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Use of Genetic Algorithm to Model Phase Equilibria of systems consisting of 3-Methylthiophene & hydrocarbons

A. Kulkarni[a], and M. H. Joshipura[b*]

[a]*Reliance Industries Limited, Jamnagar, Gujarat*
[b]*Chemical Engg. Dept., Insitute of Technology, Nirma University, Ahmedabad-382481*

Abstract

Removal of sulfur from gasoline is one of the major processes in refineries. Designing of removal process requires phase equilibrium data of the sulfur with various hydrocarbon systems. 3-Methylthiphene is an organic sulfur compound found in gasoline. In the present work VLE data of 3-Methylthiophene with various hydrocarbons were modeled using genetic algorithm. VLE data were modeled using Wilson, NRTL and Margules activity models. Margules models was found to be best amongst the studied models.

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Keywords: *Desulfurization; 3-Methylthiophen; Genetic Algorithm; NRTL, Wilson, Margules*

Nomenclature

A,b	Binary Interaction Parameter
y	vapour phase fraction
Subscripts	
exp	experimental
cal	calculate
12	interactions between compound 1 and 2

1. Introduction

The automobile industry is growing rapidly and the most undesirable outcome of the same is the air pollution due to the automobiles. There are various ways to reduce the air pollution and one of them is to have minimum impurities in the fuel used in the automobile. Sulfur is considered to be the major impurities in gasoline because [1].

- It causes the SOx in the exhaust gases, and
- Poisons noble catalyst in the automobile

* Corresponding author. Tel.: +91-2717-241911-15 Ext: 146; fax: +91-2717-241917
E-mail address: milind.joshipura@nirmauni.ac.in

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Worldwide the sulfur concentration in the gasoline is targeted to be zero in coming years. [1] The reduction of sulfur level in gasoline requires the refinery processes to be modified, specifically desulfurization process. Accurate Vapor Liquid Equilibrium (VLE) data of sulfur compounds with hydrocarbons is required for such process for both reaction and separation processes. VLE determination must be supported with good estimation models. 3-Methylthiophen is one of the organic sulfur compounds present with the gasoline. [2] Experimental determination of VLE of 3-Methylthiophene is available in the literature [1-4]. Present work is aimed to model these systems with different activity coefficient models and compare them. The binary interaction parameters for the binary systems were obtained using Genetic Algorithm.

Genetic algorithms (GAs) were developed by Holland and co-workers in 1960's [5]. GA is a method for moving from one population of "chromosomes" (e.g., strings of ones and zeros, or "bits") to a new population by using a kind of "natural selection" together with the genetics−inspired operators of crossover, mutation, and inversion.[5] Most methods called GA have following elements in common[5].

- populations of chromosomes
- selection according to fitness,
- crossover to produce new offspring and
- random mutation of new offspring

GA works on the principle of biological evolution and Charles Darwin's Theory of Survival of the Fittest. Figure 1 provides an idea about the steps to be performed for GA.

2. Database

As mentioned in the previous section few experimental data set are available in the literature for 3-Methylthiphene.[2-4]. The data generated is summarized in Table 1.

The below mentioned data base were used to obtain the binary interaction parameters for following activity coefficient models

- van Laar Model
- NRTL Model
- Wilson Model
- Margules Model

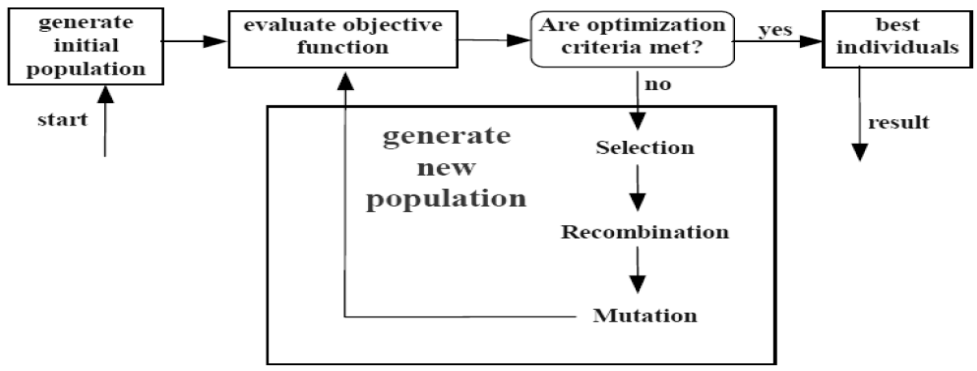

Fig. 1. Flow chart for steps performed in genetic algorithm