RECENT ADVANCES IN THE ENGINEERING ANALYSIS OF CHEMICALLY REACTING SYSTEMS

Edited by

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Recent Advances in the Engineering Analysis of Chemically Reacting Systems

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FOREWORD

It is easy to be controversial about the history and development of a scientific field, particularly one related to chemistry since it is one of the oldest and most honorable disciplines. Often papers, which had they been published later, would have had a greater impact on a field than they had at the time. This has been shown to be abundantly true in chemical reaction engineering. Since alcoholic spirits of various kinds are produced in biochemical reactors one could say that chemical reaction engineering is ancient. If one examines the older chemical engineering literature, say *Industrial and Engineering Chemistry* or the *Transactions of the AIChE*, in 1945 there is little that one would recognize as chemical reaction engineering. There was applied chemistry, to be sure, but the emphasis was different. The common tonnage chemicals had reactors that were merely built rather than rationally designed.

The first real textbook on reaction engineering was that of Hougen and Watson (1947) and at that time the name had not even been invented since that book was called "Chemical Process Principles" subtitled "Kinetics and Catalyses". Its stress was on applied chemical kinetics but it did present fixed bed reactors and the associated problems of heat and mass transfer along with a discussion of a numerical method. It is not possible to overemphasize the influence that this book had on chemical engineering both industrial and academic.

Damkohler as early as 1937 presented detailed mathematical descriptions of chemical reactors with the full transport and kinetic equations. This work in the United States, at least was largely unnoticed, unfortunately, and it is a classic example of a work appearing too early for exploitation. Denbigh in his early work developed a style and pattern which had a profound effect on reaction engineering and his papers on stirred pots, optimum temperature profiles, and polymerization reactors are classics. In the area of steady state multiplicity the work of Taffanel and LeFloch and Liljenroth anticipated the papers of van Heerden, but the latter had a greater impact since they appeared at just the right time for exploitation by others. Now mathematicians and chemical engineering theorists have entered the field in full force and the structure of these systems for lumped constant reactors is almost completely delineated. Much of this has not as yet appeared in the literature.

Single catalyst particles were considered early by Wagner but the work of Thiele opened the floodgate of work on effectiveness factors. Probably there have been more papers written on the behavior of single catalyst particles than any other subject in reaction engineering.

Chemical reaction engineering has become a mature and highly mathematical subject and even a superficial examination of the papers in this volume will verify that. This is a remarkable change from 1945, forty years ago, when it can be said that chemical engineering was a non-mathematical subject. Academic chemical engineers in their research are more and more

concerned with the structure of their systems—that is the interplay of chemical reaction and heat and mass diffusion. The structure of these systems is being developed in a way seemingly almost thought impossible a short time ago. Again mathematicians have entered the field with new results in differential and algebraic topology and the future for the theoretically inclined looks brilliant. It is possible that the whole structure of the solution space may be made evident with little or no numerical computation.

The reactor literature now is rife with papers on models for all sorts of reactor configurations for both the steady and transient states. Catalysis has become almost the exclusive preserve of the chemical engineer. Systems of reactions of enormous complexity are now routinely modelled, and, where basic data is wanting, parametric studies can be easily made. Multiphase reactors with all of the attendant problems of heat and mass transfer and fluid mechanics occasioned by diverse reactor geometry are being attacked. The some thirty papers in this volume attest to the highly developed state of an extremely complex field and to the depth that has been reached in the last twenty-five years—approximately the age of high speed computing. It is not necessary to stress what has happened during that period except to say that with the aid of the desk computer one can solve problems only dreamed of at the beginning of that period.

By now the reader should believe, I hope, that the theoretical side of reaction engineering is well in hand or will be shortly. Unfortunately the experimental and practical implementation of these results lags. Universities are not equipped to operate chemical reactors on a scale necessary to validate models appropriate to the industrial scene. The chemical and petroleum companies are loath to present proprietary results and for good reason. This is regrettable, and one cannot fail to notice that there is not one industrial paper presented in this volume.

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PREFACE

Chemical Reaction Engineering, a title coined less than three decades ago, is today one of the most popular and attractive areas of research in chemical engineering. It has assumed this role for a variety of reasons. In its totality the subject encompasses chemical kinetics, chemical reactor theory, reactor operation and dynamics, industrial reactor design, empirical determination of the effect of parameters on reactor performance, and chemical reactor technology in general. To the more discerning, however, the subject has come to denote a theoretical insight into the performance of chemical reactors for various classes of reactions, including an understanding of the chemical transformations that occur and the instabilities associated with chemical reactors. The importance of the subject has grown so rapidly that regular international conferences titled *International Seminar in Chemical Reaction Engineering* (*ISCRE*) are held alternately in USA and Europe. Another international conference was held in January this year at Pune (India), and based on the papers presented at this conference a two-volume book *Frontiers in Chemical Reaction Engineering* was brought out. A number of other conferences in related fields such as catalysis and catalyst deactivation also devote considerable attention to the reaction engineering aspects of the subjects.

This is not the proper place for listing the number of authoritative books and reviews that have appeared on various facets of chemical reaction engineering. Indeed, specific chemical and petrochemical reactions are being separately treated by some authors along with associated engineering problems. Among the other related areas which have grown almost as rapidly as the main subject itself, mention should be made of fluidization. Started originally with the hope that it might be the answer to most reactor problems, fluidization did not live up to expectations, and research in this area was waning till a decade ago when interest was suddenly revived with renewed emphasis on coal conversion reactors. The Engineering Foundation of USA conducts regular seminars on fluidization. There are then other types of reactors like immobilized enzyme reactors and polymerization reactors, not to mention the more common contacting devices for gas-liquid, liquid-liquid and gas-liquid-solid reactions in which research is continuing unabated.

A stage has been reached in the development of chemical reaction theory when one may justifiably attempt yet another collection of papers which would give a broad indication of the type of thinking presently in vogue, with a hint of the emerging directions of research in chemical reaction engineering. Such monumental works as *Chemical Reactor Theory* edited by Professors Neal Amundson and Leon Lapidus which contain authoritative articles on a number of important subjects are few, but even they do not attempt to cover the full gamut of systems and situations that one encounters while dealing with chemical reactions. The 26 papers comprising the

present volume do not also cover the entire field. No attempt has been made to restrict or define the scope of the volume, and it has been left to the authors, each an authority in his own field, to expound on a subject of his choice. It has been ensured that repetition is avoided, however.

Conceived as it has been, this volume should be regarded more as a collection of the recent works and thoughts of some leading researchers in chemical reaction engineering, rather than as a directed attempt to present chemical reaction engineering in a predetermined perspective. Notwithstanding this intentional lack of direction, it is clearly possible to classify the articles that have been received, not without some prompting suggestions from the editor, under the following categories: modelling of chemical reactions and associated mass transfer effects; parametric sensitivity and stability of chemical reactors; fluidized-bed reactors; liquid-liquid and gas-liquid reactors; three-phase reactors; polymerization reactors; and biochemical reactors.

To be sure, it is an impossible task to cover these subjects fully, and yet it is felt that the articles presented here will provide a general indication of the current thinking in some of the major areas in this rapidly widening field—widening because newer classes of systems are being included constantly. For example, polymer reaction engineering has been added, and biochemical reaction engineering has been attracting the attention of chemical reaction engineers for quite some time now. An area which has been missed here is electrochemical engineering; it was not possible to attract an article from an electrochemical engineer with bias towards reactor theory.

The accent, all too noticeable, is on analysis and theory, rather than on industrial aspects of chemical reactors. The profession of chemical engineering, being by its very definition practical, it might appear somewhat strange that this volume should be devoted exclusively to theory and analysis. Professor Amundson states in the foreword that chemical and petroleum companies do not fully give out their results, and it is likely that a vast store of information (both theoretical and practical) exists in their archives which is not old enough for publication from their point of view. This is perhaps one of the reasons for the unfortunate fact that even today many reactors are built from experience and operation at different scales rather than from theory and first principles. It is doubtful if high tonnage reactors will ever be built entirely from theory, but increasing use of theory for precisely predicting the performance of reactors, avoiding the zones of maloperation, improving the performance of reactors and optimising their operation, and delineating the zones of stability, can easily be foreseen.

The various symposia organised by *ISCRE* attempt to present the latest developments in different aspects of chemical reactor theory. The Pune conference referred to earlier also represented an attempt in this direction. The present volume may be regarded as a complementary effort—with this difference that the articles are not the outcome of a conference. In an ambitious endeavour of this nature—which is necessarily restrictive—where only 26 articles could be accommodated, it has not been possible to

invite articles from many other renowned researchers who have contributed equally to the growth of chemical reaction engineering.

I would like to record that the concept of editing a special volume in the general area of chemical reaction engineering owes its origin to my association with the Indian Institute of Chemical Engineers as editor of its journal the "Indian Chemical Engineer" from 1978 to 1983. Due to various reasons this volume could not be published as a Special Number of that journal but is being presented under the title "Recent Advances in the Engineering Analysis of Chemically Reacting Systems".

This title fully reflects the scope and contents of the articles appearing in the volume. It brings out the rather important fact that emphasis is gradually but unmistakably shifting to the theory and analysis of unsteady state operation. The analysis of steady state operation of chemical reactors has reached a stage where further research would not appear to be very rewarding. This is even more so in the case of diffusion-cum-reaction in catalyst pellets in which research of a high order has been carried out. The scholarly treatise by Professor Rutherford Aris *Mathematical Theory of Diffusion and Reaction in Permeable Catalysts* is hardly likely to be improved upon, and although no moratorium on research in this area is indicated, further studies should necessarily be restricted to unexplored aspects such as the effect of porosity and diffusivity variations in bidispersed systems rather than the development of more efficient methods of computation.

The volume starts with articles pertaining to the analysis of chemical reactions including heat and mass transfer effects, residence times in several environments and modelling of complex reactions. What is attempted here is an engineers'-eye-view (in 5 articles) of chemical transformations in the presence of physical constraints. Two articles on fixed-bed reactors then follow, highlighting the importance of parametric sensitivity and regimes of control.

Instability in chemically reacting systems has been the preserve of physical chemists, till in the early seventies chemical engineers made deep inroads in this field with their own brand of analysis. Thus in the volume we have 5 articles devoted to instability and multiplicity in chemically reacting systems. A rather noteworthy feature is that stochastic analysis appears to be gaining ground. With the availability of high speed computation facilities, there really is no reason why the more realistic stochastic approach should not replace deterministic modelling in many branches of chemical engineering.

The succeeding 11 articles are devoted to analysis of different reactor types such as fluidized-bed, gas-liquid, and three-phase reactors (including three-phase fluidized-bed reactors); one article has been included to bring out the importance of regeneration of coked catalysts using noncatalytic reaction theory.

Analysis of reacting macromolecular media forms the subject matter of the next two papers. A comprehensive and critical evaluation of diffusional effects in such media highlights the contributions in this important area. Ethanol production systems using immobilized whole microbial cells have

caught the attention of industrialists and researchers in recent years, and an article on this aspect of biochemical engineering followed by a critical evaluation of homogeneous catalysis as applied to industrial organic reactions completes the list of articles in the volume.

It is hoped that in the not-too-distant future another volume will be brough out highlighting the industrial applications of chemical reactor theory. This would provide a partial answer to Professor Amundson's lament (see *Foreword*) that the present volume does not have a single article of immediate industrial relevance (actually a couple of articles do give some industrially useful information). Nonetheless it is a fact that this volume reflects present trends in chemical reaction engineering. It is likely that the industry does take advantage of some of the newer concepts, but understandably it is chary of announcing any improvements resulting therefrom. It is not uncommon for the details of a successful application to be announced much after it has been accomplished. In some areas theory will always be ahead of practice, and hopefully chemical engineers will continue to advance theories some of which will find their way to industrial practice.

In this rather difficult task of assembling the articles and editing them I have received help from colleagues directly associated with me and also from my students. In particular I would like to record my deep sense of gratitude to Dr. B.D. Kulkarni for his continued and cheerful help.

Poona   L.K. DORAISWAMY
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CONTENTS

1. ALGEBRAIC RELATION FOR MASS TRANSPORT IN FLOWS WITH AND WITHOUT CHEMICAL REACTION

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ABSTRACT

Simple algebraic equations for the Sherwood (or Nusselt) number are developed for Falkner-Skan flows with suction at the boundary, for forced as well as natural convective mass transfer with homogeneous reactions, and for unsteady-state heat or mass transfer. Algebraic expressions have been obtained by replacing the terms of the convective-diffusion equation by their order of magnitude evaluations multiplied by appropriate constants. The values of these constants have been calulated by using rate expressions available for some limiting cases. The resulting equations predict rates within 5 to 10% of actual values.

INTRODUCTION

The analysis of mass or heat transfer phenomena in which the rate of transport is dominated by two or more processes generally requires numerical techniques (or approximate analytical techniques, such as perturbation methods, which inherently have a limited range of validity) for solving the associated transport equations. A few typical examples of such phenomena are mixed, forced and free convection of heat or mass, convective mass transfer in reacting fluids and transport problems in which external body forces exert an influence (e.g., magneto-convective flows). Since the primary focus of such studies is usually on obtaining expressions for *rates* of trasport, analytical techniques that lead directly to closed form expressions for rates are often sufficient and, in fact, desirable. A simple interpolation technique for estimating directly the rates of heat or mass transfer (Ruckenstein 1962) was applied recently to combined, forced and free convection over vertical plates and horizontal cylinders (Ruckenstein and Rajagopalan 1980) and to free convection flows over the entire range of Prandtl numbers (Ruckenstein 1980). Involved in this interpolation technique is the replacement of each term of the convective-diffusion equation by a properly scaled evaluating expression multiplied by an appropriate constant. This procedure leads to an algebraic equation for the Nusselt or Sherwood number in which the constants are determined by using the (readily available) asymptotic solutions to

the limiting cases of these problems. (Pure free convection and pure forced convection are the limiting cases in the first of the above two examples; in the second, extreme values of the Prandtl number, i.e., $Pr \to 0$ and $Pr \to \infty$, constitute the limiting cases.) In what follows, simple algebraic expressions will be provided for rates of heat or mass transfer in boundary layer flows with suction at the bounding surface, in forced or free convection in reactive flows and in unsteady convective heat or mass transfer. In the last case, unsteady-state diffusion in the absence of convection and steady-state convective diffusion form the limiting situations.

TRANSPORT PHENOMENA IN WEDGE FLOWS WITH SUCTION AT THE SURFACE

Suction (or injection) of fluids through confining surfaces is often used in controlling boundary layer development over such surfaces. The rate of suction determines the transfer coefficients (in addition to the stability of laminar flow and the possibility of separation in decelerated flows). These effects are usually encountered in transpiration cooling, transport over porous surfaces (e.g., heterogeneous catalysis) and geothermal heat transfer problems.

As an example of the application of the interpolating technique to this class of problems, we shall consider heat or mass transfer in the so-called Falkner-Skan flows (often called 'wedge flows'). This group of flow problems is characterized by free-stream velocities (outside the momentum boundary layer) that vary as a power of the distance along the wedge (measured from the leading edge); i.e., $U(x) = n_\infty x^m$. As is well-known, this class of problems admits similarity solutions both for the flow field and for the temperature or concentration field (see Schlichting, 1968) if the suction rate at the surface $(y = 0)$ is of the form

$$v(x, y)\Big|_{y=0} = v_0(x) = K\left(\frac{m+1}{2} \frac{\nu U(x)}{x}\right)^{1/2} \tag{1}$$

where v is the velocity of the fluid normal to the surface, K is a constant and ν is the kinematic viscosity. The leading terms of the power series expansions for the tangential and normal velocities (denoted by u and v, respectively) in this case are given by

$$u = A(m)U(x)^{3/2}\nu^{-1/2}x^{-1/2}y \tag{2}$$

and

$$v = B_0(m)U(x)^{1/2}\nu^{1/2}x^{-1/2} + B_1(m)U(x)^{3/2}\nu^{-1/2}x^{-3/2}y^2 \tag{3}$$

where $A(m)$, $B_0(m)$ and $B_1(m)$ are known coefficients which depend on the exponent m of the free-stream velocity.

For large values of the Prandtl (or Schmidt) number the rate of heat (or mass) transfer toward or away from the surface is controlled by the region near the wall, where the velocity field can be approximated by eqs. (2) and (3).

In this case, the following equation, in combination with eqs. (2) and (3), describes the temperature field:

$$u \frac{\partial T}{\partial x} + v \frac{\partial T}{\partial y} = \alpha \frac{\partial^2 T}{\partial y^2} \qquad (4)$$

For the following application of the proposed method we assume the boundary conditions:

$$T = T_\infty \text{ as } y \to \infty \text{ for all } x; \quad T = T_\infty \text{ at } x = 0 \text{ for all } y;$$

and (5)

$$T = T_w \text{ at } y = 0 \text{ for all } x.$$

An order-of-magnitude evaluation of the terms in eq. (4) can now be done by scalling ∂T by $\Delta T (= T_\infty - T_w)$, ∂x by x, and ∂y and y by δ, where δ is the thickness of the thermal boundary layer [given by k/h_x; k = thermal conductivity of the fluid and h_x = the local heat transfer coefficient (as yet unknown)]. Further, each term of eq. (4) is replaced by the evaluating expression multiplied by an appropriate constant, as follows:

$$u \frac{\partial T}{\partial x} \to C_1 \frac{U(x)^{3/2} \delta}{\nu^{1/2} x^{3/2}} \Delta T$$

$$v \frac{\partial T}{\partial y} \to C_2 \frac{u(x)^{1/2} \nu^{1/2}}{x^{1/2} \delta} \Delta T + C_3 \frac{U(x)^{3/2} \delta}{\nu^{1/2} x^{3/2}} \Delta T$$

and

$$\alpha \frac{\partial^2 T}{\partial y^2} \to C_4 \alpha \frac{\Delta T}{\delta^2}$$

where C_i's are constants. Substitution of the above estimates in eq. (4) and some rearrangements lead to

$$C_5 \, \text{Re}_x^{3/2} \, \text{Pr} + C_6 \, \text{Re}_x^{1/2} \, \text{Pr} \, \text{Nu}_x^2 = \text{Nu}_x^3 \qquad (6)$$

where

$$\text{Re}_x = U(x)x/\nu \qquad (7)$$

and

$$\text{Nu}_x = h_x x/k \qquad (8)$$

The coefficients C_5 and C_6 are now determined from the solutions available for limiting cases, as shown below.

Case a: No Suction

The solution for the Nusselt number in this case will determine the coefficient C_5 which arises from the contribution of bulk flow. The value of C_5 will, of course, depend on the particular form of the free-stream velocity (i.e., value of m) and is available for various values of m in Schlichting (1968)

and Eckert and Drake (1972), among others. For instance, in the case of the well-known Blasius flow ($m = 0$), one has

$$\text{Nu}_x = 0.339 \ \text{Re}_x^{1/2} \ \text{Pr}^{1/3} \tag{9}$$

which leads to

$$C_5 = (0.339)^3 \tag{10}$$

Case b: No Free-Stream Flow

In this case the governing differential eq. (4) becomes

$$v_0(x) \frac{dT}{dy} = \alpha \frac{d^2T}{dy^2} \tag{11}$$

The solution of eq. (11) under the conditions

$$T = T_w \ \text{at} \ y = 0 \ \text{and} \ T = T_\infty \ \text{as} \ y \to \infty \tag{12}$$

is then

$$T = e^{v_0 y/\alpha}[T_\infty (e^{-v_0 y/\alpha} - 1) + T^w] \tag{13}$$

It is easily seen that eq. (13) can satisfy the boundary condition for $y \to \infty$ only if $v_0 < 0$, hence only for suction. The expression for the Nusselt number then follows from the definition of h_x

$$h_x = \left(-k \frac{dT}{dy} \Big|_{y=0} \right) \Big/ (T_w - T_\infty)$$

and is given by

$$\text{Nu}_x = -(v_0 \times x/\alpha) \tag{14}$$

The particular form $v_0(x)$ specified in eq. (1) can be substituted in eq. (14), to obtain

$$\text{Nu}_x = -\left(\frac{m+1}{2} \right)^{1/2} K \ \text{Re}_x^{1/2} \ \text{Pr} \tag{15}$$

where K is a negative quantity. This implies that the coefficient C_6 in eq. (6) corresponds to

$$C_6 = -\left(\frac{m+1}{2} \right)^{1/2} K \tag{16}$$

which, for flow along a plate, reduces to

$$C_6 = -K/\sqrt{2} \tag{17}$$

The above discussion show that the Nusselt number for the combined case, denoted by, say, $\text{Nu}_{x,c}$, can be written, regardless of the value of m, as follows:

$$\text{Nu}_{x,c}^3 = \text{Nu}_{x,f}^3 + \text{Nu}_{x,s} \ \text{Nu}_{x,c}^2 \tag{18}$$

for the case of heat or mass transfer with suction at the wall. $\text{Nu}_{x,f}$ and $\text{Nu}_{x,s}$ in eq. (18) represent the expressions for Nu_x when one has only free-stream

flow (i.e., no suction) and only suction at the wall (i.e., no free-stream flow), respectively. A comparison between the values of $Nu_{x,c}$ calculated from eq. (18) and the exact, numerical results of Stewart and Prober (1962) is presented in Table 1 for $m = 0$. It can be seen from this comparison that, even though the above approach is strictly valid for large Prandtl numbers, the algebraic equation is sufficiently accurate even for $Pr \rightarrow 0(1)$, particularly when the suction rate is large ($|K| \geqslant 1$).

Table 1. Heat Transfer in Flow Along a Flat Plate with Suction at the Plate

Re_x	$Nu_{x,c}$					
	$Pr = 10; K = -5$		$Pr = 10; K = -0.5$		$Pr = 1; K = -5$	
	This work	Stewart & Prober (1962)	This work	Stewart & Prober (1962)	This work	Stewart and Prober (1962)
1×10^2	353.55	353.69	35.50	37.00	35.37	36.02
2×10^2	500.00	500.19	50.18	52.33	50.02	50.94
4×10^2	707.11	707.37	70.94	74.00	70.73	72.04
8×10^2	1000.00	1000.38	100.29	104.66	100.03	101.89
1×10^3	1118.04	1118.46	112.11	117.01	111.83	113.91
2×10^3	1581.14	1581.74	158.50	165.48	158.15	161.10
4×10^3	2236.07	2236.91	224.10	234.02	223.66	227.82
8×10^3	3162.28	3163.47	316.85	330.96	316.29	322.19
1×10^4	3535.54	3536.87	354.22	370.02	353.62	360.22
2×10^4	5000.01	5001.89	500.84	523.29	500.08	509.43
4×10^4	7071.07	7073.74	708.17	740.04	707.21	720.44
8×10^4	10000.01	10003.77	1001.34	1046.58	1000.13	1018.86
1×10^5	11180.35	11184.56	1119.48	1170.11	1118.18	1139.12

Although the above comparison is made for one special case of m, it is reasonable to consider that the equation developed can be used for other values of m as well. Finally, it is also important to note that the algebraic eq. (18) probably holds even when the velocity of suction at the wall (i.e., $v_0(x)$) assumes a form different from the one specified by eq. (1). Equation (1) is usually invoked to guarantee the applicability of similarity techniques for solving the transport equations (as done by Stewart and Prober, 1962), but it is not required for applying the interpolationte chnique. For arbitrary functional forms of $v_0(x)$, one simply has, as shown in eq. (14),

$$Nu_{x,s} = -(v_0 x/\alpha),$$

which can be used in combination with eq. (18) for predicting $Nu_{x,c}$.

MASS TRANSFER WITH HOMOGENEOUS, DESTRUCTIVE CHEMICAL REACTION

The above technique is useful for obtaining convenient expressions for mass transfer rates when a sink term (such as homogeneous reaction) enters the transport equation. In this section we shall give a few examples of such problems in both forced and natural convective flows.

Boundary Layer Mass Transfer with an *n*th Order Homogeneous, Destructive Reaction

Consider as an example the problem specified by the following equation:

$$u\frac{\partial c}{\partial x} + v\,\frac{\partial c}{\partial y} = D\frac{\partial^2 c}{\partial y^2} - k_n c^n \tag{19}$$

with

$$c = c_s \text{ at } y = 0, \quad \text{for all } x$$
$$c = 0 \text{ as } y \to \infty, \quad \text{for all } x \tag{20}$$

and

$$c = 0 \text{ at } x = 0, \quad \text{for all } y$$

Even though the velocity field can be of the form specified in the previous section in the discussion of the Falkner-Skan flows, we shall assume for the sake of simplicity that there is no suction or injection of the fluid at the boundary. Under these conditions $u(x, y)$ is given by eq. (2) and $v(x, y)$ by the second term of eq. (3).

The interpolation procedure can now be applied to eq. (19) and it can be shown that in this case one obtains

$$E_1 \text{Re}_x^{3/2} \text{Sc} + E_2 \text{Da}_{n,x} \text{Sh}_{x,c} = \text{Sh}_{x,c}^3 \tag{21}$$

where $\text{Da}_{n,x}$ is the Damköhler number for an *n*th order reaction (see below). The coefficient E_1 follows from the limiting case of mass transfer without chemical reaction as shown in the previous section. The second limiting case in this problem corresponds to mass transfer controlled by only diffusion and reaction (i.e., no convection) and is specified by

$$D\frac{d^2 c}{dy^2} - k_n c^n = 0 \tag{22}$$

and the first two boundary conditions in eq. (20). This equation can be integrated readily to obtain the concentration gradient at $y = 0$:

$$\left.\frac{\partial c}{\partial y}\right|_{y=0} = -\left[\frac{2}{(n+1)}\frac{k_n c_s^{n-1}}{D}\right]^{1/2} c_s \tag{23}$$

The Sherwood number $\text{Sh}_{x,r}$ for this limiting case follows from eq. (23) and the definition of the mass transfer coefficient, $k_{m,r}$

$$k_{m,r} = \left(-D\left.\frac{\partial c}{\partial y}\right|_{y=0}\right)\Big/ c_s \tag{24}$$

Thus,

$$\text{Sh}_{r,x} = \frac{k_{m,r}x}{D} = \left[\frac{2}{(n+1)}\frac{k_n c_s^{n-1} x^2}{D}\right]^{1/2} = \text{Da}_{n,x}^{1/2} \tag{25}$$

The above equation also defines the Damköhler number that appears in eq. (21).