The enzyme separation plant modelling, design and optimization

J. Lukic, M. Vico-Stevanovic,L. Filipovic-Petrovic, R. Beric

Abstract— A new approach for plant model building was illustrated. The use of flowsheeting in design, however, differs from its use in operations and this should be reflected in the development of the simulation procedure. In design, attention focuses on the main elements of material and heat balances, on equipment investment, and more generally, on process economics. The systems approach permits the evaluation of feasibility and global plant integration, always for a predicted behavior of the operation systems. A plant for the β-galaktosidase separation from E. Coli was used. The global optimization of the plant design was provided.

Keywords— Input data base, plant model, simulation, design, optimization, parameters.

I. INTRODUCTION

Being a key to survival in global markets including the previous needs and challenges, process engineering necessitates the today evaluation in research and teaching. It involes the whole of scientific technical knowledge necessary for physicochemical and biological transormations of raw material and energy into targeted products necessitaed by the customer.

A many number of modelling and simulation systems have been developed to aid the modelling process in engineering domains. One of the most widely used forms of simulation is that for operator training[1]-[5]. So far operator training simulators have tended to use greatly simplified models in order to ensure real time performance and most effort has been invested in the development of user interface. With the availability of much increased computing power the way is now open for the same simulation model to be used for operator training purposes. A further aspect of the extended application of simulation for operator assistance could well be achieved in conjunction with expert systems.

It many years since process modelling become a advanced tool for design work in most companies. Yet the major impact of this technology may still be in the future as more companies appreciate its values as strategic support for business operations especially in manufacturing. The means that process engineers and plant managers need even more sophisticated tools to study the behavior of the plant [6]-[12].

Thus while process flowsheeting was originally the realm of chemical engineers working in the design department the new knowledge based technology is now benefiting many others disciplines and departments so that full value is gained from the plant model[11].

In this paper the β-galaktosidase separation plant model was studied with the aim to plant design and optimization.

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II. A NEW APPROACH

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

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 [7]-[9]. Database of kinetic parameters was developed as a relational data base system which linked kinetic models and operation simulation by process models.

The steady state model, which is simpler to build, and has a wide variety of applications in its own right, it can be used directly in revamping and a wide variety of other engineering projects.

The general framework presented above generally is valid in the development of any complex computer based applications in process engineering, such as plant simulation models, or model based training systems. The life cycle concept may lead to a reliable and maintainable tool.

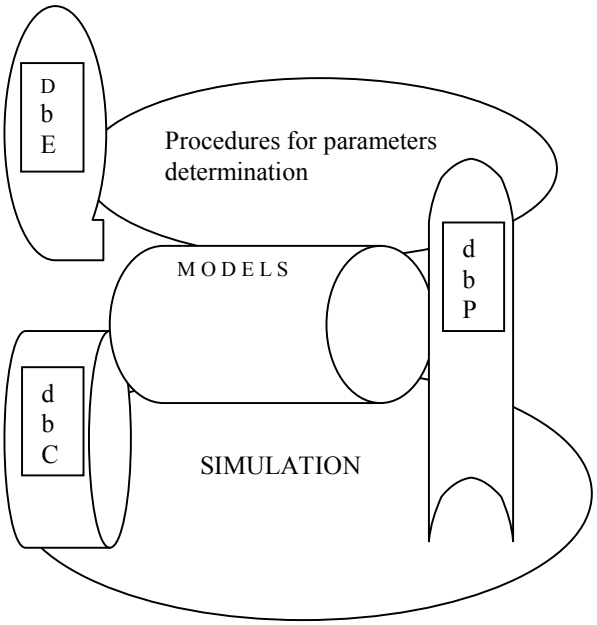
II.I Simulation methodology

Using commercial flowsheeting software, it is possible to produce a computerized tool that will permit us to learn or even "mirror" the plant behavior under different operating conditions or with different raw materials and product specifications. Such as tool is called the steady state plant simulation model. Process simulation and modeling techniques are very useful for optimizing design and operation.

Developing such as model is a preliminary and necessary stage in achieving real time plant optimization which involves treating data reconciliation and rigorous simulation simultaneously by means of optimization techniques, whose

objective is to maximize process profitability. The steady state model, which is simpler to build, and has a wide variety of applications in its own right, it can be used directly in revamping and a wide variety of other engineering projects.

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.



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

Fig. 1.Data bases network with models

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. It provides rigorous on-line modeling tools for the process design and operation and raw material and energy minimization. Raw material minimization was simulated seeking out optimal initial substances quantity. Energy minimization was provided by heat recovery simulation. This simulation integrates data bases for component data, biochemical data, and model parameters tables with structured knowledge representation subsystems.

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.

I.1. Biochemical kinetic model

The generic model were illustrated by actually implementation biochemical reaction.

The synthesizing procedure is generated and ranked database facts and clauses, kinetic parameters database and kinetic models which defined bioreaction and product concentration changes [10]-[11].

General kinetic model:

$$E + S \xrightarrow{k1} ES \underset{k-1}{\overset{k2}{\rightleftarrows}} P + E \quad (1)$$

$$\frac{dc_{ES}}{dt} = k_1 \cdot c_E \cdot c_S - k_{-1} \cdot c_{ES} - k_2 \cdot c_{ES} \quad (2)$$

and product rate

$$\upsilon = \frac{dc_P}{dt} = k_2 \cdot c_{ES} \quad (3)$$

where E is enzyme, S- substrate, P-product , c- concentration, k-specific biochemical constant, and v –bioreaction rate.

I.2. Bioreaction operation model

It is assumed that fermentation occurs in the liquid phase and the contents are perfectly mixed. Product capacity depends from initial flow rate and composition, bioreaction conditions and different size of fermentor volume [12].

Overall flow rate balancing:

$$F_i - F_O = \frac{dV}{dt} \quad (4)$$

Biomass growth:

$$\mu_X c_X - \alpha_X c_X - F_O c_X = V \frac{dc_X}{dt} \quad (5)$$

Substrate rate,

$$F_i c_S - F_O c_S - \frac{\mu_X}{Y_{X/S}} - \frac{q_P}{Y_{P/S}} - m c_X = -V \frac{d}{dt}(c_S) \quad (6)$$

Product rate,

$$q_P c_X - F_O c_P - K_p c_P = V \frac{d}{dt}(c_P) \quad (7)$$

where V is microbial broth volume, F- flow rate, concentration, X - biomass, S- substrate, P-product, μ_X - specific speed biomass growth, α_X - specific speed biomass death, q_P -specific speed of the product formation, m – specific speed substrate consumption for biomass maintainance, $Y_{X/S}$ - coefficient of the substrate conversion in biomass, $Y_{P/S}$ -coefficient of the substrate conversion in product, K_P - average values of microbial population, and t – time.

III. PROCESS PLANT MODEL

The plant simulation model should mirror the behavior of a complex plant subject to constraints in feedstock, products, equipment capacities, operational parameters, and utilities consumption. It's objectives include to:

-Provide comprehensive report of material and energy streams;
-Determine the correlation between the chemical reactors and separation systems;
-Study the formation and separation of byproducts and impurities;
-Support preventive maintenance by tracking performance of key equipment over time, and its relation to the buildup of impurities;
-Improve to robustness to plant operation;
-Asses how to eliminate wastes and prevent environment pollution;
-Evaluate plant flexibility to changes in feedstock or products;
-Validate process instrumentation and enhance process control,
-Update process documentation and prepare future investments, and
-Optimize the economic performance of the plant.

The achieve these goals, the rigorous simulation model must be tuned. This demands reliable plant data stream compositions, temperatures, pressures, and so on. These are obtained from test runs during steady state operation.

The knowledge based system which automated the process enabling engineers to perform modelling and simulation study was investigated. Input data bases linked with routines for process units models. Generic data base of parameters was developed as a relational data base which link process plant model.

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, variables, behavior rules, and initial conditions.

The overall mass balance:

$$\sum_{i=1}^{NM} s_i \partial_i F_i = 0 \qquad (8)$$

Substream mass balance:

$$\sum_{j=1}^{NSS}\sum_{i=1}^{NM} s_i F_i f_{ij} = 0 \qquad (9)$$

Component mass balance:

$$\sum_{k=1}^{NC}\sum_{j\neq 1}^{NSS}\sum_{i\neq 1}^{NM} s_i F_i f_{ij} z_{i,j,k} = 0 \qquad (10)$$

and overall energy balance

$$\sum_{i=1}^{NM} s_i \partial_i F_i h_i + \sum_{i=1}^{NH} s_j \partial_j H_j + \sum_{i=1}^{NW} s_k \partial_{ki} w_k = RHS \qquad (11)$$

equation i, where $s_i = +1$, for inlet streams and $s_i = -1$ for outlet streams, ∂_i is stream scale factor, F_i mass flow stream i, f_{ij} is mass fraction of substream j in stream i, z_{ijk} is mass fraction of component k in substream j of stream i, NM is number of inlet and outlet material streams, NH is number of inlet and outlet heat streams, NW is number of inlet and outlet work streams, NSS is number of substreams within material streams, NC-number of components specified on the components main or components group forms, h_{ij} is enthalpy of stream i, H_j is flow of heat stream j, w_k is work of the work stream k, RHS is right hand side of the energy balance equation (11).

Having defined the relevant compounds, the elementary and enthalpy balance can now be defined. There are the following relevant elements and corresponding elementary balances for C,H,O,N,S and enthalpy balance need to be formulated.

Carbon balance: $6r_s + r_c + 19r_P = 0$ (10a)

Hydrogen balance:

$$10r_s + 2r_w + 24r_P + 6r_N + 2r_{sacid} = 0 \qquad (10b)$$

Oxygen balance:

$$5r_s + 2r_o + 2r_c + r_w + 4r_{sacid} = 0 \qquad (10c)$$

Nitrogen balance: $2r_N + r_P = 0$ (10d)

Sulfur balance: $r_{sacid} + r_P = 0$ (10e)

Enthalpy balance:

$$-235r_s - 94r_c + 68r_w - 19r_N - 194r_{sacid} + rH = 0 \qquad (11a)$$

The input component data base and data base of kinetic parameters have developed as a relational data base system which linked with simulation by process models.

A reactor simulation with detailed kinetics and a realistic flow model may be executed better with specialized software (Savkovic-Stevanovic et.al., 2007). In fact, in flowsheeting only need an accurate description of the transformation linking the input the output of the reaction system. This again highlights the differences between design and operations, in the design mode, the modeling of chemical reactors focuses on the main products rates.

Fact, the time behavior, like catalyst activity, or impurities generation, is difficult to estimate. In contrast, in operations, a detailed knowledge of the bioreaction systems is available, but its interaction with other equipment items is still unknown.

The abio reaction system for given bioreactor operating conditions as function of variable input stream is the key feature that need in modelling the biochemical reactor in flowsheeting. A set of stoichiometric, independent biochemical reactions has been formulated and molar extent of reaction used as the reaction coordinate.

For the examined plant in which E.Coli growths and β-galaktosidase separates flowsheeting is shown in Figure 3. Figure 4 shows the process plant flow diagram with optimal process units.

The use of advanced modelling technique for an actual automated equipped involved the continuous steady state nature of the processing units starting from the crude tanks and ending in the component tanks.

IV.THE SEPARATION PLANT DESIGN

The use of flowsheeting in design, however, differs from its use in operations and this should be reflected in the

development of the simulation procedure. In design, attention focuses on the main elements of material and heat balances, on equipment investment, and more generally, on process economics [7]-[10]. The systems approach permits the evaluation of feasibility and global plant integration, always for a predicted behavior of the bioeaction systems. While a deeper systems analysis of the plant would be worthwhile, considering that the basic design could be responsible for more than 80% of the cost of investment and operation, a detailed simulation and constrained, however, by the project schedule and lack of data.

The input components data base and design process parameters data base have developed as a relational data base system which linked with process models by simulation.

In fact, in flowsheeting only need an accurate description of the transformation linking the input the output of the bioseparation system [11]. Optimization in design specification was achieved (Fig.2). This again highlights the differences between design and operations, in the design mode, the modelling of bioreactors focuses on the main products rates. In this paper design mode was considered.

The separation plant for continuous β-galactosidase separation from constituent mutant E.coli requists sterilizator, fermenter, centrifuge, rotation vacuum filter as shown in Fig.3. Microbial cells concentration in the 5-step periodic centrige and destroys in the high pressure homogenizator. Cells separte from the mixture by rotation vacuum filter.

The input component data base and data base of parameters have developed as a relational data base system which linked with operation simulation by process model.

Fact, the time behavior, like enzyme activity, or impurities generation, is difficult to estimate. In contrast, in operations, a detailed knowledge of the systems is available, but its interaction with other equipment items is still unknown.

Thus, such a simulation can be particulary useful for retrofit projects, where in may provide insights that lead to relative reduction in impurity levels.

V. PLANT OPERATION

The handling of impurities, often neglected or unknown in the design phase, is one of the most important aspects of plant operations. Some impurities have their origin in the raw materials, others are produced by thermal decomposition or other actions in the process. They cause drops in performance, equipment fouling, and product losses, and may lead to environment pollution. Only a global plant simulation allows the quantitative identification of their values.

In operation, in contrast, attention centers mainly on product flow rate and specifications, but also plant troubleshooting, controllability, and maintenance. The performance of bioreactors and separation systems impose the rules of the game. They are independent and time variable to some extent. Only a detailed plant simulation enables an understanding of these interdependencies and their quantitative evaluation. Thus, the exact knowledge of a detailed material and energy balance is by far more important in operations than in design. Even the flow rates of trace impurities are relevant, because they may impact equipment maintenance and environment protection. The material and energy balance as well as the operational characteristics of a plant are highly interconnected, and well suited for a system analysis.

VI. FLOWSHEETING RECYCLE STRUCTURE

To develop a plant simulation model, should be first developed a Simulation Flow Diagram- SFD. It is close to but not identical with the process flow diagram-PFD, because of modeling limitations or flowsheeting convergence constraints. This means that the simulator should be provided with capabilities assuring flexibility both in modelling as well as in flowsheeting procedures, for instance.

Transfer of information between units, such as heat exchanger duty and mechanical work or between streams:full access to stream and unit variables, both in retrieving as well as in modifying mode, powerful user programming capabilities, and flowsheet split/merge features.

Unfortunately, the technical literature provides little information about structural analysis of a large plant for simulation purposes. First, the recycle structure of a large flowsheet may be analyzed by means of some simple structures. These typically are structured loops, crossed loops, and interconnected loops.

Flowsheet decomposition involves selection appropriate tear streams. The basic concept in tearing has bean review in references (Savković-Stevanović, 2007). Most commercial simulators provide automatic procedures tear stream identification and for generation of the calculation sequences.

VI.THE OPTIMIZATION METHOD

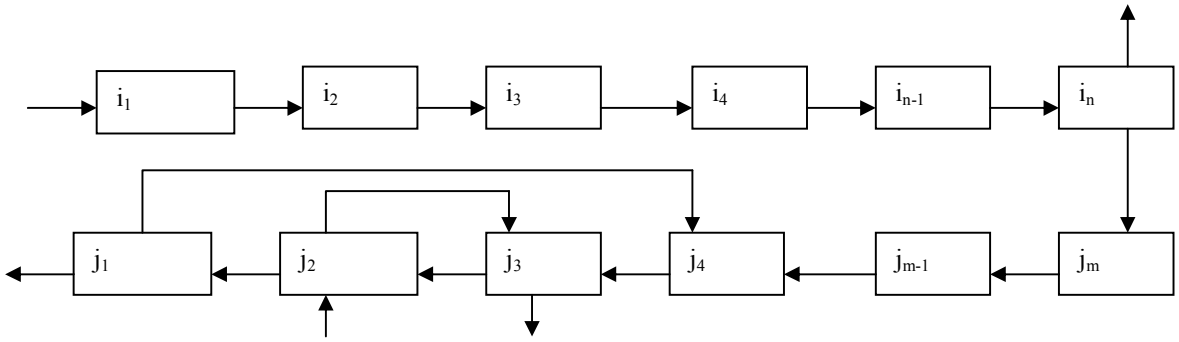
The material and energy streams network can be optimized by any algorithm of the linear programming optimization method. This procedure finds the maximum of multivariable, linear function subject to linear constraints involving eqs.(1)-(4).

$$\text{Maximize } F = C_1X_1 + C_2X_2 + ... + C_NX_N \qquad (12)$$

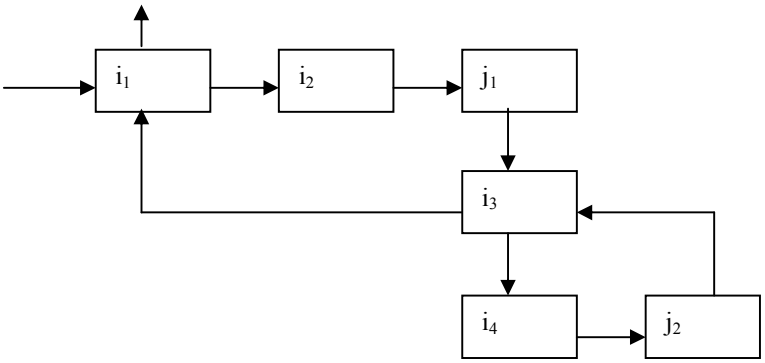
Subject

$$\text{to } A_{1i}X_1 + A_{12}X_2 + ... + A_{iN}X_N \leq, =, \geq B_i \qquad i = 1,2,....,M \qquad (13)$$

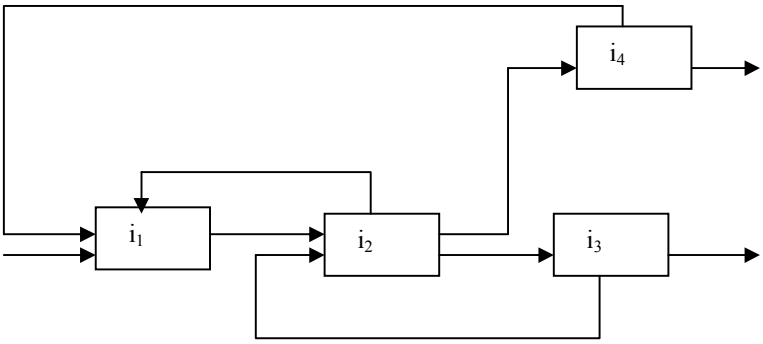
$$X_1, X_2, ..., X_N \geq 0.$$



a) Structured loops

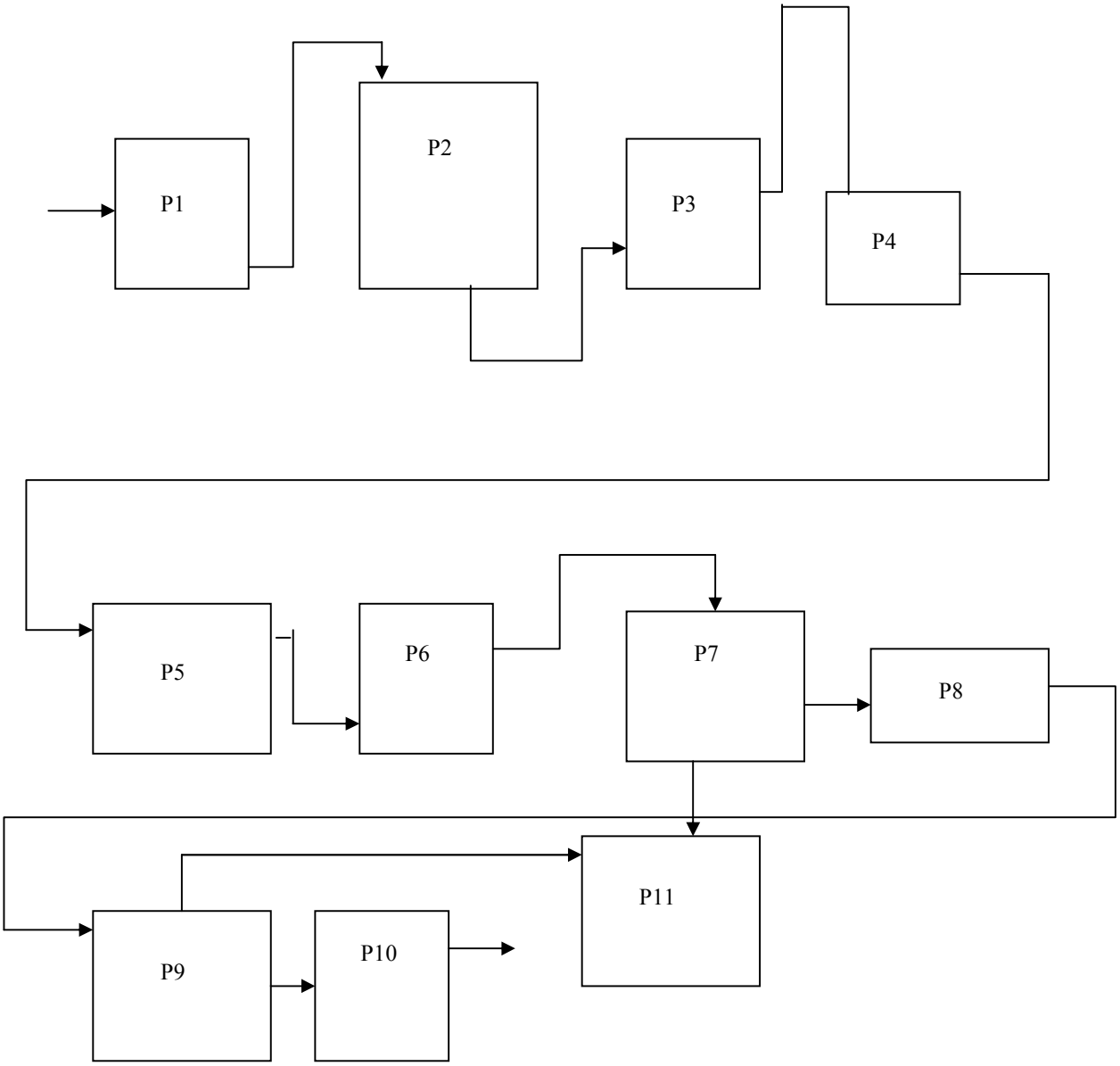


b) Crossed loop



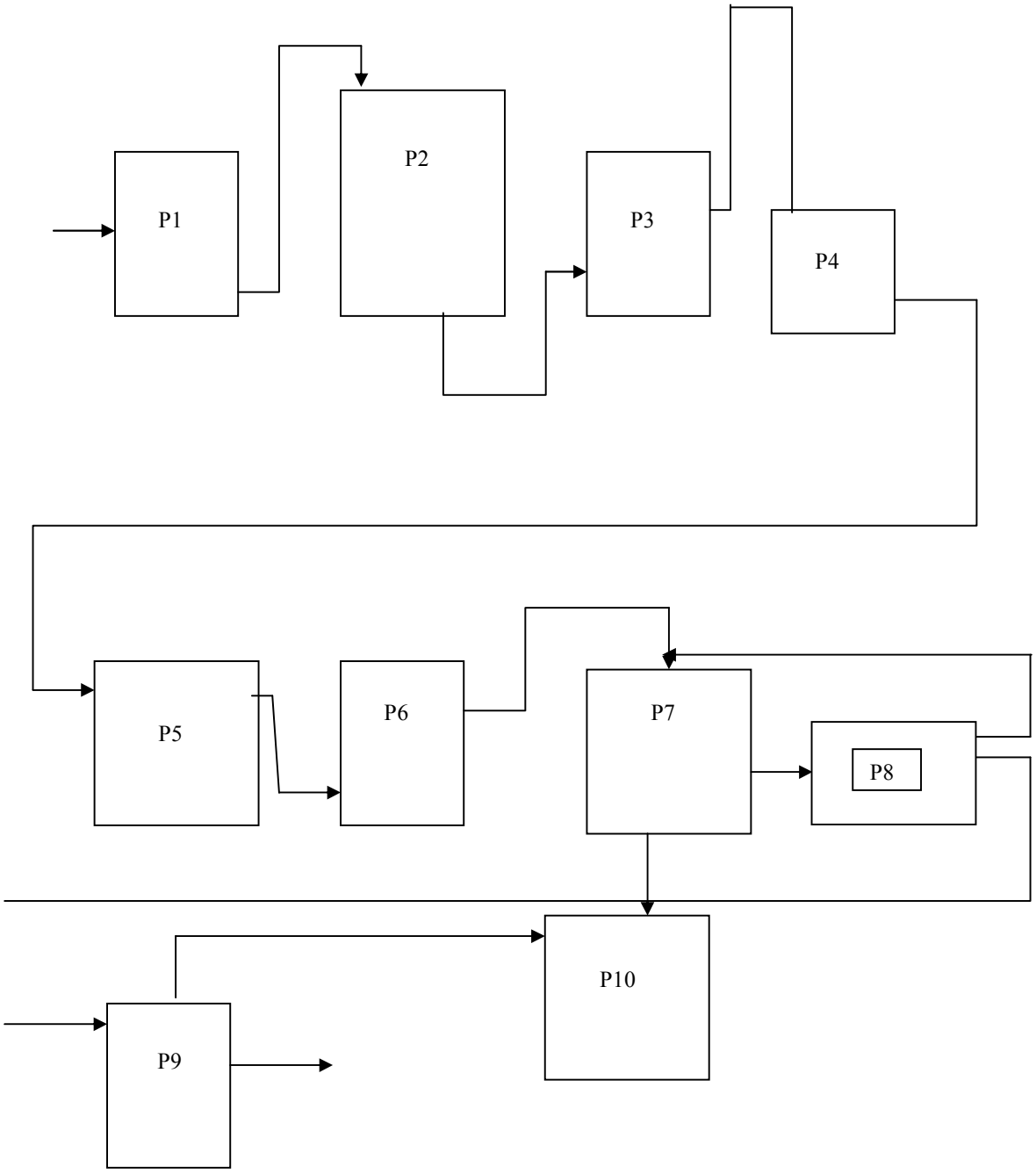
c) Interconnection loops

Fig.2 The flowsheeting structures



P1- sterilizator, P2-fermenter, P3-heat exchanger, P4-centrifuge, P5-homogenizator, P6-heat exchanger, P7- mixer tank, P8- rotation vacuum filter, P9- mixer tank, P10-centrifuge, P11- container.

Fig.3 The bioseparation plant scheme



P1- sterilizator, P2-fermenter, P3-heat exchanger, P4-centrifuge, P5-homogenizator, P6-heat exchanger, P7- mixer tank, P8- rotation vacuum filter, P9- centrifuge, P10-container.

Fig. 4 The optimized flowsheeting scheme

where the $A_{ij,}$ B_i, and C_j are given constants and the X_j are the decision variables.

The method is an iterative technique that tends to find the global optimum of the objective function within the feasible region established by the constraints. The simplex method is very suitable to use.

In this paper recuperation streams were implemented in the optimal material and energy streams network of the enzyme separation plant.

Design process scheme after plant streams optimization has shown in Fig.4.

The input component data base and process parameters data base have developed as a relational data base system which linked with process models by simulation.

In fact, in flowsheeting only need an accurate description of the transformation linking the input the output of the system. Optimization in design specification was achieved.

VII. CONCLUSIONS

The results of this paper have shown power of the process model for generating different separation operations. Dynamic simulation can early in design phase to avoid costly post-startup modifications.

The obtained results are shown superiority of the modelling aided process operation tool and illustrate recycle flowsheeting structures. Current and future work therefore includes continuous update of models, rules properties and problems.

In this paper knowledge based process design of the β-galaktosidase separation plant was studied. The simulation flow diagram was developed.

Process plant simulation models were constructed and collected for plant design and operation. The knowledge based system which automated the process, enabling engineers to perform modelling and simulation was built.

A relational data bases which including component data base and data base of biokinetic parameters have developed. This relational data base system has linking with operation simulation by process models.

ACKNOWLEDGMENT

The authors wish to express their gratitude to the fund of Serbia for Financial Support.

Notation

c- concentration, kg/ dm^3
E-enzyme
F- flow rate, dm^3 /h
h_{ij} is enthalpy of substream j in stream *i*
H_j -flow of heat stream *j*
f_{ij} -mass fraction of substream *j* in stream *i*
k-specific biochemical constan, h^{-1}
K_P - average values of microbial population
m – specific speed substrate consumption for biomass maintainance, h-1
P-product
r-conversion rate, mole/h
S- substrate
$s_i = +1$, for inlet streams, and $s_i = +1$ for outlet streams
t – time , h
V-volume,dm^3
v –bioreaction rate
X-biomass
$Y_{X/S}$ - coefficient of the substrate conversion in biomass
$Y_{P/S}$ -coefficient of the substrate conversion in product
z_{ijk} - mass fraction of component *k* in substream *j* of stream *i*

Greek symbols

μ_X -specific speed biomass growth, h^{-1}
α_X - specific speed biomass death, h^{-1}
q_P -specific speed of the product formation, h^{-1}
∂_i - stream scale factor

Index

C-carbon
E—enzyme
i-input
N-nitrogen
o- output
P- product
S-substrate
X-biomass
W-water
O-oxygen
H-hydrogen

Abbervation

NM-number of inlet and outlet material streams
NH -number of inlet and outlet heat streams
NW- number of inlet and outlet work streams
NSS- number of substreams within material streams
NC-number of components specified on the components main or components group forms.
RHS- is right hand side of the energy balance equation (11).

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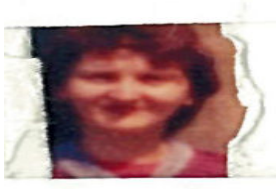

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