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“‘The stars are made of the same atoms as the earth.’ I usually pick one small topic like this to give a lecture on. Poets say science takes away from the beauty of the stars – mere gobs of gas atoms. Nothing is “mere.” I too can see the stars on a desert night, and feel them. But do I see less or more? The vastness of the heavens stretches my imagination – stuck on this carousel my little eye can catch one-million-year-old light. A vast pattern – of which I am a part – perhaps my stuff was belched from some forgotten star, as one is belching there. Or see them with the greater eye of Palomar, rushing all apart from some common starting point when they were perhaps all together. What is the pattern, or the meaning, or the *why?* It does not do harm to the mystery to know a little about it. For far more marvelous is the truth than any artists of the past imagined! Why do the poets of the present not speak of it? What men are poets who can speak of Jupiter if he were like a man, but if he is an immense spinning sphere of methane and ammonia must be silent?”

Richard P. Feynman

“The most exciting phrase to hear in science, the one that heralds the most discoveries, is not ‘Eureka!’ (I found it!) but ‘That’s funny...’”

Isaac Asimov

University of Alberta

Constrained Optimization of Nonlinear Chemical Dynamical Systems

by

Sachin Kansal

A thesis submitted to the Faculty of Graduate Studies and Research in partial fulfillment of the requirements for the degree of **Master of Science**.

in

Process Control

Department of Department of Chemical and Materials Engineering

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University of Alberta

Faculty of Graduate Studies and Research

The undersigned certify that they have read, and recommend to the Faculty of Graduate Studies and Research for acceptance, a thesis entitled **Constrained Optimization of Nonlinear Chemical Dynamical Systems** submitted by Sachin Kansal in partial fulfillment of the requirements for the degree of **Master of Science** in *Process Control*.

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J. Fraser Forbes

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Martin Guay

. . . .

G. Galileo

Date: . . . .

To Love, Peace, and the Brotherhood of Man

Acknowledgements

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Abstract

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2.2.1 Model Selection

— choice of the model which captures the important process behavior yet is not overly complex and computationally expensive to implement

2.2.2 Process Measurements

— choice of instrumentation which makes the real-time implementation possible and yet doesn't require all new instrumentation for the existing batch process plants

Chapter 3

Optimization in Flat Output Space

3.1 Introduction

The dynamic optimization of batch processes ......

Table 3.1: Model Parameters for the CSTR

α	=	30.828	hr^{-1}
β	=	86.688	hr^{-1}
δ	=	3.522×10^{-4}	$m^3.K.KJ^{-1}$
γ	=	0.1	$K.KJ^{-1}$
T_{in}	=	104.9	^oC
c_{in}	=	5.1×10^3	$mol.m^{-3}$
k_{10}	=	1.287×10^{12}	hr^{-1}
k_{20}	=	9.043×10^6	$m^3(mol.hr)^{-1}$
E_1	=	9758.3	
E_2	=	8560.0	
ΔH_{AB}	=	4.2	$KJ.mol^{-1}$
ΔH_{BC}	=	-11.0	$KJ.mol^{-1}$
ΔH_{AD}	=	-41.85	$KJ.mol^{-1}$

3.2 Differentially Flat Systems

Differential flatness is a concept that applies to underdetermined system of ODEs. A general underdetermined system ...

Remark 1 *It is clear from above, that a solution connecting any two generic points in the original system space can be found. Thus flat systems are controllable.*

3.3 Overview of the Process

The nylon polymerization reaction can most clearly be described in terms of equivalent or functional groups [Steppan et al., 1987; 1990Steppan *et al.*, 1987 Steppan *et al.*, 1990] as follows: ....

The above model is analyzed in the exterior calculus setting of Guay et al., 1991 and the flat ouputs for the above model, similar to the ones calculated by Rothfuss et al., 1996, are found to be:

$$
\begin{aligned}
y_1 &= T \\
y_2 &= \frac{c_{in} - c_A}{c_B}
\end{aligned}
$$

Chapter 4

Summary and Conclusions

4.1 Contributions of this Thesis

4.2 Recommendations for Industrial Application

4.3 Directions for Future Work

4.3.1 Academic Research Directions

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Bibliography

Steppan, D.D., M.F. Doherty and M.F. Malone (1987). A kinetic and equilibrium model for nylon 6,6 polymerization. *J. Appl. Poly. Sci.* **33**, 2333–2344.

Steppan, D.D., M.F. Doherty and M.F. Malone (1990). Wiped film reactor model for nylon 6,6 polymerization. *Ind. Eng. Chem. Res.* **29**, 2012–2020.