# MODELING, SIMULATION AND CONTROL OF RUNAWAY REACTION IN A BATCH REACTOR

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# MODELING, SIMULATION AND CONTROL OF RUNAWAY REACTION IN A BATCH REACTOR

by

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**Submitted in fulfillment of the requirement of the degree of**

DOCTOR OF PHILOSOPHY

to the


INDIAN INSTITUTE OF TECHNOLOGY DELHI
NEW DELHI, INDIA
SEPTEMBER 2010

# CERTIFICATE

This is to certify that the thesis titled "**MODELING, SIMULATION AND CONTROL OF RUNAWAY REACTION IN A BATCH REACTOR**", being submitted by **KARRI RAMA RAO** to Indian Institute of Technology, Delhi for the award of Degree of Doctor of Philosophy is a record of a bonafide research work carried out by him. Mr. Karri Rama Rao worked under our guidance and supervision for his doctoral work and to our knowledge, the thesis submitted by him has reached the requisite standard.

The thesis or any part thereof has not been submitted to any other university or institute for the award of any degree or diploma

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# ACKNOWLEDGEMENTS

I am blessed with all nice people around me throughout my life. While working on research project for past five years, many people have influenced my life and my thought processes. It is almost an impossible job to acknowledge them in a couple of pages or for that matter in limited number of words.

It is with great pleasure that I express my indebtedness, deep regards, whole hearted gratitude and thanks to my respected supervisor Prof. D. Phaneswara Rao for his support, guidance and giving necessary information, and continuous inspiration for completing the project.

I am also indebted to Dr. Ch. Venkateswarlu, Scientist – F, Indian Institute of Chemical Technology (IICT) for his kindly acceptance as co-supervisor and allowing me to work at IICT under his supervision. I am very thankful for his patience, inspiration, guidance and constant encouragement at each and every stage of my research work.

I would also like to thank Dr. James Gomes, Prof. K.D. P. Nigam and Dr. A.K. Saroha for being a part of my dissertation committee.

I would like to express my thanks to Dr. U. Sreedevi, and Prof. S.K. Gupta for their inspiration, moral support and valuable suggestions when I am down with low confidence. I am also thankful to faculty members of the Chemical Engineering Department for smooth sail in the department.

A person, without her, this accomplishment would have been incomplete, is my wife, Soni. Her encouragement, her support, care and love at each stage of life helped me in academic as well as non-academic life. I have learned and will continue to learn lots of

things from her. Her affection and emotional support during some of my difficult days has provided me an invaluable experience in our life.

My daughter Yajnasri is an angel for us. She entered in my life when I started my research work. Watching her grow day by day gives me the most enjoyable experience of my life. After long tiring day, when I reach home, her one smile rejuvenates my spirits. She might not have idea how much she has contributed towards our thinking and way of life.

There is no way that this section on acknowledgements could even come close to completion without mentioning all my friends who made my stay in Department memorable. My special thanks for my labmates, Ajit, Devika, Bala, Pradeep,..list is almost endless. I really wish to express my most sincere thanks to all you guys. I would like to specially thank Kishore, Elavarasan and Pradeep for allowing me to work in their lab which helped me a lot for my research work. My sincere thanks for all our 'Telugu Group' in Nalanda and IP Aparments. I would like to mention Kishore, Srinu and Babu sir for their encouragement throughout all these years.

I would like to thank scientists at IICT Mr. Anand, Mr. Jayant and fellow research scholars, Mr. Kiran, Mr. Ganesh for making my stay pleasant in Hyderabad.

I would like to express my regards to Mrs. Rama Devi, Mr. Gopal Singh, Mr. Ch. Durga Prasad Rao, Mr. Pala Ramesh, Mr. Sarva Rao, Mr. Mohan Kumar, my colleagues of M.V. G. R college of Enggs for their encouragement. My special regards to Mr. K.V.L. Raju (Principal) and Mr. G. L.N. Raju (Director) for encouraging me to pursue research career.

My sincere thanks to Dr. Vladan Babovic, my employer at the Singapore Delft Water Alliance (SDWA), for providing me the post doctoral fellowship at National University of Singapore. I would like to take this opportunity to thank all the staff members and colleagues at SDWA for making me a part of their organization.

I am also thankful to the supporting staff members of the Postgraduate Research Laboratory, Mr. Nayak and Mr. Ashish, for their assistance in the laboratory.

In the end, I would like to say that all of this could be possible only because of constant love and encouragement by my mother (Kannathalli), my brother (Narayana), my sister's Lakshmi and Lalitha, my brother in-laws, and all my family members and friends back home.

Last but not the least; I am so thankful to my father-in-law (Mr. L.V.Rao) and mother-in-law (Mrs. Prameela) for their kind support and patience.

I also wish to express my thanks to all other friends who have helped me directly or indirectly in completing the research project.

It's the birth of my cute prince (baby Jayant) who brought me luck in defending my thesis.

Finally, I would like to thank the main person who is my aspiration behind the research career; he is none other than my dad, who has left me during my childhood. I pray for his soul.

May 2011 KARRI RAMA RAO

# *Abstract*

Batch reactors are widely used to manufacture specialty chemicals, polymers, food and agricultural materials, biochemical and pharmaceuticals, coatings and composites etc. Set-point tracking of batch reactor systems is challenging because these are highly nonlinear and dynamic in nature in contrast to continuous reactors, which operate at steady state conditions when there is no disturbance.

As the system variables like temperature and reactant concentration in the reactor vary with time, the batch operation can pose safety problems if the reactions are exothermic in nature. The trajectory of the system depends on initial operating conditions or system parameters. For an exothermic reaction, if the initial reactant or coolant temperature is increased above a threshold value while keeping all other variables constant, the exothermic reaction can proceed at a very rapid pace and the temperature may attain a very high peak value before dropping down to the coolant temperature and at the peak temperature, the limiting reactant may get exhausted. This drastic change in system behavior with respect to small changes in a critical parameter beyond a threshold value which is called as runaway and such a system is said to be parametrically sensitive.

The aim of this work is to avert the runaway behavior and to design an effective control strategy to a batch reactor where a highly parametric sensitive exothermic reaction involving hydrolysis of acetic anhydride in the presence of sulfuric acid as catalyst and acetic acid as solvent is carried out. For this a mathematical model is developed and is verified with the experimental runaway behavior. To control the runaway behavior at the desired isothermal temperature, various advanced controllers are

implemented and bench mark is made by comparing with conventional controller. The effectiveness of the advance controller with various orders is evaluated by applying the controller to control the temperature of runaway batch reactor. The result of these controllers hence dictates the use of advanced controllers in chemical industry to avert major disasters. These results also indicate that by knowing the region of operating conditions that lead to runaway for a particular reaction system, appropriate controller system and safety measures can be designed to avert runaway and prevent losses.

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