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# Computer aided operation and design of the cationic surfactants production

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**Abstract**

In this paper process operation simulation of the cationic surfactants based on quaternary ammonia salts were provided. The component data base integrates with data base of the kinetic parameters and structured knowledge representation for the surfactant subsystem alkyl-di-methyl-benzyl-ammonium-chloride production. Simulation was carried out for various operation regions and conditions, different reactors size and production rate. Steady state and unsteady state process behaviors were simulated.

**Keywords:** Surfactant kinetic models, kinetic parameters, elementary transition, dynamic of product formation

## 1. Introduction

In the analysis and operation of processing systems simulation is a major technique [1-2]. The traditional simulation technique are often inflexible and provide limited means to the user. In fact, such technique can not clearly simulate the dynamic behavior of the real processes.

There exists considerable success in developing expert aided simulation systems. Intelligent simulation highlights the potential to meet with the demand. The technological advance in simulation has addressed to research interest of intelligent simulation.

Process operation simulation for the cationic surfactants: lauryl-, miristyl-, cetyl-, and octyl - di - methyl - benzyl - ammonia - chloride production were performed in this paper.

## 2. Integrated expert aided simulation

The segregation of the databases, knowledge base systems and inference engine in the expert system allows us to organize the different models and domain expertise efficiently because each of these components can be designed and modified separately.

The knowledge representation of differential models is described using semantic network. The knowledge extending involves initial knowledge $K_0$, and gain operator *go* as following:

$$K = go(K_0) \tag{1}$$

The model generation methodology is a blend of several problem solving paradigms, and hierarchical dynamic goal system construction serves as the basis for model generation. Database protocol manages all data bases, reports and tables as linking objects.

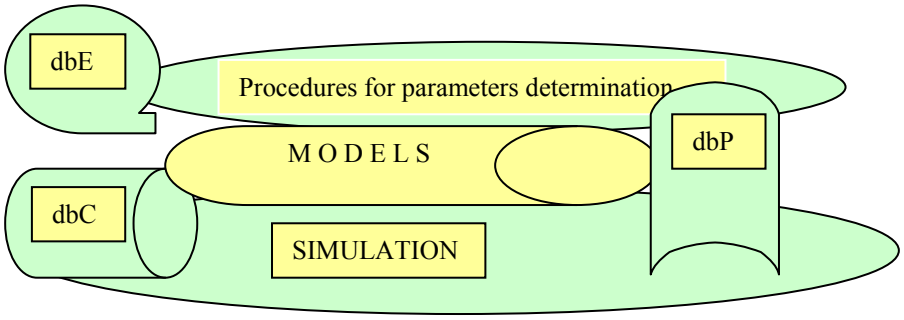
## 3. Paper approach

A new approach in the computerized modeling is represented directly by the structure of the elementary transitions referring to the various phenomenological defined chemical reactions.

The knowledge based system which automated the process, enabling engineers to perform modelling and simulation study was built. Input component data base and experimental database was linked with routines for kinetic parameters determination [3-5]. Database of kinetic parameters was developed as a relational data base system which linked kinetic models and operation simulation by process models.

### *3.1. Simulation methodology*

The models manager operations performs real time process operations on various levels. Model manager shows how do you seek out a new way to the operation life cycle model and how do you make process history. It provides rigorous on-line modeling tools for the process design and operation and raw material and energy minimization. Raw material minimization was




dbE – data base of the experimental data, dbC-component data base, dbP-parameters data base

Figure 1.Data bases network with models

simulated seeking out optimal initial reactants ratio. Energy minimization was provided by heat recovery simulation.

This simulation integrates data bases for component data, chemical reaction data, dynamic data and model parameters tables with structured knowledge representation subsystems.

### *3.2. Chemical reaction models*

The generic model were illustrated by actually implementation chemical reaction of the first and second order for surfactants production based on quaternary ammonia salts. The network kinetic models for cationic surfactants formation can be made.

The synthesizing procedure is generated and ranked database facts and clauses, kinetic parameters database and kinetic models which defined reaction and product concentration changes. General kinetic model for the surfactant reactions is derived as following:

$$A_1 + B_1 \rightarrow^{k_1} C_1$$
$$A_2 + B_2 \rightarrow^{k_2} C_2$$
$$A_3 + B_3 \rightarrow^{k_3} C_3$$
$$\ldots\ldots\ldots\ldots\ldots\ldots$$
$$A_n + B_n \rightarrow^{k_n} C_n \qquad (2)$$

For reactants,

$$\frac{dc_{Ai}}{dt} = \frac{dc_{B_i}}{dt} = -k_i c_{A_i}^{n_{A_i}} c_{B_i}^{n_{B1i}} \quad (3)$$

and products

$$\frac{dc_{Ci}}{dt} = k_i c_{A_i}^{n_{A_i}} c_{B_i}^{n_{B_i}}$$

where $A_{i\,(i=1,..4)}$=(lauyl-chloride, miristyl-chloride, cetyl-chloride, octyl-chloride) , $B_{i(i=1)}$ =(NN'-di-methyl-benzyl-amine) and $C_{i(i=1,...4)}$ =(lauryl-di-methyl-benzyl-ammonium-choride, miristyl-di-methyl-benzyl-ammonium-choride, cetyl-di-methyl - benzyl - ammonium - choride, octyl - di- methyl - benzyl - ammonium -choride), $k_i = k_0 e^{-E/RT}$ , $n$ is reaction order and $c$ is component concentration.

The structural model is generated according to several levels decomposition of the process unit into phases and components. The simulation begin with system definition. Definition includes components, input and output attributes, state variables, behavior rules, and initial conditions.

It is assumed that reactions occur in the liquid phase and the contents are perfectly mixed. Product composition depends from initial reactants concentration, reaction conditions and different size of reactor volumes.

### *3.3. Case study*

As a case study the cationic surfactants based on quaternary ammonium salts production were used. The lauryl-, miristyl, and octyl-di-methyl-benzyl-ammonium-chlorides formation are occurring at the temperature of 77-90$^{o}$C. The separation of products from raw materials has been carried out.

### *3.4. Results and discussions*

Reaction progress curves were simulated. Process sensitivity analysis was performed by dynamic simulation for various conditions. Through a stability study is predicted the behavior in the start up and product periods.

Simulation was carried out for various operation regions and object functions. Dependence of the component concentration and composition with time for various reactions was performed as shown in Figure 2-3. The computer supported cooperative work with databases management and mathematical modelling and simulation of the process operation provides intelligent operation management support system.

The dynamic simulated results are shown in Figure 2. Figure 3 shows component compositions changes for steady state operation.

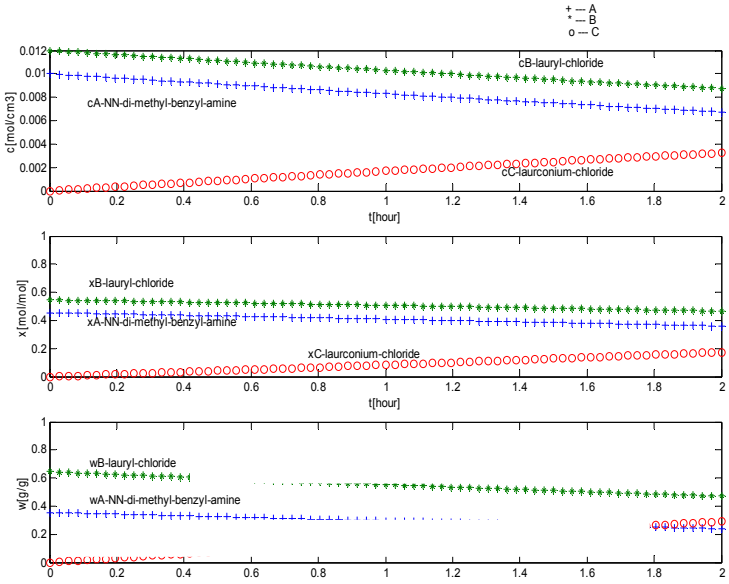



Figure 2.Unsteady state simulation for reactants initial mole ratio 0.5($A_1$):1.0 ($B_1$)when "alkyl-=lauryl-" and reactor volume 5dm$^3$

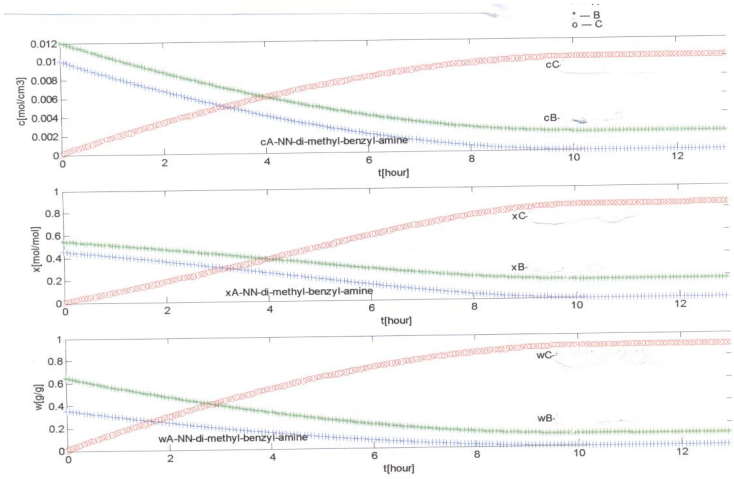



Figure 3. The steady state simulation results for reactant initial mole ratio 2.5(A):3(B) when "alkyl=octyl" and reactor volume 50dm$^3$

Experimental data of the lauryl -, miristyl -, and octyl – di – methyl - benzyl-ammonium-chloride have been taken from reference [3,5] for energy activation, acceleration factor, reaction order and specific rate constant determination. Those kinetic parameters for cetyl- di – methyl benzyl-ammonium-chloride formation have been predicted. Because of that this surfactant simulator is superior to the numerous dynamic simulators that are commercially available.

## 4. Conclusions

The results of this paper have shown power of the process model for generating different cationic surfactants operations.

The obtained results are shown superiority of the computer aided process operation tool and illustrate ability for discovering a new surfactant product. This simulation coordinate all symbolic reasoning systems and numerical routines in an integrated intelligent system.

Current and future work therefore includes continuous update of models, rules properties and problems. The obtained results in this paper can be applied in the others domain.

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