# STOCHASTIC MODELLING OF REACTION-DIFFUSION SYSTEMS


By

Y. S. SRINIVAS


SUBMITTED
IN FULFILMENT OF THE REQUIREMENTS FOR THE DEGREE OF
**DOCTOR OF PHILOSOPHY**


DEPARTMENT OF CHEMICAL ENGINEERING

INDIAN INSTITUTE OF TECHNOLOGY, DELHI


1989

# CERTIFICATE

*This is to certify that the thesis entitled 'Stochastic modelling of Reaction-Diffusion Systems' being submitted by Mr. Y.S. Srinivas to the Indian Institute of Technology, Delhi for the award of the degree of 'Doctor of Philosophy' is a record of bonafide research work carried out by him. Mr. Y.S. Srinivas worked under our guidance for the submission of this thesis which to our knowledge has reached the requisite standard.*

*The thesis or any part thereof has not been submitted to any other University or Institution for the award of any degree or diploma.*

*(Dr. B.D. Kulkarni)*

*(Dr. S.Subrahmaniyam)*

*DEDICATED*

*TO*

*MY PARENTS*

# ACKNOWLEDGEMENT

I am deeply indebted to **Dr. B.D Kulkarni**, Deputy Director, National Chemical Laboratory, Pune-8, for suggesting the problems, inspiring guidance and constant encouragement throughout the course of this investigation. I am extremely grateful to **Dr. S. Subrahmaniyam**, Department of Chemical Engineering, Indian Institute of Technology, Delhi, for the stimulating discussions, and the help during the course of this work.

My sincere thanks are due to Prof. L.K. Doraiswamy, F.N.A., Director, National Chemical Laboratory, Pune - 8, for giving me support to carry out this work at NCL. Also I take this opportunity to thank Dr. R.A. Mashelkar, F.N.A., Distinguished Scientist, NCL, for his encouragement and providing research facilities in the Chemical Engineering Division.

I would like to express my gratitude to Mr. P.S. Ananthanarayanan, General Manager, Balmer Lawrie & Co. Ltd., Madras, for his help in submitting this thesis.

I would like to thank all my colleagues in the Division of Chemical Engineering at NCL, especially Dr. V.K. Jayaraman, Dr. V. Ravi Kumar, Dr. S.S. Tambe, and Mr. S.R. Inamdar. I am thankful to Mr. K. Radhakrishnan for preparing this manuscript.

I would also like to thank the Council of Scientific and Industrial Research for the award of a research fellowship during the tenure of this work, and the Director, NCL, for permitting me to present the work in the form of a thesis.

**Y.S. Srinivas**

## ABSTRACT

The scope of the present work includes study of some representative problems in chemically reacting systems which can bring out the essential features of reaction-diffusion systems, with noise affecting the system properties in a multiplicative fashion. Systems which exhibit instabilities in the form of limit cycle behavior and dissipative structures which form spatial patterns have been modelled stochastically.

Effect of external noise on a trimolecular scheme viz. the Brusselator model has been studied. A one dimensional spatial stochastic model incorporating multiplicative noise (of the Gaussian type) in the diffusion component of one of the concentration variables has been formulated and two different characteristic lengths have been chosen for analysis. The bifurcation diagram for each characteristic length has been initially obtained and the stability analysis performed. Stochastic model simulations in each one of the steady state regions with differing strengths of noise were subsequently carried out. It was observed that new solution branches are brought about for certain noise intensities and correlation times.

A detailed stochastic analysis of the regions of multiple steady states in a nonisothermal nonadiabatic tubular reactor was investigated for differing extents of noise levels. A pseudo-one dimensional homogeneous model with first order kinetics was employed and the solution diagram generated. Solutions in these different regimes of the bifurcation diagram were chosen and the influence of external noise (Gaussian type) on the nature of the system was investigated extensively. The stochastic analysis revealed a total reversal of stability (kinetic to diffusion regime and *vice-versa*), with the three unstable steady states.

The influence of both white and nonwhite Poisson noise on oscillating reacting systems has been analytically evaluated. The external noise was incorporated in the macroscopic equations and stochastic differential equations were formulated. The governing Fokker-Planck equations (of reaction-diffusion type) were derived for the case of exactly solvable limit cycle for both single and two variable cases. These systems were investigated in the presence of Poisson noise , with case examples, and the results were compared with those for the Gaussian noise. The results suggest that noise parameters can generally alter the stationary solution and that noise cannot always be ignored.

# CONTENTS