

# A multistage, multiphase and multicomponent process system modelling

T. Mosorinac and J. Savkovic-Stevanovic

**Abstract**—In this paper an integrated modelling method was presented. At transfer phenomena modelling, the interphase and intercomponent transfer mechanisms were investigated by integrated modelling. Modelling method started with system definition, elements identification and their interrelations definition according to goal state. The general multistage process information structure, which enables the integrated modelling was built. The process models were generated for batch, semi-batch and continue multistage process units. Using the advanced method, one can evaluate by multi-convergence criteria dynamic state and steady state of the multistage system. For the process models distillation and absorption multistage with and without chemical reaction were used. As a virtually process representation a multistage, multicomponent distillation process was used. The obtained results show benefits of the integrated modelling method.

**Keywords**—Multistage unit, integrated modelling, multiphase, multicomponent, simulation, parameters definition.

## I. INTRODUCTION

THE concomitant advances in theory, mathematical modelling, numerical methods and measuring systems, bring the new perspectives to the physical phase dynamics, chemical dynamics and moving in space computing. Using the advanced method, one can evaluate by multi-convergence criteria dynamic state of the complex system. The obtained results demonstrate characterization of the equilibrium and non-equilibrium states and transition between them and how it can be used to predict the stability of dynamic system. Dynamic behavior of the moving liquid and vapor phases and their interactions were computed. Need to examine, more sites at which there is significant cross-interactions between phases.

The quantitative approach to modelling and inference involve computing the path coefficients between the variables and using the resulting equation to predict the change in the cause [1],[2].

Although the quantitative approach has proven very useful for dealing with many real-world problems, it is neither sufficient nor necessary under some circumstances. Furthermore, because in reality, there may not exist enough quantitative knowledge to permit full quantitative modelling, abstract qualitative models are worthwhile to explore.

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Qualitative modeling has become one major line of research toward the representation of deep models in knowledge based systems.

An approach refers to the technique which predicts the possible qualitative behaviors of a system on the basis of the model comprising the predefined transfer parameters and constraint predicates.

These parameters and constraints are abstracted from the mathematical equations describing the system dynamic behavior. This model provides a snapshot of the qualitative characteristics of the system at each defined time frame, and is especially useful when we want to know the dynamic trends [3].

Distillation is probably the most widely used separation process in the chemical and allied industries, its applications ranging from the rectification of alcohol, to the fractionation of crude oil. Though the emphasis is on distillation processes, the basic construction features, and many of the other variables, also apply to other multistage processes, such as stripping and absorption. A good understanding of methods used for correlating vapour-liquid equilibrium data is essential to the understanding of distillation and other equilibrium staged processes.

In this paper the integrated modelling method for multistage, multiphase and multicomponent systems for distillation and absorption processes was developed.

## II. MODELLING APPROACH

Scientists are interested in discovering functional relationships among physical phenomena in order to explain their behavior. Over the years, scientists have studied two aspects isolation of the variables which represent cause phenomena and those which represent effect phenomena, and determination of the magnitude and direction of change in effect phenomena corresponding to a change in cause phenomena [1].

The identified variables along with their functional relationships can serve as a useful computational model for making inference.

As a step toward a complete knowledge representation scheme for modelling support, it has combined the decomposition, taxonomic and coupling relationships in a knowledge representation scheme called the system entity structure. Previous works identified the need for representing the structure and behavior of systems, in a declarative scheme related to frame theoretical and object based formalisms. The elements represented are motivated, on the one hand, by system theory concepts of decomposition, how a system is

hierarchically broken down into components and coupling how these components may be interconnected to reconstitute the original system. On the other hand, systems theory has not focused on taxonomic relations, as represented for example in frame hierarchy knowledge representation schemes. In the system entity structure scheme, such representation concerns the admissible variants of components in decompositions and the further specializations of such variants.

The two areas of model development and analysis are addressed through the discussion of generic modelling and simulation environment. The knowledge based simulation environment is an expression of some control law. To the extent that the rule base is derived from set of assumptions about the environment and performance expectations, it is a belief system. However, in the existing form, the goals are not expressed and the underlying assumptions are not evident. Consequently, they are opaque to the analyst and cannot be directly applied to the learning process. When expressed in hierarchical form the relationship that exist between goals and subgoals provide a basis for relating overall goal based system performance to specific assumptions about the variability and contribution of the supporting subgoals. In this form, the belief system is a full expression of some control theory in that the system's relationship with the environment, as expressed in a set of feasible state conditions, can be related either in overall system performance measures to be relationships and the subgoals that support them.

A number of methodologies and modelling and simulation systems have been developed to aid the modelling process in chemical engineering domains [2]. Simulations in chemical engineering are more effective because of power to make possibilities to knowledge keep on with changeable technologies, products and the other sources. For multistage, multiphase and multicomponent system general informations for model building are shown in Fig.1.

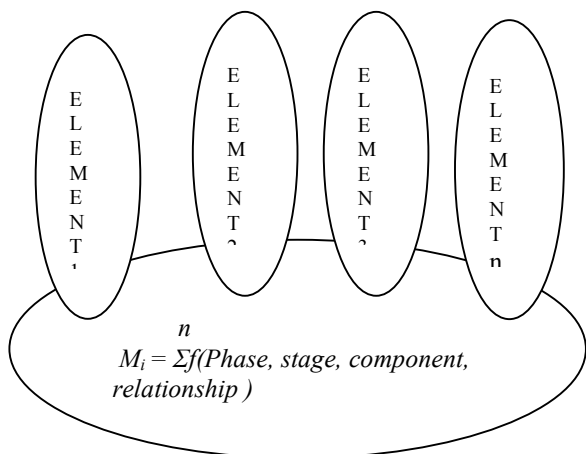


Fig.1 Model building

If the system incorporated other phenomenas as a chemical reaction these effect will be aided.

Various rules can be applied to this system based on the transitivity relationships of the qualitative variables.

To organize the logic of the rules, states variables must be defined within the system. Three types of state variables can be defined within a given component. The first are those variables whose values can be controlled by the system, are controllable variables. The second set of state variables are those variables whose values are observable to the system operator. Last are those variables whose values are not immediately discernible by the system operator such as inner pressure, temperatures, and so on.

Symptoms are appearing in various flooding elements.

### III. MULTISTAGE PROCESS UNIT MODEL

Let consider process system of the gas and the liquid phases flow through the fixed bed solid particles[4],[5]. A multiphase flow system has shown in Fig.2. The main state variables characterizing of the system are liquid flow rate L, gas (vapour) flow rate G and hold up M.

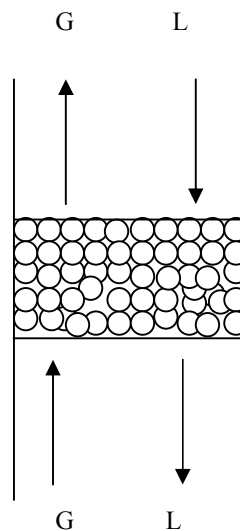


Fig.2 Gas and liquid flow through the solid particles

Modelling is the bridge between real system and a model, while simulation is the connection to a computational device that can activate the mechanism within the model. Most simulation attempts are based on models that have a time dimension. This makes the models and in turn the simulation dynamics.

$$G-L=dM/dt \tag{1}$$

where M is hold up.

The qualitative model for systematic cause-event analysis was made, and discrete state of variables were defined.

L (low, medium, high).

G (low, medium, high).

M (low, medium, high).

Need to discover the new system state after random disturbance.

In the first step the rule base is forming and set the data base to the given causes. In the second step the goal oriented strategy is using to infer the value of the attribute concerned.

IF L is low AND G is high THEN  
 M will decrease.  
 IF L is high AND G is medium THEN  
 M will increase.  
 IF G is high AND L is high THEN  
 M is medium.  
 IF H is high AND G is low THEN L  
 is high.  
 IF H is medium AND L is low THEN G  
 is low.

All the rules and the given facts are asserted in the clause base. The performance of the program depends on both the clausal order and the goal order. Since always place facts on top of rules, if the value of the given attribute is already known.

IV. MULTISTAGE, MULTIPHASE AND MULTICOMPONENT SYSTEM MODELLING

Modelling method started with system, subsystem, elements, and their interrelations definition according to goal state. It follows methods and procedures formulation for model development.

In this case for a multistage, multiphase and multicomponent system development can use distillation unit operation, absorption unit operation and chemical reaction unit operation[6]-[8].

Any multistage unit with distillation or absorption unit operation can be defined.

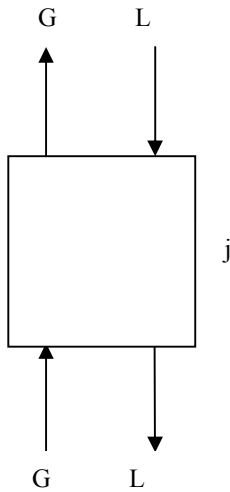


Fig.3(a) Multistage process unit elements

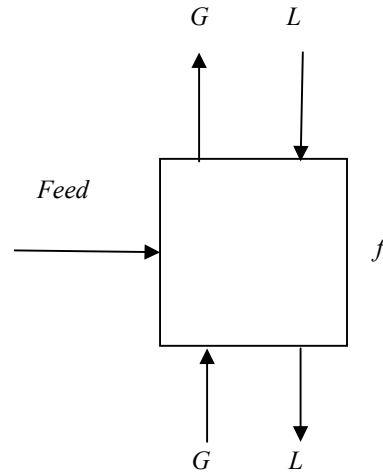


Fig.3(b) Multistage process unit elements

Mathematical model for dynamic response for an element *j* Fig.3(a) in multistage, multiphase and multicomponent integration is defined as:

$$L_{j+1} + G_{j-1} - L_j - G_j = \frac{dm_j}{dt} \quad (1)$$

$$L_{j+1}h_{j+1} + G_{j-1}H_{j-1} - L_jh_j - G_jH_j = \frac{du_j}{dt} \quad (2)$$

$$L_{j+1}x_{j+1,i} + G_{j-1}y_{j-1,i} - L_jx_{j,i} - G_jy_{j,i} = \frac{dm_{j,i}}{dt} \quad (3)$$

where *m* hold up on the stage, *H* is enthalpy of the gas phase, *h* is enthalpy of the liquid phase, *u* accumulated energy on the stage, *x* the liquid phase mole fraction composition, and *y* is the gas phase composition.

Mathematical model for dynamic response for the feed element Fig. 3(b) in multistage, multiphase and multicomponent integration is defined as:

$$F_j + L_{j+1} + G_{j-1} - L_j - G_j = \frac{dm_j}{dt} \quad (4)$$

$$F_jh_{Fj} + F_jH_{Fj} + L_{j+1}h_{j+1} + G_{j-1}H_{j-1} - L_jh_j - G_jH_j = \frac{du_j}{dt} \quad (5)$$

$$F_jx_{Fj,i} + F_jy_{Fj,i} + L_{j+1}x_{j+1,i} + G_{j-1}y_{j-1,i} - L_jx_{j,i} - G_jy_{j,i} = \frac{dm_{j,i}}{dt} \quad (6)$$

where *F* is the feed flow rate.

If chemical reaction operation has integrated with distillation or absorption operation in multistage unit than mathematical model can be defined for element  $j$  Fig.3(a) as following, assuming that chemical reaction occurs only in the liquid phase.

$$L_{j+1} + G_{j-1} - L_j - G_j + m_j(v_j) = \frac{dm_j}{dt} \quad (7)$$

$$L_{j+1}h_{j+1} + G_{j-1}H_{j-1} - L_jh_j - G_jH_j + \Delta h(v_j) = \frac{du_j}{dt} \quad (8)$$

$$L_{j+1}x_{i,j+1} + G_{j-1}y_{i,j-1} - L_jx_{i,j} - G_jy_{i,j} + m_{i,j}(v_{i,j}) = \frac{dm_{i,j}}{dt} \quad (9)$$

where  $v$  is chemical reaction rate.

Mathematical model for dynamic response for a feed element  $f$  Fig.3 (b) in multistage, multiphase and multicomponent integration with chemical reaction is defined as:

$$F_j + L_{j+1} + G_{j-1} - L_j - G_j + m_j(v_j) = \frac{dm_j}{dt} \quad (10)$$

$$F_jh_{Fj} + F_jH_{Fj} + L_{j+1}h_{j+1} + G_{j-1}H_{j-1} - L_jh_j - G_jH_j + \Delta h(v_j) = \frac{du_j}{dt}$$

$$F_jx_{Fj} + F_jy_{Fj} + L_{j+1}x_{i,j+1} + G_{j-1}y_{i,j-1} - L_jx_{i,j} - G_jy_{i,j} + m_{i,j}(v_{i,j}) = \frac{dm_{i,j}}{dt} \quad (11)$$

V. THE SEPARATION PROCESS DEVELOPMENT

Information system design started with synthesis which including basic blocks, their models, their behavior and interrelations with their functions.

The general objective of distillation is the separation of substances that have different vapor pressures at any given temperature. The word distillation refers to the physical separation of a mixture into two or more fractions that have different boiling points.

If a liquid mixture of two volatile materials is heated, the vapor that comes off will have a higher concentration of the lower boiling material than the liquid from which it was evolved. Conversely, if a warm vapor is cooled, the higher boiling material has a tendency to condense in a greater proportion than the lower boiling material.

Distillation application in various chemical reactions has the goal to separate product from the reaction system to be able to continue moving chemical reaction equilibrium and increase yield. Also, distillation can be applied in chemical engineering for obtaining high purified products and increase product quality.

The general objective of absorption is the separation of substances bases on different solubility at a given temperature.

From a light gas stream pollution may be removed by contacting the gas stream with a heavy liquid stream in a countercurrent, multiple stage column. Since absorption is a heat liberating process, the liquid is customarily introduced at a temperature below the average temperature at which the column is expected to operate.

V.1 DISTILLATION COLUMN OPERATION

The separation of the liquid mixtures by distillation depends on differences in volatility between the components. The greater the relative volatilities, the easier the separation. The distillation columns scheme is shown in Fig. 4. Vapour flows up to column and liquid counter currently down to column. The vapor and liquid are brought into contact on stages, plates or packing. part of the condensate from the condenser returned to the top of the column to provide liquid flow above the feed point, reflux and part of the liquid from the base of the column is vaporised in the reboiler and returned to provide the vapour flow.

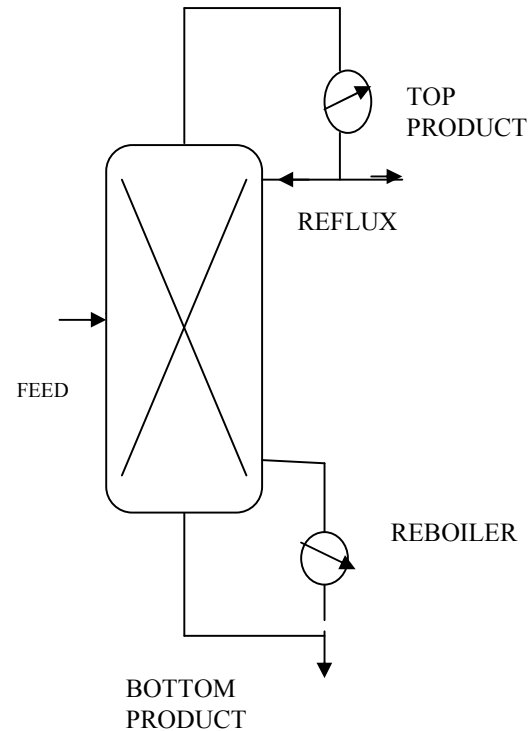


Fig. 4 Distillation column scheme

The more volatile components are stripped from the liquid and it is known as the stripping section. Above the feed, the concentration of the more volatile components is increased and it is called the enrichment, or more commonly, the rectifying section. Fig.4 shows a column which producing two product streams, referred to as tops and bottoms, from a single feed. Columns are occasionally used with more than one feed, and with side streams withdrawn at points up the column. This does not alter the basic operation, but complicates the analysis of the process, to some extent.

If the process requirement is to strip a volatile component from a relatively nonvolatile solvent, the rectifying section may be omitted, and the column would then be called a stripping column.

In some operations, where the top product is required as a vapour, only sufficient liquid is condensed to provide the reflux flow to the column, and the condenser is referred to as a partial condenser. When the liquid is totally condensed, the liquid returned to the column will have the same composition as the top product. In a partial condenser the reflux will be in equilibrium with the vapour leaving the condenser. Virtually pure top and bottom products can be obtained in a single column from a binary feed, but where the feed contains more than two components, only a single pure product can be produced, either from the top or bottom of the column. Several columns will be needed to separate a multicomponent feed into its constituent parts.

The reflux ratio,  $R$  is normally defined as the ratio of flow returned as reflux and flow of the top product taken off. The number of stages required for a given separation will be dependent on the reflux ratio used.

In an operating column the effective reflux ratio will be increased by vapour condensed within the column due to heat leakage through the walls. With a well lagged column the heat loss will be small and no allowance is normally made for this increased flow. If a column is poorly insulated, changes in the internal reflux due to sudden changes in the external conditions, such as a sudden rain storm, can have a noticeable effect on the column operation and control.

Total reflux is the condition when all the condensate is returned to the column as reflux, no product is taken off and there is no feed.

At total reflux the number of stages required for a given separation is the minimum at which it is theoretically possible to achieve the separation. Though not a practical operating condition, it is a useful guide to the likely number of stages that will be needed.

Columns are often started up with no product take off and operated at total reflux until steady conditions are attained. The testing of columns is also conveniently carried out at total reflux.

Minimum reflux is very important operation parameter. As the reflux ratio is reduced a pinch point will occur at which the separation can only be achieved with an infinite number of stages. This sets the minimum possible reflux ratio for the specified separation.

Optimal process separation needs optimal reflux ratio. Practical reflux ratio will lie somewhere between the minimum for the specified separation and total reflux. The operator must select a value at which the specified separation is achieved at minimum cost. Increasing the reflux reduces the number of stages required, and hence the capital cost, but increases the service requirements, steam and water, and operating costs.

The optimum reflux ratio will be that which gives the lowest annual operating cost. No hard and fast rules can be given for the selection of the design reflux ratio, but for many

systems the optimum will lie between 2 - 5 times the minimum reflux ratio.

Significant parameter is feed point location. The precise location of the feed point will affect the number of stages required for a specified separation and the subsequent operation of the column. As a general rule, the feed should enter the column at the point that gives the best match between the feed composition, vapour and liquid in two phases, and the vapour and liquid streams in the column. In practice, it is wise to provide two or three feed point nozzles located round the predicated feed point to allow for uncertainties in the design and data, and possible changes in the feed composition after start up.

Except when distilling heat sensitive materials, the main consideration when selecting the column operating pressure will be to ensure that the dew point of the distillate is below that which can be easily obtained with the plant cooling water.

Vacuum operation is used to reduce the column temperatures for the distillation of heat sensitive materials and where very high temperatures would otherwise be needed to distill relatively nonvolatile materials.

When calculating the stage and reflux requirements it is usual to take the operating pressure as constant throughout the column. In vacuum columns, the column pressure drop will be a significant fraction of the total pressure and the change in pressure up the column should be allowed for when calculating the stage temperatures. This may require a trial and error calculation, as clearly the pressure drop cannot be estimated before an estimate of the number of stages is made.

## V.2 ABSORPTION COLUMN OPERATION

Strippers are used to remove relatively light gases from a heavy oil stream by contacting it with a relatively light gas stream such as steam. The sketch of a typical stripper is shown in Fig. 5.

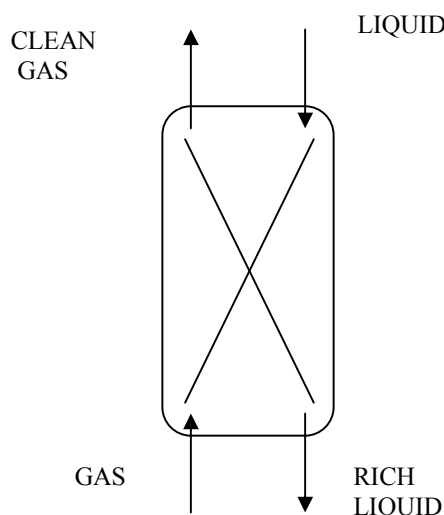


Fig. 5 An absorber column scheme

The total flow rate of the gas inlets at the bottom of the column is called rich gas. The absorber liquid plus the material that it has absorbed leave at the bottom of the column, the

stream is called rich liquid. The treated gas leaving the top of the column is called stripped gas such as shown in Fig. 5.

VI. SEPARATION OF THE MULTICOMPONENT MIXTURES BY DISTILLATION WITH MULTIPLE STAGES

A conventional distillation column is defined as one that has one feed and two product streams, the distillate D and bottoms B.

Summarized mathematical model is as follows:

$$y_{ji} = K_{ji} x_{ji} \quad 1 \leq i \leq c, 0 \leq j \leq N + 1$$

$$\sum_{i=1}^c y_{ji} = 1 \quad 0 \leq j \leq N + 1$$

$$\sum_{i=1}^c x_{ji} = 1 \quad 0 \leq j \leq N + 1$$

$$G_{j+1} y_{j+1,i} - L_j x_{ji} - D x_{Di} = \frac{dm_{ji}}{dt} \quad \text{for}$$

$$1 \leq i \leq c, \quad 0 \leq j \leq f - 2$$

$$F_f y_{fi} + F_F y_{Fi} - L_{f-1} x_{f-1,i} - D x_{Di} = \frac{dm_{f-1,i}}{dt} \quad 1 \leq i \leq c$$

$$G_{j+1} y_{j+1,i} - L_j x_{ji} - B x_{Bi} = \frac{dm_{ji}}{dt} \quad \text{for}$$

$$1 \leq i \leq c, f \leq j \leq N$$

$$F x_{Fi} - D x_{Di} - B x_{Bi} = \frac{dM_i}{dt} \quad \text{for}$$

$$1 \leq i \leq c$$

$$G_{j+1} H_{j+1} - L_j h_j - D H_D + Q_c = \frac{du_j}{dt} \quad \text{for}$$

$$0 \leq j \leq f - 2$$

$$G_f H_f + G_F H_F - L_{f-1} h_{f-1} - D H_D + Q_c = \frac{du_{f-1}}{dt}$$

$$G_{j+1} H_{j+1} - L_j h_j - B h_B + Q_R = \frac{du_j}{dt} \quad \text{for } f \leq j \leq N$$

Eqs.(12)

First consider the case in which the following specifications are made for a column at steady state operation: 1) number of plates in each section of the column, 2) quantity, composition and thermal condition of the feed, 3) column pressure, 4) type of overhead condenser, total or partial, 5) reflux ratio, L<sub>0</sub>/D, or

V<sub>1</sub> or L<sub>0</sub> and 6) one specification on the distillate such as the total flow rate D. Steady-state operation means that no process variable changes with time. In this case right side terms in system equations (12) are equal zero. For this set of operating conditions, the problem is to find the compositions of the top and bottom products. Thus, by solving this kind of problem the characteristics of the top and the bottom products can be determined.

Inspection of this set of equations shows that the equations are a logical extension of those state for the binary mixture system.

As in the case of the material balances for any one component, the number of independent energy balances is equal to the number of stages ( $j = 1, 2, 3, \dots, N, N+1$ ). In this case the total number of independent equations is equal to  $(2c+3)(N+2)$ , as might be expected from the fact that an adiabatic flash is represented by  $(2c+3)$  equations. When it is supposed that the vapor and liquid streams form ideal solutions, the enthalpy per mole of vapor and the enthalpy per mole of liquid leaving stage j are given by the following expressions:

$$H_j = \sum_{i=1}^c H_{ji} y_{ji}, \quad \text{and} \quad h_j = \sum_{i=1}^c h_{ji} x_{ji} \quad (13)$$

where the enthalpy of each pure component i in the vapor and liquid streams leaving plate j are represented by H<sub>ji</sub> and h<sub>ji</sub>, respectively.

For column at unsteady state operation, each holdup specified gives rise to an additional multiplier parameter. For each time period, successive approximations of the temperature at the end of the time period are made until a temperature profile is found such that the component material balances and the enthalpy balances are satisfied as well as the specification for the column.

VII. SEPARATION MIXTURE BY ABSORPTION

The classical absorption based on the assumption that stage of the column is perfect stage, that is, the gas leaving each stage is in equilibrium with the liquid leaving. Also, it is assumed that the absorption factors for each component i do not vary with stage number, that is, A<sub>ji</sub> = A<sub>j</sub>.

Summarized mathematical model for absorber is:

$$y_{ji} = K_{ji} x_{ji} \quad \text{and} \quad \text{absorption factor } A_{ji} = L_j / G_j K_{ji}$$

$$L_{j+1} + G_{j-1} - L_j - G_j = \frac{dm_j}{dt}$$

$$L_{j+1} h_{j+1} + G_{j-1} H_{j-1} - L_j h_j - G_j H_j = \frac{du_j}{dt}$$

$$L_{j+1} x_{j+1,i} + G_{j-1} y_{j-1,i} - L_j x_{j,i} - G_j y_{j,i} = \frac{dm_{j,i}}{dt}$$

Eqs.(14)

For steady state operation condition right hand side terms in system equations (14) are equal zero.

The procedures developed and demonstrated here constitute different methods for solving the component

material balances, the equilibrium relationships, and the enthalpy balances which are required to describe absorbers and strippers.

The methods are developed for existing absorbers that is, the number of stages is fixed and it is desired to determine the separation that can be effected at a specified set of operating conditions. The set of specifications considered are pressure, gas flow rate, gas phase compositions, liquid phase rate, liquid phase compositions, inlet temperature, outlet temperature, and total number of stages.

The problem to be solved consists of finding the solution sets of total flow rates, compositions, and temperatures corresponding to a given set of specifications. Many procedures are presented for solving problems of this type. In the presentation of these procedures, both perfect stages and perfect heat transfer are assumed. Perfect heat transfer means that the gas and liquid streams leaving each stage possess the same temperature. The temperatures may vary, however, from stage to stage.

### VIII. THE MULTICOMPONENT SEPARATION

For a case study the distillation column was used.

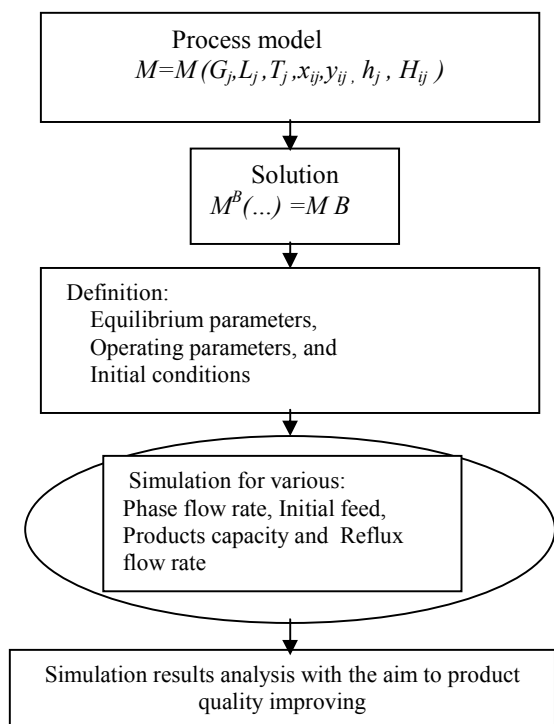


Fig. 6 The integrated algorithm for simulation

The main specification variables characterizing of the process are the feed flow rate  $F$ , benzene composition in the feed  $x_F$ , distillate flow rate  $D$ , benzene composition in the distillate  $x_D$ , reflux flow rate  $L_R$ , bottoms flow rate  $B$ , and bottoms benzene composition  $x_B$ .

The process simulation algorithm and manipulative and object variables illustration have shown in Fig. 6.

A distillation column with fifteen theoretical stages for benzene recovery from the mixture of toluene and xylene was

used as shown in Fig. 7. The column operate under steady state conditions.

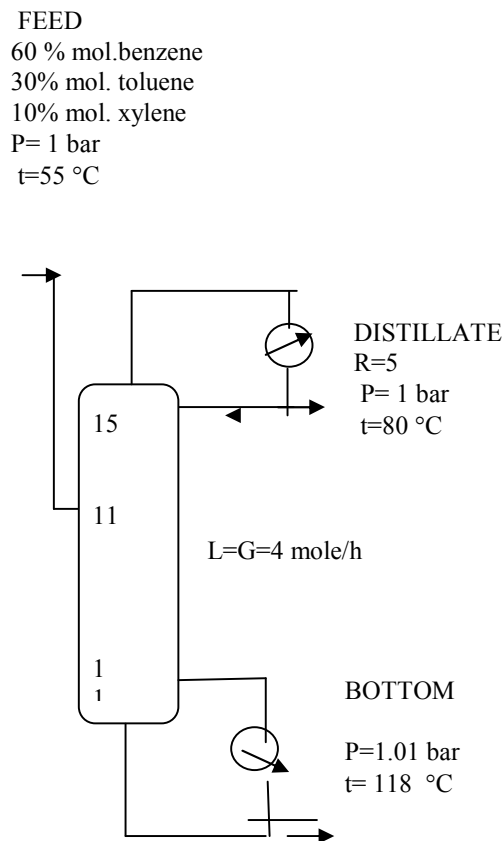


Fig.7 Scheme of distillation simulation

#### VIII.1. THE METHOD FOR THE DETERMINATION OF BUBBLE POINT AND DEW POINT TEMPERATURE

For temperature profile and the components mole fractions profiles in all phases calculation the  $K_b$  method was used [7], [8].

Relative values of the equilibrium constant are independent of temperature [9], the expression given by the first three equations in the eqs. system (12), may be rearranged in a manner such that trial-and-error calculations avoided in the determination of the bubble point and dew point temperatures.

The ratio  $K_i/K_b$  is called the relative volatility  $\alpha_i$  of component  $i$  with respect to component  $b$ , that is,

$$\alpha_i = \frac{K_i}{K_b} \quad (a)$$

where  $K_i$  and  $K_b$  are evaluated at the same temperature and pressure. Component  $b$  may or may not be a member of the given mixture under consideration. when  $x_i$ 's and the pressure  $P$  are given and it is desired to determine the bubble point

temperature, the formula needed may be developed by first rewriting the first expression eqs.(12) as follows:

$$y_i = \left(\frac{K_i}{K_b}\right)K_b x_i = \alpha_i K_b x_i \quad (b)$$

Summation of the members over all component  $i$ , followed by rearrangement yields:

$$K_b = \left(\frac{1}{\sum_{i=1}^c \alpha_i x_i}\right) \quad (c)$$

Since the  $\alpha_i$ 's are independent of temperature, they may be computed by use of the values of  $K_i$  and  $K_b$  evaluated at any arbitrary value of  $T$  and at the specified pressure. After  $K_b$  has been evaluated by use of equation (c) the desired bubble point temperature is found from the known relationship  $K_b$  and  $T$ .

If the  $y_i$ 's are known instead of the  $x_i$ 's, then the desired formula for the determination of the dew point temperature is found by first rearranging equation (b) to the following form:

$$K_b x_i = \left(\frac{y_i}{\alpha_i}\right) \quad (d)$$

and then summing over all components to obtain:

$$K_b x_i = \sum_{i=1}^c \left(\frac{y_i}{\alpha_i}\right) \quad (e)$$

Although there exists many systems whose  $\alpha_i$ 's are very nearly constant and equations (d) and (e) are applicable for the determination of the bubble point and dew point temperatures, respectively, the greatest use of these relationships lies in their application in the iterative procedures for solving multicomponent distillation problems.

## VIII.2 COMPUTATION PROCEDURE

For computation procedure which was using the constant molar overflow is assumed and the material balance and equilibrium relationship equations are solved stage by stage starting at the top or bottom of the column. To define a problem the following variables must be specified, or determined from other specified variables, according to Lewis-Mathison method[10].

- Feed composition, flow rate and condition
- Distribution of the key components
- One product flow
- Reflux ratio
- Column pressure
- Assumed values for the distribution of the non-key components.

The usual procedure is to start the calculation at the top and bottom of the column and proceed toward the feed point. The initial estimates of the component distributions in the products are then revised and the calculations repeated until

the compositions calculated from the top and bottom starts mesh, and match the feed at the feed point.

In general, the Lewis –Matheson method has not been found to be an efficient procedure for computer simulation, other than for relatively straightforward problems. It is not suitable for problems involving multiple feeds, and side streams, or where more than one column is needed.

The method is suitable for interactive programs run on small computers. The computer solving the stage equations, while control of the iteration variables, and convergence is kept by the designer.

## IX. RESULTS AND DISCUSSION

The obtained results for feed composition 60% mole fraction of benzene, 30% mole fraction of toluene and 10% mole fraction of xylene, feed flow rate 4.0 mole/h, reflux number  $R=5$ , feed stage  $f=11$  and total number of theoretical stages  $N=15$  are shown in Fig. 8 to Fig.10.

Fig. 7 shows operating conditions of the distillation column.

Fig.8 shows temperature profile through the column.

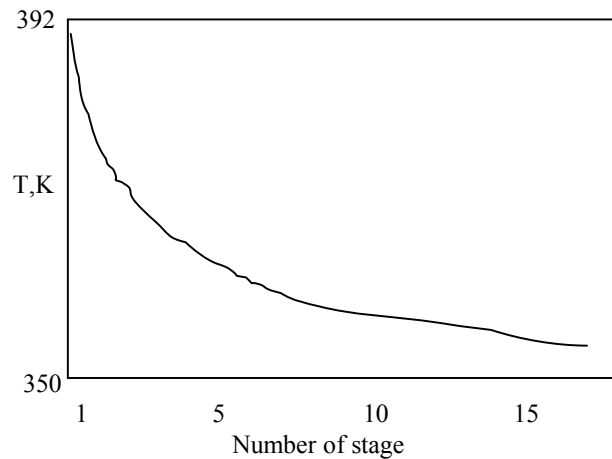
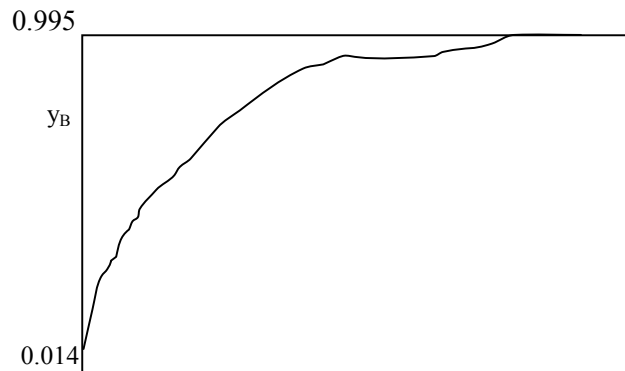


Fig.8 Temperature changing with stages of the column

In Fig.9 the benzene composition profile of the vapour phase through the stages is shown.

Fig.10 shows the benzene composition profile in the liquid phase per stages.





1                      5                      10                      15  
number of stage

Fig.9 The benzene composition profile in the vapor phase by stage to stage

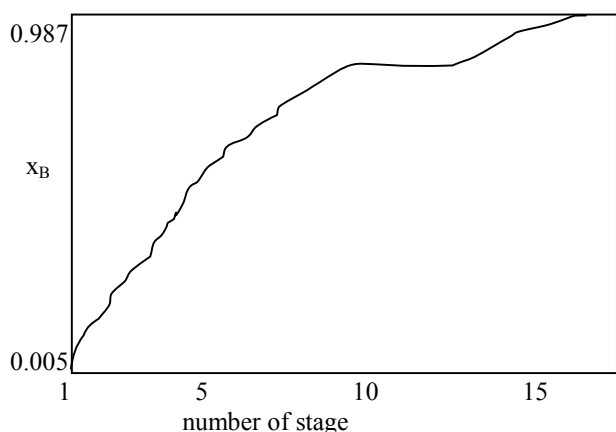


Fig.10 The benzene composition profile in the liquid phase by stage to stage

On the feed stage appears decreasing of the benzene composition in the both of the liquid and vapor phases, because of different feed composition from composition on the stage.

Analysing the obtained results in Fig.9 and Fig.10 can reduce operating cost for the same product quality.

## X. CONCLUSION

The obtained results show power in structuring multistage process units and multistage column building. Models help to build intelligent decision support system and allows to efficiently build the new integration. The results in this paper has directly applications in design, operation and optimization of the multistage columns. Adding or reducing stages can establish optimal system according to required separation. Also, by adding different stage can develop the new separation process system.

## ACKNOWLEDGEMENT

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## Notation

A-absorption factor  
B-bottoms flow rate, mole /h  
c-total number of component  
D-distillate flow rate, mole /h  
G-gas phase flow rate, mole /h  
L-liquid phase flow rate, mole/h  
H-enthalpy of the dgas phase  
h-enthalpy of the liquid phase

F-feed flow rate, mole/h  
K-equilibrium constant  
m-stage holdup, mole  
M-total holdup, mole  
Q- ehergy of heating or cooling, J/h  
T-temperature, K  
u-energy accumulation,J  
v-reaction rate  
x-composition in the liquid phase, mole/mole  
y-composition of the gas phase, mole/mole

## Index

c-condenser  
i-component  
j-stage  
f-feed  
R-reboiler

## Greek symbol

$\Delta h$  –heat of chemical reaction

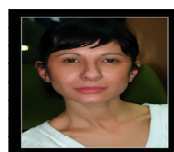
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