in a completely rigorous fashion for a multicomponent reacting continuum in both integral and differential forms. The role of the material control volume in isolating diffusive fluxes is noted throughout.

2. Constitutive theory

Non-equilibrium thermodynamics provides the most practical and unifying tool for the derivation of linear constitutive equations. The previously-obtained equations of change are utilized in the entropy balance equation for a material control volume, and the diffusive flux and rate of production of entropy are readily identified. This actually provides a good basis for discussion of the nature of diffusional phenomena in general (heat, mass or momentum) which is the very foundation of the Transport Phenomena approach. Linear phenomenology is then introduced to arrive, with relatively little effort, at the transport coefficients and driving forces as given in equations (18.4-1) to (18.4-13) of BSL. This development is particularly desirable since it clearly elucidates the role of chemical potential (isothermal) gradients (or concentration and pressure gradients) and body forces in mass diffusion processes. With a slight variation of the above development, Stefan-Maxwell type equations are obtained and are utilized to introduce in a concise fashion the concept of effective diffusivity for dilute multicomponent systems. At this point homework problems are assigned which bring out certain important features of mass and energy transport in multicomponent systems.

For a brief illustration of approaches developed within the framework of Rational Mechanics, the most general stress-strain relationship for a purely viscous (Stokesian) fluid is derived. The principles of *"material indifference"* and *"isotropy"* are of main concern here. How isotropy leads to symmetries that restrict the form of the constitutive equation involves a very instructive argument which is given in detail. We thus arrive at equation (3.6-11) of BSL, which is used as the starting point for a number of homework assignments in non-Newtonian fluid flow. Finally molecular mechanisms are considered from the simple kinetic theory approach given in BSL. An elementary, one-dimensional random walk is discussed and a diffusion process is obtained in the limit as a stochastic process. The main aim in these discussions is to provide the basis for interpretations of diffusivities in terms of the frequency and distance (velocity) of fluctuation processes, since these concepts are also useful in turbulent phenomenological theories.

3. Transition to components

Flexibility in choice of a co-ordinate system is important for the most convenient solution of any transport problem. Furthermore, the transition from the general vector equations to component forms must be thoroughly understood. These goals are achieved by discussing some elements of differential geometry for orthogonal curvilinear co-ordinate systems. Explicit general expressions for the vector differential invariants are obtained in terms of the *"physical components,"* by referring their co-ordinate-free representations to a *local cartesian basis*. Finally the importance of an intelligent choice of co-ordinate systems, which takes advantage of the symmetries of the problem, is illustrated by examples of simple diffusion problems in elliptic geometries and of convective diffusion in stagnation flow (material co-ordinates). An immediate application follows by introducing the concept of the stream function, which is then related to the physical components of the velocity vector by satisfying the equation of continuity in a general orthogonal curvilinear system for two-dimensional or axisymmetric incompressible flow. In this part, and throughout the course, topics on the algebra and calculus of tensors are reiterated whenever possible to provide the student with the required familiarity.

In class, emphasis is placed on ideas and their complete and logical evolution rather than mere enumeration of results.

B. APPLICATIONS

BY THIS TIME THE students have solved a large number of problems and they have seen the abstract developments of the theoretical foundations. At this point they are ready and, in fact, anxious for the in-class applications which they were promised at the beginning of the course. Again the basic economy of ideas is emphasized. It is essential, nevertheless, that the student be introduced to a number of important chemical engineering applications in addition to the specialized topics of multicomponent diffusion and non-Newtonian flow which were treated earlier. The general areas of interphase transfer at fluid-fluid and fluid-solid interfaces in both stratified and dispersed (bubbles-drops-suspensions) systems are in the center of such interest and, in addition, provide unlimited opportunity for instructive discussions. The basic problems are posed at the outset for both deterministic and stochastic (chaotic) systems. Their solutions are discussed throughout the remainder of the course in terms of the possible variety of approaches.

In all applications, an effort is made to reduce the procedure to a number of elementary steps. Simplifications are introduced at two levels, and in both, a clearly-understood list of the restrictions imposed by the simplifying assumptions is compiled. We first simplify the vector equations (change-constitutive) as we utilize them to understand the *"physics"* of the specific problem. This examination leads also to the most convenient co-ordinate system. Further simplifications are then introduced in the component forms of the equations. The boundary conditions are then discussed in light of the requirement for a well-posed mathematical model.

The classification of applications is in terms of the interplay between convection and diffusion, on the one hand, and between deterministic (laminar) and stochastic (turbulent) systems on the other. Methods of obtaining fundamental knowledge of the physical processes in stochastic systems are discussed. Convection-diffusion considerations are an important input for these discussions as well as for the analysis of deterministic systems. Now the homework assignments are more closely related to the lecture material than before.

1. Similarity—Interphase Transfer

We start with a brief account of dimensional considerations. The "natural" units which are provided by the physical parameters that "enter" the problem are discussed. The concept of self-similarity is then introduced and illustrated by obtaining "universal" solutions for the propagation of a strong shock wave in the atmosphere, the flow of a heavy fluid over a spillway, and for gas absorption into a turbulent liquid with high turbulent intensities (recent results obtained by the author and co-workers). The general problem of transfer across a free turbulent interface is posed in detail. Open channel (natural stream) flows, annular and bubbly pipe flows, film flows and agitated dispersed (bubble) systems are identified as important special cases, and the desirability of a unified approach is thus illustrated. On the other hand, the nature of variations between these systems is discussed in terms of the physical motions involved and their interaction with the diffusion processes near the gas-liquid and comparatively solid-liquid interface. A qualitative discussion of the origin of hydrodynamic instabilities that lead to periodic motions (waves) and turbulence is given. The physical meaning of eddies, large and small scale motions, correlation and dissipation of turbulent energy is briefly discussed. The quantitative treatment, however, of these topics is postponed till the end of the course.

Similarity is then used for the reduction of partial differential equations. Problems in unsteady diffusion and unsteady convective diffusion are solved and discussed. Invariance of a partial differential equation under certain transformations of the independent variables is utilized as an elementary example of the Group Symmetric origin of the method but also as a practical means of uncovering the precise form of the similarity transformation. In terms of these solutions, penetration and renewal concepts for turbulent interfaces are discussed. The previously-obtained universal solution is reinterpreted in terms of quasi-deterministic models of turbulent interfaces. This discussion leads to a rational look at the limitations of the *"correlation"* approach in general.

Non-equilibrium thermodynamics provides the most practical and unifying tool for the derivation of linear constitutive equations.

2. Negligible convection

Rigorous elimination of the convective terms is initially carried out for cases in which $\mathbf{V} \cdot \nabla \mathbf{V} = 0$, $\mathbf{V} \cdot \nabla \psi = 0$ ($\mathbf{V} \perp \nabla \psi$) or $\mathbf{V} \equiv 0$. A large number of solutions, previously-obtained in the homework problems on conduction, diffusion and rectilinear flows, is recalled. The linearity property and resulting superposition are pointed out and help enlarge the class of available solutions. Some multi-dimensional diffusion problems (including source terms) that help familiarize the student with Carslaw and Jaeger and Crank are solved as homework assignments.

The *approximate* elimination of the convective terms occupies most of the discussion. Important classes of fluid mechanical approximations, such as creeping flow and lubrication theory, are introduced and applied to specific problems. Stokes' solution for creeping flow around a solid sphere is worked out in detail and the "paradox" of the corresponding problem for a cylinder is discussed. Oseen's improvement of Stokes' solution is then given. The two solutions are then interpreted. Stokes' approximation involves a symmetric diffusion of vorticity from the sphere while Oseen's improvement incorporates (approximately) convection of vorticity by the main flow. This consideration leads to the genesis of the boundary layer concept which is taken up next. Prior to that, however, the film concept is examined and the effects of mass transfer on temperature and concentration profiles are pointed out by means of BSL's treatment of interphase transfer at high mass transfer rates.

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the system allowed to come to equilibrium again. Again the oxygen pressure was measured, and the liquid O/K ratio calculated. The data indicate that at any given temperature level the oxygen partial pressure depends only on the liquid O/K ratio. Data are shown below at 500, 600, and 650°C for various O/K ratios.

	Partial Pressure of Oxygen, atm.		
O/K ratio	500°C	600°C	650°C
1.0	0.018	0.070	0.13
1.1	0.10	0.13	0.21
1.2	0.26	0.26	0.31
1.3	0.43	0.40	0.43
1.4	0.61	0.55	0.60

There is essentially nothing known about the structure of the liquid phase. It is black, probably has a high electrical conductivity, and contains some or all of the following species, K^+, O_2^-, K_2O, K_2O_2, KO_2, etc.

We need, immediately, an accurate value for the energy evolved or absorbed if a reaction occurs so that the liquid melt absorbs oxygen isothermally at 600°C and changes the O/K ratio from 1 to 1.4. Express your answer on a basis of 1 gram-atom of potassium.

Also, from the data given, please formulate a simple process flow diagram to remove oxygen from air and indicate possible problem areas.

4. Concentrated sulfuric acid (100%) is to be mixed with water before being added to a batch reactor. For optimum control of the reactor, the dilute acid should be fed between 5 and 10°C. The inlet reactor concentration is to be 20 wt % acid. To minimize heat exchange equipment, it has been suggested that the dilution step be carried out by pouring the concentrated acid over the requisite amount of ice (4 lbs.). Assuming we adopt this scheme and also precool the concentrated acid originally to 0°C, what specifications would you place on the heat exchange equipment to bring the dilute acid to 10° C?

Freezing points of sulfuric acid solutions, partial pressures of water over sulfuric acid solutions, and ice vapor pressure data are attached if needed.

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3. Boundary layers

The classic *exact* solution for laminar flow induced by an infinite rotating disc is derived in detail to illustrate more clearly how convection may limit the growth of a diffusion layer. At this point the student is ready to be convinced of the rationale for the boundary layer assumptions. Laminar boundary layers of momentum, mass, energy are considered in detail for flat plates and solid spheres. The role of the Reynolds, Schmidt and Prandtl numbers in these phenomena is emphasized, especially as a means to understand the limitations of the boundary layer assumptions.

Previously tackled problems of transfer at turbulent interfaces are re-examined in terms of boundary layer concepts and solutions. In particular, renewal concepts are discussed in terms of the small penetration approximations as well as eddy models.

4. Negligible diffusion

The complete solution of a boundary layer situation requires adequate consideration of the diffusion-free region of the domain. The usually non-trivial case is concerned with the fluid mechanical problem. The concepts of inviscid (ideal) flow and irrotational flow are introduced and contrasted. The vorticity-free flow ($W \equiv 0$) around a growing bubble in a *viscous* fluid illustrates this distinction and elucidates how solid surfaces, in general, act as vorticity sources for viscous fluids. Here the ideas are clarified by considering the boundary conditions required for a well-posed problem of a flow starting from rest when it is cast as ideal flow in terms of the velocity potential on the one hand or is described by the Navier-Stokes equation on the other.

The remainder of the material covered in this section is concerned with construction of irrotational flows while the depth and extent of coverage depend largely on how far behind schedule we are at this point.

5. Hydrodynamic Stability—Turbulence

The physical concepts associated with system isolation from surroundings and random inputs form the basis for application of small perturbation analysis of stability. Due to time limitations, a semi-rigorous derivation of the Orr-Sommerfeld equation is given, and the origin of turbulence is discussed in terms of random inputs at random time. Statistical and phenomenological approaches as well as physical models are illustrated and contrasted in terms of potential and purpose. The physics of turbulent motions are recalled from previous discussions and are placed on a more concise and, whenever possible, quantitative basis. Turbulent intensity, correlations, Fourier decomposition and the turbulent energy spectrum are introduced for this purpose. Finally the well known quantitative results of the Universal Equilibrium theory are introduced to define characteristic length and velocity scales for this range. Scalar transport in turbulent flows is now discussed in terms of large and small scale motions and comparisons with experiments are given for stratified and dispersed systems. The course is completed with a brief discussion of interfacial turbulence.

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