DYNAMICS DAYS SOUTH AMERICA 2010
International Conference on Chaos and Nonlinear Dynamics

INPE – National Institute for Space Research
São José dos Campos – SP – Brazil – July 26-30, 2010

A NOVEL NON-SMOOTH BIFURCATION IN A CHEMICAL PROCESS DAES SYSTEM

Gerard Olivar[1], *Juan B. Restrepo*[2], *Angelica M. Alzate*[3]

[1]Universidad Nacional de Colombia Sede manizales, Manizales, Colombia, golivart@unal.edu.co
[2]Universidad Nacional de Colombia Sede manizales, Manizales, Colombia, jbrestrepob@unal.edu.co
[3]Universidad Nacional de Colombia Sede manizales, Manizales, Colombia, amalzatei@unal.edu.co

keywords: Applications in Engineering,Bifurcation theory and analysis,Differential Algebraic Equations

1. INTRODUCTION

The use of Differential algebraic equations is common in the dynamic simulation of chemical engineering plants and apparatus that deal with physical equilibrium, special cases of that would be the the Liquid-Liquid equilibrium and the Vapor-Liquid-Liquid equilibrium that are systems that are described by piecewise smooth non linear differential algebraic equations with non trivial discontinuity frontiers, the analysis of shortcut design chemical engineering models such as residue curves and liquid-liquid contactors leads to the appearance of bifurcations over the discontinuity frontier.

2. DAE BIFURCATIONS

The most common DAE bifurcations is know as singularity inducted bifurcation [1], it consist on the the sudden change of sign of eigenvalues without crossing zero, it is common on electrical engineering systems. By far the most common bifurcation in chemical engineering systems is the fold bifurcation [2**?** –4], in many cases meaning the non operability of an specific apparatus under certain conditions , in many other cases it mean the appearance of multistability.

As said before the appearance of fold bifurcations is common, but the use of piecewise smooth systems to describe chemical engineering apparatus is not, neither is the appearance of a theoretically consistent fold bifurcation over the discontinuity surface as an important operation parameter is varied.

3. CHEMICAL ENGINEERING LIQUID-LIQUID CONTACTOR

A liquid-liquid contactor is widely used in chemical engineering plants to perform extractions [5], the operation principle is to take advantage of the different solubility of some chemical species in two insoluble solvents, those are put in intimate contact allowing the solute to pass from one to the other, another class of extraction is the auto inducted reaction extraction where during a reaction two immiscible species are formed creating a two phase system, taking advantage of the immiscibility of the two formed chemical species using a liquid-liquid contact equipment can mean an enormous rise in the productivity(specially for reversible chemical reactions) and avoid energy consumption in the further process steps [6, 7].

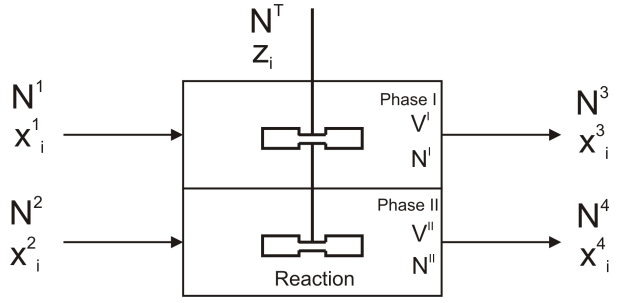

Figure 1 – Auto inducted liquid-liquid Contactor

4. APPEARANCE OF BIFURCATION

The study case of the Biodiesel auto inducted liquid extraction (see Figure 2) is representative for being one of the new applied technology cases where the novel DAE bifurcation appear. The transformation of fats and vegetable oils (triglycerides) into long chain fatty acid esters by the reaction with an alcohol generally methanol or ethanol in presence of a catalyst, is the base of industrial production of biodiesel and it is called transesterification[8–10], from the modeling of the reactor for the production of biodiesel from sunflower oil using enzyme as catalyst several bifurcation diagrams were obtained, both operation parameters R (see Figure 3) and D (see Figure 4) where varied, which are the relation of reactives at the inlet of the reactor and the dilution rate respectively. A special case of a fold nonsmooth bifurcation was obtained showing that it falls over the discontinuity surface (see Figure 5).

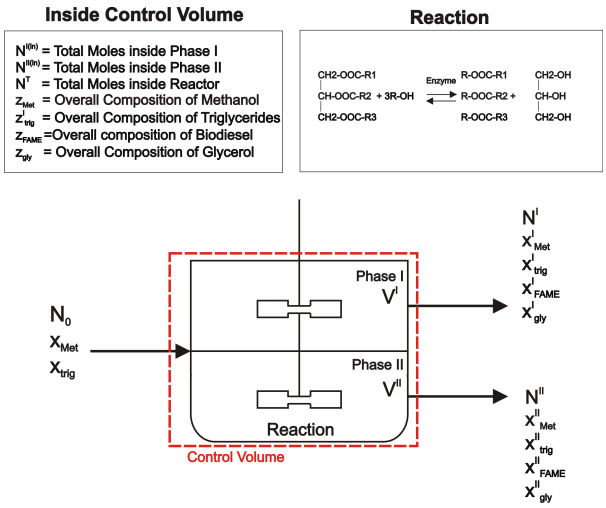

Figure 2 – Auto Inducted liquid-Liquid Extractor for the Production of Biodiesel

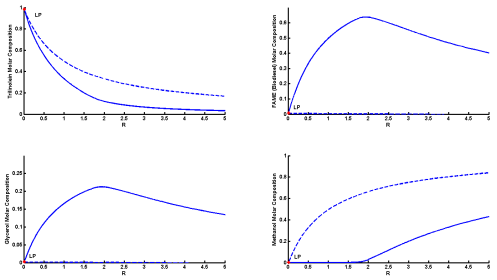

Figure 3 – Bifurcation diagram obtained varying R

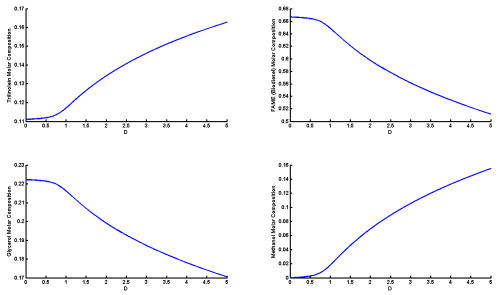

Figure 4 – Bifurcation diagram obtained varying D

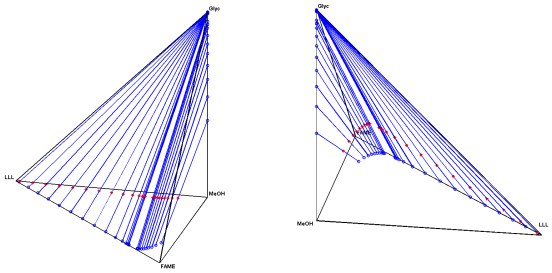

Figure 5 – Space state representation of the bifurcation diagram physical equilibrium tie lines

References

[1] Z.W. Marszalek, W. Trzaska. Dae models of electrical power systems and their bifurcations around singularities. In *Decision and Control, 2004. CDC. 43rd IEEE Conference on*, 2004.

[2] Willy J. F Govaerts. *Numerical Methods for the Bifurcation fo Dynamical Equilibrium*. SIAM, 2000.

[3] Yuri A. Kustnetzov. Applied mathematical sciences. In *Elements of Applied Bifurcation*, number 112. Springer-Verlag, 1995.

[4] Rüdiger Seydel. Interdisciplinary applied mathematics. In *Practical Bifurcation and Stability Analysis*, number 5. Springer-Verlag, 1994.

[5] Robert Ewald Treybal. *Liquid extraction*. McGraw-Hill, New York, 2nd ed edition, 1963.

[6] Luis Fernando Gutiérrez Mosquera. *Estudio y Diseño de Procesos Reacción Extracción Simultáneos*. PhD thesis, Universidad Nacional de Colombia Sede Manizales, 2007.

[7] Luis Fernando Gutierrez Mosquera Carlos A.Cardona, Luis Geronimo Matallana Perez. Aplicación de la destilación reactiva en la producción de biocombustibles. Ponencia en la Cuarta conferencia internacional sobre energía renovable, ahorro de energía y educación energética, 2005.

[8] F. Kovács L. Gubicza Beláfi-Bakó, K. and J. Hancsók. Enzymatic biodiesel production from sunflower oil by *Candida antartica* lipase in a solvent-free system. *Biocatal. Biotransf.*, 20:437–439, 2002.

[9] D. Combes Dossat V. and A. marty. Continuos enzymatic transesterification of high oleic sunflower oil in a packed-bed reactor: influence of the glycerol production. *Enzyme. Microb. Tech.*, 25:194–200, 1999.

[10] Juan Lanz Cristina Gonzlez, Jos M. Resa and M. Angeles Fanega. Properties of mixing of systems that contain sunflower oil with ketones. *J. Chem. Eng. Data*, 47:1116–1122, 2002.