SPECIAL TOPICS IN TRANSPORT PHENOMENA

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Preface

This monograph comes out of a long history of two things: on the one side, teaching a course on transport phenomena, which one of us (GA) has done for a longer time than he cares to confess; on the other side, working together, which the other one of us probably thinks has gone on for too long already, though the time involved is significantly less than what was being talked about before.

Teaching transport phenomena is a strange experience. There is so much conceptual content in the subject that one has no hope whatsoever of covering any reasonable fraction of it in a two-semester course; and yet, that's exactly what one is called upon to do. There is a redeeming feature, however: a textbook which is so obviously a classic, its contents so obviously what one is expected to teach to the students, that in a way the task is made easy by telling the students, on the very first day of class, that they will eventually be expected to have mastered Bird, Stewart and Lightfoot — BSL. At least, they know exactly what is expected of them. This does make things easier, or at least not so overwhelmingly difficult that one would give up in despair, but still, let's face it: who has ever covered BSL in two semesters?

However, one goes on and tries to teach something. The content of BSL is just too much, so one tries to extract concepts and concentrate on those, the details being left to BSL. One of us has done that for too long, and has found out after a while that he wasn't teaching BSL at all — he was teaching concepts which the students found challenging, though they had difficulty tracking them down in BSL. And yet, one still expects students to have grasped BSL, doesn't one? And on the other hand, one becomes quite fascinated with the concepts — or the special topics, or the ideas — one has been concentrating upon, and one doesn't know exactly what is going on. Unless one is lucky (as one of us has been) in having among his students the other one of us — a student who seems to have no problem mastering BSL on her own, and finds the discussion of special topics, concepts, or whatever, a challenging experience in the classroom.

Well, how can all this be translated into a monograph, if at all? When one writes a book, one has an audience in mind. But this turns out to be the ideal situation if one considers a monograph whose audience is intended to be the population of graduate students in chemical engineering. This is just the audience one wants: an audience who has mastered BSL already, so that one can concentrate on what one thinks, perhaps wrongly, to be rather interesting special topics, challenging conceptual issues, things which are, let's face it, just shear fun. Fun to teach, fun to think about, fun to write about - without (thank God for BSL) having to worry about all the nitty gritty details. Or, for that matter, about the concepts at the first level of conceptual development, or even the second or the third one. Isn't it rather nice to be able to concentrate on very special cases? Particularly if one can try to show that they are not that special after all?

Now when we teach, not abstractly, but concretely in the classroom, we have a few problems of a down to earth nature. When we need to do some algebra, we have two choices. One, we get it all done on transparencies so there are no sign mistakes and everything runs smoothly. Well, we can do that, and by the time our collection of transparencies is large enough, we think of writing a book which is supposed to be in competition with BSL. People have done that, and it has been a mistake — you can't beat BSL at their own game. The other choice is to be cavalier about algebra, miss the signs, and ask students to work it out themselves at home whenever a problem arises — that works beautifully, but one doesn't get a collection of slides to stimulate one to write a book.

There is another thing about actual teaching in the classroom: one interacts with students. One says something and a student objects to it. Now 90% of what students say in class is just meant to make themselves look like conscientious students and that is entirely irrelevant. But the remaining 10% — that's what makes teaching in the classroom worthwhile. If it weren't for that, one might as well bury BSL in a computer data bank, require students to access it and work out all the problems, and be done with it. Should anyone still think there's some use in an instructor actually walking up to the lectern and saying something, one could choose the best one to do so, videocassette him or her, and put the videocassette in the computer data bank as well. The whole point about teaching is the interaction with students; and so we instructors, short of declaring bankruptcy, have to maintain that such interaction is absolutely crucial. Now we have already admitted that such interaction may have any meaning only in 10% of the cases — can we say anything more?

Perhaps yes, and we have tried to do so in this monograph by introducing three characters: Sue, Ralph, and Bob. Bob is an engineer, a no-nonsense type, one who knows life and isn't going to be taken in by any too-sophisticated argument. He keeps our feet on the ground; his observations are frustrating at times, particularly when one is trying to discuss a subtle conceptual point, but he compels us to always point out the practical significance of what we are discussing, and that is healthy. Ralph is the typical good student. He never makes a mistake in algebra, he knows all the formulas in the books, he remembers everything. He is perhaps the most frustrating of the useful students — getting him to accept a new viewpoint is very, very hard indeed. He knows BSL by heart, and he enjoys those problems which are marked with a subscript of 5, very difficult. He knows he can work those out much better than anybody else in the class. Ralph keeps us from being sloppy — or at least he tries very hard to do so. Our third student, Sue, is — let's face it — the one we prefer, though we would never tell her. She has just slipped by her undergraduate work, because she didn't work very hard. Should she do any algebra, she is guaranteed to make a terrible mess of it. She is very fuzzy about the content of the books she has studied in her undergraduate days — just the opposite of Ralph. That makes it easy for her to accept new viewpoints: she hasn't mastered the old ones well enough to cherish them. And she's smart. She is, in fact, a totally imaginary character: we all hope that a student will ask the question we want to be asked, and it never happens. Sue is our dream of a student, who always asks that question. If one only could get a Sue in one's class in real life, everything would just be absolutely wonderful.

Now why Bob, Ralph and Sue? Because about a third of the students in chemical engineering nowadays are female. Half of the authors of this monograph is female, but with only two authors it's hard to match the one-third ratio exactly, and half is the closest approximation one can obtain. We do, however, have a great advantage: we don't need to worry about our grammar being considered sexist. We use "he" and "she" interchangeably, without worrying about percentages; we never feel the need to use him/her, which we find annoying in the extreme.

We have talked about BSL earlier. We assume our reader has studied at least some parts of it. What else do we assume our reader has studied? Well, let's first answer an easier question: what else do we hope our reader has, well, not studied, but at least leafed through. We hope he has read a classic which unfortunately isn't read much at all, "Dimensional Analysis" by P.W. Bridgman, Yale University Press, 1922. She would also have done well reading

"Diffusion and Heat Exchange in Chemical Kinetics" by D.A. Frank-Kamenetskii, Princeton University Press, 1955 (we do not even hope our reader knows Russian), and "Physicochemical Hydrodynamics" by B. Levich, Prentice-Hall, Englewood Cliffs 1962. "Process Fluid Mechanics", same Publisher, 1980, and "Process Modeling", Longman 1986, by M.M. Denn would also be on our list of favourites (Mort Denn is great — he slips in the word "process" no matter what he is writing a book about. We haven't been able to find a reasonable way of doing the same ourselves). And, since we are dreaming, "Rational Thermodynamics", Springer-Verlag 1984, by C.A. Truesdell wouldn't hurt by any means. Now that's what we would hope our reader has read, but not what we'll assume she has in fact read — except BSL. That, dear reader, you should have studied, and if you haven't, well, it's just tough luck.

In a preface, one is supposed to acknowledge help received, isn't one? Help has been received, mainly by students. Clever ones, who asked challenging questions; less clever ones, who had the courage to say they hadn't quite understood what was going on; some students who worked on some special problem for their senior thesis in Naples, and were able to prove that the simple problem intended for a senior thesis was a difficult one worth a higher level thesis; some students who worked for a PhD thesis, and were able to show that the sophisticated problem given to them was really trivial, and managed to get a PhD because they thought of their own problem afterwards; students of the Bob type, who kept our feet on the ground; of the Ralph type, who obliged us to do our algebra correctly; and wouldn't it be nice in real life to be able to thank also a student of the Sue type?

There is another category of acknowledgements we need to make. We started on this project because courses titled something like "Special Topics in Transport Phenomena" are commonplace in many chemical engineering departments. So, at the very beginning, we wrote to friends in a large number of such departments asking for their advice on what should go into a book with such a title. We received a large number of very thoughtful replies, and these have been taken into account. The number of people who replied is too large for a list to be given here, but our sincere thanks go to all entries in this non-existent list.

Naples, Italy, and Nottingham, UK

Foreword

The publication of this monograph has taken longer than expected, even though it was almost in its final version a couple of years ago. Many events have happened in the meantime, and there was a time when we almost gave up on its publication. It has been only after the untimely decease of Gianni that I started to think again about it.

As the reader can see from the Preface, Gianni taught transport phenomena for many years and — as he himself used to admit — he was teaching concepts instead of details; students could find the details in the Bird, Stewart and Lightfoot book — very hard work indeed. Having been a student of his myself a long time ago, I found Gianni's lectures extremely difficult, but amazingly challenging: I always wanted to attend his lectures again after graduation, just to enjoy them without the fear of eventually having to pass the exam. Of course I never managed to do that, and when a few years later I was team-teaching with him, I appreciated that his teaching habits were still unchanged — and the feelings of the students too. This is why I was eventually convinced that this monograph deserves to be published: it collects somehow Gianni's way of teaching and some of the concepts he tried to transfer to students.

Chapter 6 was re-written later. In our original project we meant to furnish very general concepts about the hydrodynamics of granular materials. At that time the field was not yet so popular, and basic concepts were still in the development stage. When I reconsidered the possibility of publishing this monograph, I realised that many very good books on the subject had come out in the meantime (such as, for instance, the book by J.P.K. Seville, U. Tüzün and R. Clift, "Processing of Particulate Solids", Blackie Academic & Professional, 1997; and the one by L.-S. Fan and C. Zhu, "Principles of Gas–Solid Flow", Cambridge University Press, 1998). Therefore, there was no reason to repeat in one chapter what was already available and published in a much more complete way. Chapter 6 has been completely re-written with the help of Tommaso Astarita, and the reader will find it somewhat different in style from the other chapters. Chapter 6 now deals with new results obtained by ourselves on compressible flow of granular materials, a very challenging topic which is still at its exordium, and which looks very promising in new developments. A flavour of "granular" thermodynamics is given too.

A number of people must be acknowledged for their help in writing Chapter 6. Many thanks go to Tommaso for contributing most of the results on compressible flow of granular materials, and for sketching most of the figures. I would like to thank Renee Boerefijn for providing useful comments, and Yvonne Campbell for typing most of Chapter 6 quickly and professionally.

Many thanks go to Samir Khan for sketching the majority of the graphs.

Finally, a special thank you goes to Ari Kummer for his invaluable help and support during the latest part of the work, which is always the most difficult and demanding.

Raffaella Ocone
Edinburgh, 2001

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Chapter 1

Introduction to Methodology

1.1 INTRODUCTION

On the first reading of this chapter, the reader will probably get the impression that we do not follow an organized line of thought—we wander here, there, and everywhere. Well, in a sense we do, but there is a hidden line of thought, which hopefully will become apparent to our readers on the second reading. This is meant to be a provocative chapter, one which hopefully will provide ample food for thought, and we hope our readers get quite mad with us no later than halfway through. We also hope they'll forgive us by the end.

What is the scope of the chapter? We analyze several apparently unrelated problems, and all of them are formulated in the simplest possible form (don't worry, there are complexities aplenty), in fact in such a simple form that in most cases an analytic solution to the governing equations can be obtained. The purpose is to extract from these simple problems some lessons of presumably general applicability: the reader is asked not to skip the remarks, which may mostly appear trivial in connection with the specific problems considered, but will later be seen to be anything but trivial. We also try, on more than one occasion, to find out something about the solution of a problem without actually solving it, or to find an approximate solution. This may appear futile when an exact analytical solution is available, but it is meant to pave the way for doing that kind of thing when an exact solution is not available. For the problems at hand, the powerfulness of these techniques is reinforced by comparison with the exact solution.

A very important aim of this Chapter is to convince the reader that the subjects of Transport Phenomena and of Thermodynamics are not mutually exclusive ones; in fact, they are strongly intertwined, much more so than is usually thought. The usual attitude in this regard is to think that Thermodynamics tells us what the equilibrium conditions are; if the actual conditions are not equilibrium ones, knowledge of thermodynamics allows us to establish what the driving force for a transport process may be, and that is all the coupling between the two subjects that there might be. Well, the situation is significantly more complex than that. This is an important conceptual point, and it becomes more clear if the analysis is uncluttered by irrelevant complexities. This is the main reason for formulating all the problems in the chapter in their simplest possible form which leaves the conceptual content still there.

Now, is there some kind of simplification which we might do once and for all? Indeed there is: a geometrical one. It so happens that the space we live in, which we may perhaps be willing to regard as an Euclidean one (an assumption which certainly makes life easier) is, however, no doubt endowed with an embarrassingly large number of dimensions: three. Following the old rule of thumb that there really are only three numbers, 0, 1 and ∞ (perhaps only 0 and ∞ in fluid mechanics, we consider high Reynolds number flows, low Reynolds number flows, and an instructor who deals with the case where the Reynolds number is about unity is regarded as fussy in the extreme — whoever remembers what Oseen contributed to fluid mechanics?) we come to the conclusion that our space is awkwardly close to having infinitely many dimensions. Do we really need to bother about this as soon as we begin? Perhaps we may avoid the issue. Geometry has a nasty tendency to make things complex even when they are not; or, if things are conceptually complex, geometry tends to mask this interesting kind of complexity with the trivial one of having three dimensions to worry about: just as the complex game of chess. Perhaps we can stick to the deceptively simple game of checkers, without, as Edgar Allan Poe rightly observed, losing any of the conceptual subtleties, in fact keeping them in the sharp relief they deserve: we may stick, for the time being, to spatially one-dimensional problems, where all quantities of interest are functions of at most one spatial variable, say X. However, we do not want to degenerate to the silly simplicity of tick-tack-toe, and so we will not make the steady state assumption, so that time t is, in addition to X, an independent variable.

All problems in engineering science are formulated on the basis of two types of equations: *balance* equations and *constitutive* equations. A balance equation can be written either for a quantity for which a general principle of conservation exists (such as mass, linear momentum, angular momentum, energy, etc.), or for a quantity for which no such principle exists (like entropy, or the mass of one particular component in a reacting mixture), provided its rate of generation is included in the balance equation. We begin by considering the former case.

Let $F(X,t)$ be the flux of the quantity considered, i.e., the amount of it crossing the surface orthogonal to X at X per unit time, and let $C(X,t)$ be the concentration, i.e., the amount of the quantity considered per unit volume. The unsteady state balance equation takes the form:

$$\partial F/\partial X + \partial C/\partial t = 0 \tag{1.1.1}$$

Now there are several subtleties with Eq. (1.1.1) and some of these will be discussed later on. However, for the time being we are happy with it as it stands, and we ask ourselves the following question.

Suppose the system is initially at equilibrium, with $C = 0$ everywhere (if it has some value other than 0, it can always be set to zero by normalization).

Remark 1.1.1

Normalizing C to an initial value of zero is more than simply trying to make the algebra a little less cumbersome. When a problem is essentially linear, we want to keep it that way; now, mathematically a problem is linear if boundary conditions are homogeneous (a linear combination of the dependent variable and its derivatives is zero). This can be accomplished, for sufficiently simple problems, by appropriate normalization.

Correspondingly, $F=0$ initially:

$$t < 0, \; X > 0, \; F = C = 0 \tag{1.1.2}$$

At time zero a jump of C is imposed at $X=0$, say:

$$t > 0, \; X = 0, \; C = J \tag{1.1.3}$$

where J is the imposed jump. The question which we ask is: what are the functions $C(X,t)$ and $F(X,t)$ at $X > 0, t > 0$?

Remark 1.1.2

This shows that we are focusing on the propagation of an imposed jump. It will be seen that this is in fact a very interesting problem, and indeed one can immediately ask oneself an interesting question: under what conditions will the imposed jump propagate as such (i.e., staying a jump?).

And under which conditions will it, if it does stay a jump, decay in amplitude?

It is perhaps obvious that Eqs. (1.1.1–3) do not give enough information to answer this question. What is needed is a *constitutive equation*: an equation which assigns the value of $F(X,t)$ in terms of $C(X,t)$, so that the problem becomes a mathematically well posed one.

However, before discussing constitutive equations, it is useful to define a dimensionless concentration $c = C/J$, so that Eqs. (1.1.1–3) become:

$$\partial F/\partial X + J\partial c/\partial t = 0 \tag{1.1.4}$$

$$t < 0,\ X > 0,\ F = c = 0 \tag{1.1.5}$$

$$t > 0,\ X = 0,\ c = 1 \tag{1.1.6}$$

Remark 1.1.3

Since initially both F and C are zero, why did we choose to consider the case where a jump of C is imposed, rather than a jump of F? Mainly because of tradition. Indeed, it will often be useful to consider what may be called the dual problem, where a jump Q of the flux F is imposed. In that case, a dimensionless flux $f = F/Q$ comes to mind straightaway, but there is no immediate concentration scale available to define a dimensionless concentration.

1.2 THE CLASSICAL PLUG FLOW REACTOR

Suppose we have a plug flow reactor (PFR) without knowing it is a PFR (we are allowed to be silly that early in the game), and we wish to determine its Residence Time Distribution by measuring the response to some forcing function on the feed. We choose a step forcing function. Specifically, the PFR is fed with a steady state mass flow-rate of pure water, and at time zero we switch the feed to one of water containing a concentration J of ink. We monitor the transparency of the exit stream as a function of time; we are willing to assume that the transparency, when appropriately normalized, is proportional to $1–c(L,t)$, where L is the axial length of the PFR. (Of course,