ANALYTICAL AND NUMERICAL STUDIES OF SOME TRANSPORT PHENOMENA

by

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DEDICATED

TO MY PARENTS ...

CERTIFICATE

This is to certify that the thesis entitled

ANALYTICAL AND NUMERICAL STUDIES OF SOME TRANSPORT PHENOMENA

which is being submitted by **Ms.VIDHYA BALASUBRAMANIAN** *alias* **B. VIDHYA LAKSHMI** *for the award of the degree of* **DOCTOR OF PHILOSOPHY in MATHEMATICS** *to the* **INDIAN INSTITUTE OF TECHNOLOGY, DELHI,** *is a bonafide record of research work done under our guidance and supervision.*

The thesis has reached the standard fulfilling the requirements of the regulations relating to the degree. The results obtained in this thesis have not been submitted to any other University or Institute for the award of any degree or diploma.

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ABSTRACT

The thesis contains seven chapters and is broadly divided into three sections. **Chapter 1** *contains a survey of literature related to all the three sections.*

In **PART I**, *the transport of a reactive contaminant in a mildly curved tube under the influence of heterogeneous chemical reaction is considered. In particular, the combined action of secondary flows and homogeneous/heterogeneous reaction on the development of concentration profiles/longitudinal diffusion coefficient is studied. The contents of this part include* **Chapters 2, 3** *and* **4**. *The main emphasis in these chapters is to obtain the description of the transport phenomena of solutes in the presence of secondary flows and heterogeneous reaction using the analytical (perturbation and derivative expansion procedures) and spectral finite difference method of analysis.*

Chapter 2 *deals with the dispersive transport of a heterogeneously reactive tracer in a mildly coiled tube. The study extends the analysis of dispersion of a passive tracer in a straight circular tube first reported by Taylor [1953]. The analysis shows that in the interphase transport of reactive species, the effective dispersion coefficient is significantly different from that of Taylor due to mild effects of wall absorption. Mild effects of wall absorption is considered because in that case, the loss of solute at the boundary will not be quite considerable and hence there may be sufficient amount of solute left in the flow by the time, the Taylor limit is applicable. Moreover, the effect of wall absorption is to cause appreciable radial concentration gradients. This puts a bound on the values of the wall absorption parameter for which the one dimensional Taylor dispersion model is valid. Therefore, a perturbation series solution is obtained to find the modification in the effective dispersion coefficient due to secondary flows and mild absorption effects. The constraints imposed by the perturbation techniques are removed using a numerical scheme based on spectral method. Results are found to be applicable for a time at which the Taylor dispersion model holds. The results corresponding to the straight tube are found for a time at which the Taylor dispersion model holds and are verified with* Sankarsubramanian *and Gill [1973]. It is found that the combined effect of curvature and wall reaction is to reduce the longitudinal dispersion coefficient considerably. Finally, it is observed, that the Taylor model restricted the analysis to weak effects of wall absorption only and hence*

there is a need to look for the generalized dispersion model to incorporate the moderate effects of wall absorption as well.

In **Chapter 3**, *the combined effect of secondary flows and moderate effects of irreversible boundary reaction on the dispersion process is analysed based on the generalized dispersion model proposed by Gill and Sankarasubramanian [1970]. The study describes the development of dispersive transport following the injection of a tracer in terms of the three effective transport coefficients viz. the exchange, the convection and the dispersion coefficients. Unlike the corresponding straight tube analysis (Gill and Sankarasubramanian [1973], Phillips et. al. [1995]) where the exchange coefficient is found to be independent of the velocity distribution, the present analysis shows its dependence on cross stream velocity distribution (secondary flow effect). Second order corrections (in terms of the Dean number) for the asymptotic large time evaluations are also made for the convection and dispersion coefficients. In the absence of any interface transfer, the results are in agreement with Erdogan and Chatwin [1967], with the exchange coefficient approaching zero and the other two coefficients attaining their proper values. At the other extreme, it is shown that for rapid wall reaction mechanism in the presence of mild secondary flows, the exchange coefficient is enhanced, while the convection and the dispersion coefficients are reduced. For moderate values of the absorption parameter, the retention effects are found to be the rate determining processes and the secondary flows have negligible effect, thus confirming the earlier results of Jayaraman et. al. [1998] for the case of secondary flows with absorbing curved walls.*

In **Chapter 4**, *the bulk concentration distribution in a Newtonian fluid for the secondary flow in a curved tube with bulk/wall reaction is obtained for a range of parameter values using an axially marching spectral finite difference scheme. The results predominantly illustrate that for fixed extent of secondary flows there is an improvement in the performance of the reactor as the effect of bulk and wall reaction mechanisms intensify in the system. For the same magnitude (moderate effects) of bulk and wall reaction mechanisms, there appears to be an increased conversion/performance in the homogeneous case. For small values of the reaction parameters, the improvement in the performance (3%) is more due to the interface transfer than bulk reaction. But, for* *moderate values of the non-dimensional reaction parameters (around 10), the enhanced performance (28 %) is more due to the bulk reaction than wall reaction. As the effects of secondary flow dominate, there is an improvement in the performance of the reactor irrespective of the reactivity of the solute. The results agree with those of Mashelkar and Venkatasubramanian [1985] for the case of non-absorbing walls. It is also observed that the approach of isoconcentration profile to the stream line pattern occurs at a lower value of the curvature parameter in the presence of wall reaction.*

The study is extended to examine the modifications in the tracer response measurements due to the power law rheology of the flowing fluid. The salient observation, irrespective of the reactivity of the solute, is that the performance of the reactor is improved in the case of pseudoplastic fluids compared to dilatant fluids. This improvement is further enhanced due to the presence of mild interface transfer.

PART II *contains* Chapters 5 *and* 6. Chapter 5 *deals the hydrodynamics of the phenomenon of steady state, fully developed, incompressible flow of a Newtonian fluid flowing through a lid driven square cavity. This study is extended in* Chapter 6 *to capture the time development of the complex vortex structure formed due to the impulsive movement of the lid in a square cavity. The governing nonlinear vorticity equations in* Chapter 5 *are elliptic whereas in* Chapter 6, *they are parabolic in nature. The emphasis in these chapters is to adapt and implement two new compact, 9 point, higher order finite difference formulae for the corresponding equations. The numerical scheme reported in* Chapter 5 *is a fourth order method and that given in* Chapter 6 *behaves like a fourth order method for fixed mesh ratio. These schemes reduce the execution time considerably (compared to the earlier methods) and utilise optimal storage for the implementation of the algorithm.*

In Chapter 5, *following Mohanty [1989], a compact, nine point, fourth order method is constructed and implemented for the simulation of the recirculation phenomenon (vortex formation) due to a lid driven square cavity. The results have been compared with Gupta [1991] and with the other solutions available in the literature. The results illustrate the well known features of the driven cavity, including, a primary vortex in the central part of the cavity and secondary vortices in the lower part. We find from the numerical experiments that for the values of Reynolds number reported by Gupta [1991],* *the rate of convergence of the present algorithm is much faster. The execution time of the algorithm has reduced to almost one half of that reported by Gupta [1991].*

In **Chapter 6**, *following Jain et. al. [1992], a high order, nine point finite difference method is implemented to simulate unsteady flows in a two dimensional square cavity due to the impulsive movement of the lid. For fixed mesh ratio, the method behaves like a fourth order method. The results of the analysis have been compared with Soh and Goodrich [1988] who have applied Crank-Nicolson type method (which in effect behaves like a second order method) to solve the problem. The time development of the vortex structure and its asymptotic approach to steady state is clearly captured by the numerical means. The use of time extrapolation for obtaining the starting values at every time level, considerably reduced the number of iterations required per time level. The dimensional drag exerted on the lid at every time level was computed by Simpson's rule. It was observed that as time progressed, there was initially a rapid fall in the numerical drag value, which assumed a steady value at later times. The patterns of development of the flow field, vorticity and streamline contours obtained for different values of the Reynolds number were also found to be in excellent agreement with Soh and Goodrich [1988] and Natarajan [1992].*

PART III *contains* **Chapter 7** *which deals with the numerical simulation of the propagation of a non-linear Schrödinger wave in the presence of damping and homogeneous effects. The main emphasis is on the construction and implementation of two moving variable mesh schemes, in order to track the travelling wave solutions like solitons. The variable mesh methods could find the location of the peak as well as the maximum amplitude of the soliton very accurately. These schemes offer a large reduction in the storage requirements and execution time as compared to the earlier methods.*

Chapter 7 *deals with the construction of variable mesh methods, following the procedure given in Jain et. al. [1984], for the solution of a strongly dispersive system in which the asymptotic time evolution of the slow modulations in the amplitude under perturbed conditions is governed by the non-linear Schrödinger equation. The methods generate a variable mesh with fine non-uniform mesh spacing wherever it is necessary (near the peak of the soliton) and a coarser mesh spacing where the solution is not as critical. The superposition of the variable mesh is based on the* *geometric description of the solution in order to track the travelling wave solutions like solitons so that the location of the peak as well as the maximum amplitude of the soliton is predicted more accurately. The basic approach is to locate the soliton in the solution and then place a non-uniform mesh there. In otherwords, the non-uniform mesh is not fixed, but moves along with the soliton. In this way, the nodes remain concentrated in the regions of rapid variation of the solution. Also, the redistribution of the nodes, the possible addition of new nodes and the interpolation of the dependent variables from the old mesh to the new mesh are all done at a fixed time. For the solution of the perturbed NLSE with appropriate initial condition, two moving variable mesh schemes of orders* $O(k + h_m)$ *and* $O(k + h_m^3)$, *where* k *is the time step and* h_m *is the maximum of the non-uniform mesh spacings, are constructed and implemented. The results have been compared with those obtained using the uniform mesh (Peranich [1987]). The variable mesh schemes predicted the location and the amplitude of the moving soliton accurately.*

Contents