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Economic and Mathematical Models of Optimizing Some Activities in the Petrochemical Industry

Economic cybernetics and computing electronic technique applied in the petrochemical industry allow the more efficient treatment of the ever more complex flow, from extraction and processing till the turning to account of the crude oil.

The methods and models of economic cybernetics and the electronic technique applied relatively recently in some major activities in the field of petrochemistry have led to the finding of optimum solutions with respect to the multiple and complex technical and economical aspects. As a result of a fruitful cooperation in the domain of scientific research between the laboratories of the Department of Economic Cybernetics and some industrial units there has been possible that a significant group of concrete questions in the field of petrochemistry should be optimized by using modern methods of analysis and modelling as well as the modern computation technique. Thus, their implementation in the production process has led to results with particularly valuable implications for the national economy.

Without going into details, from the multitude of the problems solved within the framework of these collaborations we present further the problem of the modelling of the olefins manufacturing technological process, the problem of the optimization for gasoline blends, the problem of petroleum-product transportation, as well as a system of routines used for statistical and mathematical modelling.

I. OPTIMIZATION OF THE OLEFINS MANUFACTURING TECHNOLOGICAL PROCESS

General features of the modelling of technological processes

The continuous growth of the complexity of chemical processes and the objective trend towards increasing their efficiency are making ever more necessary the introduction in the production process of the most up-to-date techniques and methods, which most assuredly allow the obtaining of the economic optimum. The experience of the researchers within the laboratories of the Department of Economic Cybernetics, with the cooperation of the specialists from industry, shows that the optimization of phenomena and processes must blend the technical aspects with those economic into a unitary system, the substantiation of which is constituted by a mathematical form containing the functions of manifestation of all influential factors of the respective phenomenon or process.

In the approach of the mathematical modelling of the olefins manufacturing, of the gasoline blends, as otherwise in other simulation processes, there have been visible some stages, with precise functions and delimitations, which are being pointed out in the concrete applications that we present further.

The analysis and the establishment of the objectives for the olefins manufacturing form

The whole modelling process for the olefins manufacturing has been divided into two partial processes — thermal cracking reactor line and separation line —, which has allowed the inclusion in the form of some intermediate variables and, at the same time, has eased the process of the elaboration of the form itself. The very minute analysis of the process has allowed the detection and selection of the dependent and argument variables.

An important aspect of the analysis stage was the establishment of the objectives to which the elaborated form had to reply. This has allowed the selection of the structure of the form, the choice of variables, the establishment of the form response accuracy, the methodology for deducing the equations as well as the fact that there is involved a management form and not a design one of the respective process.

Without going into the classification and interpretation of the variables of this process, we consider that this stage rigorously effected has ensured to the largest extent the veracity of the form.

Designing, collecting and checking of data

In the stage of designing the model there have been inventoried all the factorial and resultative variables, from among which there have been selected those of whose participation in the process is significant.

From the experience gained in the modelling of this chemical process it has resulted that there are particularly important the checking and adjust-

ing of the measuring, control and analysis apparatus of each factor participating in the process. For instance, it has been practically ascertained that the utilization of diaphragma type flow transducers does not provide the necessary accuracy, a fact for which these have been replaced by others of numerical type with turbine. Similarly, for high temperature measuring there have been necessary the checking and gauging of the common thermocouples into a precise field.

In the data collecting stage in the process there have been used standard type forms, with precise filling instructions. This collection was effected by the operating personnel of the process, following a briefing and the direct guidance and leading of the modelling group. This stage has been greatly eased by the availability of the process analysers, which allowed the effection of analyses at short intervals of time.

In the stage of the checking of data there have been used statistical and mathematical indicators, which allowed the specification of the variation intervals of variables, the exclusion of erroneous experiences, the completion of experiements, as well as of the checking of material and energetic balances etc.

The study of connections and the elaboration of the model

The collected data have been submitted to a complex correlation and regression analysis with a view to establishing the intensity and the form of the existent links between the factorial and the resultative variables. Only by a correct interpretation of the most corresponding connections and forms, there could be precisely determined the characteristic equations of the process. In the modelling of this process there has been tested a large number of simple and multiple linear equations, polynomial quadratic, cubic, reverse equations etc.

Owing to the complexity and to the large volume of computations, it was necessary to use the IBM 360 electronic computer of the laboratory of the Department of Economic Cybernetics, utilizing especially the WIEZOR and REMUS routines, worked out by the research workers of these laboratories.

As a result of a complex analysis of all the stages of the olefins manufacturing process, there has been regarded as advantageous the constitution of the overall model from three partial models:

— model for pyrolysis furnace;
— model of acetylene catalytic hydrogenation;
— model of ethylene separation by fractional distribution.

Since the efficiency functions of the three partial models were of a technical nature, the overall model of the process has been constituted by taking into account the economic side and taking the cost price as criterium.

Simulation and refining of the model

For each model there has to be established the degree of conformity with the real process for which it was designed. For this, the checking of the model of olefins manufacturing technological process included two stages. In the

first one the model has been tested round the current operating values of the process in the *furnace-form* way, while the second stage involved the model simulation all through the variation field, in the *model-furnace* way.

The model refining has been a stage of improvement, adjustment and simplification of the already tested and simulated model. In the concrete case of the pyrolysys furnace, the model refining has led to a decrease of its error by approx. 10%.

Model implementation

This last stage of the whole modelling activity is meant to make the actual link between model and process. The stage is achieved depending on the existence of a computer, namely on the fact if the model will run off-line or it is a stage preceding an on-line running. At the same time, this stage serves also to obtain some new information on the model-process link, with a view to improving the model.

Although the efficiency of implementing such a model is difficult to be established, as a result of the qualitative variation of raw materials and the specification of all qualitative and quantitative leaps in new conditions, in the case of pyrolysis furnace form, one of the indicators of economic efficiency is the rise of ethylene output by 8.6% as against designed capacity.

II. OPTIMIZATION OF PRESCRIPTIONS FOR GASOLINE BLENDS

The experience of the technological process modelling group within the laboratories of the Department of Economic Cybernetics has enabled to outline the idea according to which the modelling and optimization of the prescriptions for gasoline blends is a component part of a general model, which starts from the processing of crude oil, is being continued with the refining and processing in chemical installations and ends with the turning to account of the obtained products.

Taking into consideration the fact that the overall model of crude oil-derivates is an extremely complex one, the respective modelling can be achieved only by successive steps, each step being a sub-system of the general system. This is justified, on one hand, by the fact that each stage marks the limits of a distinct area within the whole flow, and on the other, for the fact that the modelling activity implies a very large volume of work.

The problem of gasoline blends is put as a result of the fact that through the crude oil refining there are not being directly obtained marketing products, but chemical compounds which have to be subsequently combined. Their blending is being done in such a way as to achieve finished products which should correspond from the qualitative standpoint to the STAS requirements. This thing is particularly complex, since the components which are participating in the blending have different qualities and the difficulty consists not in the physical process of blending but in the establishment of the quantitative proportion of each component, so that from different qualities should be obtained the quality imposed by STAS.

If as related to the mathematical model for gas-oils there is a broader opinion concerning the utilization of linear equations, as far as the model for gasolines is concerned we are of the opinion that there is necessary to use equations determined by help of the statistical methods. This can be perfectly achieved under the conditions of ensuring some measuring and control instruments of the most exacting quality and in the conditions of using an electronic computer.

The mathematical model of the optimization of prescriptions for gasoline blends has been constituted of three large categories of equations and namely:

— equations related to quality;
— equations related to quantity;
— equation of efficiency function.

The quality equations referred to octane number, distillation at (10cc, 50 cc, 50 cc, 100 cc), density and steam compression features.

These equations have been established on a statistical way with ratios of the type:

$$Y = \sum_i K_i \theta_i x_i$$

where:

Y represents the blend feature;
K_i — the influence coefficient of each factor i on the resultative variable Y;
θ_i — the features of component i;
x_i — the amounts from each component i.

The most difficult problem consists in the determination of the regression coefficients K_i, which are being established with the aid of the correlation method within the following stages:

— *designing and realization of a plan of experiments* which should cover the whole feature variation area of all components and in the assumption of small and random variations;

— *processing and analysis of data* obtained on the basis of the achievement of the plan of experiments by help of REMUS routine (for the establishment of the quantities of selective multiple regression);

— *elaboration of quality functional equations*;

— *laboratory testing of functional equations.*

The quantity equations are being constituted as a result of some constraints to be imposed in the process, such as the inclusion of cushion stock in the blend, the inclusion of some components within some limits as a result of the insufficient room for storing the components in installations or the limitation of volume blending following the insufficient space for storing the finished products.

The efficiency function equation raises itself also some problems, because, usually, there is not a unanimously accepted opinion concerning the selection as an efficiency criterium of the cost minimization, benefit maximization or total production maximization.

Since the strips obtained during the blending process are qualitatively different, especially with regard to octane number, the mathematical form of the prescription of gasoline blends is to be conceived as a whole; the qualitative constraints of each gasoline type are being constituted in stages specific for each type, while the quantitative constraints are formed on the entire model.

Also, the efficiency function relates to the overall model of gasolines.

From the practical experience of the research workers in the laboratories of the Department of Economic Cybernetics there could be pointed out several drawbacks on the line of utilizing and extending the mathematical modelling of gasoline blends, such as:

a) the costs of components are not in conformity with their quality, which lead to erroneus results in the case of choosing as efficiency functions the cost minimization or benefit maximization;

b) insufficient storing capacities which make impossible the optimization of blends in continuous flow;

c) lack of measuring, control and analysis instruments, which influences not only the modelling process of gasoline blends, but also the achievement of other models from the whole set of processes within the crude oil-derivates line;

d) big range of component features, as a result of the raw material variation, instability of refining processes etc. This variation can be minimized through an optimization model of the respective processes.

III. OPTIMIZATION OF PETROLEUM-PRODUCT TRANSPORTATION

The system of the transportation plan from refineries to users, put into operation as far back as 1970, is based on the classical model of transportion, in which the efficiency function is constituted by the transportation cost. It is a three-dimensional model of transportation and is solved by factorization in usual bidimensional problems of transportation.

Following the monthly exploitation of the system there are obtained from the computer, on the basis of the worked out form, the ensuing states:

— operative plan of transportation;
— state of transportation expenses;
— list of users;
— summary on counties of optimized petroleum products.

The transportation operative plans are being worked out for each of the ten supplying refineries and they constitute optimum solutions of the transportation model elaborated at the level of the national economy, ensuring in this way the rational and operative utilization, without manual intervention and systematizations.

The computation methodology and the contents of these plans are in agreement with the practical necessities of the Ministry of Transports and Telecommunications, of the supplying refineries and of the enterprises for delivering the petroleum-products within PECO centre.

The state of transportation expenses is emphasizing their volume at the level of the whole national economy as well as distributed for each of the 40 products and for each refinery.

The list of users is the state by which there are marked all the institutions which are receiving petroleum-products on the basis of this plan, ordered in alphabetical order within the framework of each IDPP and located throughout the country.

The summary on counties reflects, on the basis of the transportation operative plan, the volume of the main petroleum-products (gasolines, gas-oils, oil, black oil, fuel) transported from refineries to the 39 counties of the country and to the municipality of Bucharest.

Besides these states, the system can provide, upon request, other states too, such as the unitary costs of transportation from refineries to users, the distancies from refineries to users etc.

The PECTORAF routine system, elaborated by the research workers of the Department of Economic Cybernetics, is making use of a large volume of information organized on permanent and semipermanent card files. The information from the permanent card files are those related to users, addressee stations, products, refineries and IDPP. The information from the semi-permanent card files are mainly concerning the necessary quantities for each user and are kept only for the interval between two transports of transportation plan.

A picture of the efficiency of the system can be given comparatively. If we take as a reference point the month of February 1970, in which the transport plans were calculated, both manually and electronically, the annual estimated efficiency was of 6.3 million lei saving of costs (in the conditions of optimizing only 6 products and for 2500 users). For the year 1974 the saving of costs is categorically higher, as a result of the fact that the present system optimizes the transportation of 40 products to 4100 beneficiaries.

Another big advantage of the system is the fact that it allows the reduction of a significant volume of work, both in the field of collecting, recording, checking and conveying the data on the information circuit, as well as in the elaboration of the transportation plans.

There is also positive the fact that the transportation operative plans are edited in a fast way by the computer, they do not require a manual intervention and become final documents for the Railway System, the PECO centre and refineries.

The analysis of correlation and regression by help of REMUS routine (Selective Multiple Regression)

At the foundation of the statistical and mathematical modelling of problems I and II lay a system of routines for the processing and interpretation of the experimental data collected from the flux or subsequent to making some planned experiments. The centre element of this system is the REMUS routine for the analysis of the multiple correlation and regression. As this routine can also be used in other problems in which there rises the necessity of processing some data (in petrochemistry or in another field), we present it further.

The theory of correlation provides the research worker with a methodology of searching the interdependence and connection in which there are

found the phenomena of nature, society or economy. The complexity of the investigated phenomena and processes imposes the accurate determination of the evolution equations of these, depending on one or several factors, as well as the necessity of expressing their essence under the form of synthetic indicators. With the help of correlation there can be characterized numerically the form of connection, its intensity and direction, as well as the degree of influence of the various factors. Based on these one can express the tendency of growth or decrease of a resultative variable to the extent of the increase or the decrease of one or several factorial variables.

The multple possibilities of practical application of the theory of correlation in the most diverse fields being well known, within the framework of the laboratories of the Department of Economic Cybernetics there has been created the REMUS routine. It combines the facilities offered by the theory of correlation and the mathematical statistics with those of the electronic computers with a view to penetrating into the essence of phenomena and processes met with in practice.

The REMUS routine has as a main function the establishment of regression equations — linear or nonlinear — of a variable depending on other variables.

This routine, setting out from the series of statistical data of the variables characterizing the phenomenon under study, calculates and inverts the covariance matrix, calculates the possible correlation coefficients (multiple and pairs), the coefficients of regression and other statistical indicators used both in the analysis of factors, as well as for the establishment of the algebrical and transcendental regression surfaces.

Besides the computation of evolution equations and of the stated indicators, the routine allows, on the basis of a combined dispersional analysis, the selection of the most influential variables and the determination of the most significant equations for the levels of significance 10%, 5%, 1% and 0.1%.

Since the REMUS routine is computing for each tested equation the coefficient of correlation, the multiple determination, the deviance and the coefficient of variation, it gives the user the possibility of choosing the most adequate equation.

On the basis of data generator, by very simple orders, the user is able to make alterations on the variables of logarithmical, exponential, reverse, radical nature, reaching up to the editing of diagrams.

To illustrate the particularly high facilities of this routine, we specify, just as an example, that an equation of COBB-DOUGLAS or LOGISTICS type is computed from a set of data by one order only. Moreover, it displays very simple facilities of introducing the data, taking or not taking remarks into computation and inserting of comments.

The multiple possibilities of the routine to determine the linear, polinanial, nonlinear and transcendental regression surfaces have permitted its utilization in various domains by many research workers of the laboratories of the Department of Economic Cybernetics.

Among the most special utilizations we enumerate:

— determination of mathematical modelling for pyrolysis furnace;

— determination of quality constraints at the model of prescriptions for gasoline blends;
— determination of the model of a fractional column;
— determination of the model of a hydrogenation reactor;
— prognosis computations of several phenomena;
— determination of labour norms.

As a result of the possibilities offered by the REMUS routine, an increasing number of productive and research units and central institutions such as CHIMPEX — Constanța, the Department of the Ministry of Agriculture, the Institute for the study of international conjuncture, apply for the utilization of this program.

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MODELES ECONOMIQUES-MATHEMATIQUES D'OPTIMISATION DE CERTAINES ACTIVITES DANS L'INDUSTRIE PETROCHIMIQUE

Les méthodes et les modèles de la cybernétique économique et la technique électronique de calcul, utilisées dans la recherche scientifique applicative dans le domaine de la pétrochimie, ont conduit à des solutions optimales en ce qui concerne les multiples et complexes aspects technico-économiques.

Les auteurs, présentent le modelage du processus de fabrication des oléfines, l'optimisation des mélanges de produits pétroliers, l'optimisation du transport de ces produits ainsi qu'un système de programmes utilisé dans le modelage statistique-mathématique.

On présente les modéles et les systèmes élaborés, ainsi que les résultats obtenus par suite de leur application dans la production.

ЭКОНОМИКО-МАТЕМАТИЧЕСКИЕ МОДЕЛИ ОПТИМИЗАЦИИ ОТДЕЛЬНЫХ ВИДОВ ДЕЯТЕЛЬНОСТИ В НЕФТЕХИМИЧЕСКОЙ ПРОМЫШЛЕННОСТИ

Методы и модели экономической кибернетики и электронная техника расчета, применяемые в прикладных научных исследованиях в области нефтехимической промышленности, привели к изысканию оптимальных решений в отношении многочисленных и сложных технико-экономических аспектов.

В настоящей статье представляются: задача моделирования процесса производства олефинов, задача оптимизации смесей нефтепродуктов, задача оптимизации перевозки нефтепродуктов и система программ, применяемая при статистико-математическом моделировании.

Представляются разработанные модели и системы, а также результаты, полученные при их применении на производстве.

29.5.1974