The Third International Conference "Problems of Cybernetics and Informatics"
September 6-8, 2010, Baku, Azerbaijan. Section #3 "Modeling and Identification"
www.pci2010.science.az/3/11.pdf

METHODS OF CALCULATIVE EXPERIMENT FOR SETTING THE PROBLEMS OF MODELING AND OPTIMIZATION OF CHEMICO-TECHNOLOGICAL PROCESSES

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Acceleration of periods and reduction of sizes of development of new chemical-technological in many promote automation optimal architecture of experimental researches with application of a computer. If first from these interdependent among themselves directions it is coupled to creation on the basis of a computer of loop systems of managements for computerized machining the measuring information and digital control by operation of a pilot unit in real time on teams with a computer [1] application of methods of planning of active experiment is typical of the second direction with use of optimal composition plans [2, 3]. On the basis of these methods in the last years are the series of programs and program complexes have found the application in the calculating experiment [4, 6].

In the present operation results of development of the dialogue system from an application package on optimal methods of design of experiments are given. The system is oriented on its use with a PC and ensures carrying out of the following main operations:

Formation of an initial matrix design of experiments, its expert estimation and handing over on the display screen or immediately in a control system of installation of the information on conditions of its operation; reception quantitative and quality indicators about the propped process appropriate to a delivered set of tests and their machining; a determination of the equations reqrechin models of the process and inspection of its adequacy to experimental data; choice of criterion of optimization and a determination of optimal area of passing of the process.

The designed application package is fulfilled on a modular approach that allows to improve and expand it in lead of new programs.

At the first stage operation of an application package starts with scheduling factor experiment. The User in the conversational mode executes operations on lead in a computer number of factors n, meanings of their zerolevels *Z* and intervals of variation δ z, and also sizes of the cod K, defining desirable of the plan. Depending on the task possibility of formation of a scheduled matrix with a maximum number of factors $n \prec 7$ for complete factor experiment (CPE), fractional factor experiment (FFE), and also central orthogonal composition plan (COCP) and Rota table central composition plan (RCCP) is provided. In the last two cases to a nucleus of the plan sizes of star-shaped shoulders and number of experiments at the centre of the plan (see fig.1) are follow-up defined.

At the second stage of an application package it is applied to machining of the function of the response, the investigated process in the same sequence which has been recommended a computer at their carrying out. When the computer is included in a digital control system by a pilot unit in which chromatographic methods of the analysis of resultants of reaction are used, in an application package the padding handler of the chromatographic information, and quantity indicators of composition of analyzed products, choice and filing in a computer memory of percentage of a unknown quantity a component in the resultants of reaction, perceived in consequent accounts in the capacity of meanings of the function of response of the optimized process is stipulated.

Under injected experimental data in a computer are regressive equation of model of probed with use of one of four handlers; choice of a necessary handler is stipulated by the type of the given plan of carrying out of experiment. For machining results of experiments delivered under plan (CPE), (FFE) or (RCCP)? M1 proqrams, M2, M3, M4 are used accordingly. With their help the evaluation of coefficients of the appropriate equation of regressions is carried out,

the significance of coefficient on a Stewdent test number is mustered and the degree of reproducibility of delivered experiences is evaluated; thus obtained regressive equation with significant coefficients is mustered on adequacy on a Fisher's ratio test. If the obtained equation presents the process inadequately possibility to complete the realized plan up to the composition plan more highly the order is given the user and to realize a padding series of experiment. At acknowledgement of adequacy of model the further data handling by programs of optimization is manufactured with the purpose of a determination of optimal conditions of passing of the probed process.

At a linear aspect of model to a determination of optimal solution are applied a method of steep climbing on response surfaces (L1 program) and a simplex method (L2 program) (see fig.2).

For a determination of best values in a case regressive second-kind equations, are used included in application packages of the program which implement algorithms random search (L5 program), method of coordinate descent (L6 program), a method of movement on canonical surfaces (L4 program), [2, 3, 7]. L3 program intended for search of a maxima not to a linear function n is included in an application package, variable by a gradient method.

The search algorithm on the basis of a gradient method composed in view of limitations:

$$f(\bar{z}) = 0, \quad \bar{z} \cdot \in Q\{z_{i\min} \le \bar{z} \le z_{i\max}, 1 \le i \le n\}, \tag{1}$$

where $\bar{z} = (z_1, z_2, ..., z_n)$ is a vector of controlled parameters [3].

The given algorithm realizes movement to an optimum in a direction of the greatest variation of a function F, i.e. in a direction of a gradient of optimized criterion. In the capacity of an optimization the functional of the following aspect is applied:

$$F = \sum_{i=1}^{n} \left[f_i^{\ni}(\bar{z}) - f_i^{p}(\bar{z}) \right]^2 \tag{2}$$

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The sequence of choice of handlers of experimental data is defined by the structural code. With its help the user creates «a computational chain» called programs. The structural code looks like target number IML where the first dogit points a linear aspect reqressionnoy models, second – one of possible processing methods of datas of active experiment, and the third –one of possible methods of optimization.

The worked out methods have been used for modeling and optimization of the process of oxidative transformation zeolite catalysts.

Calculative complex has a universal character and can be used for numeric and analytic modeling, as well as for automatic management of chemico-technological processes, that makes possible to reduce the volume and duration of the held investigations.

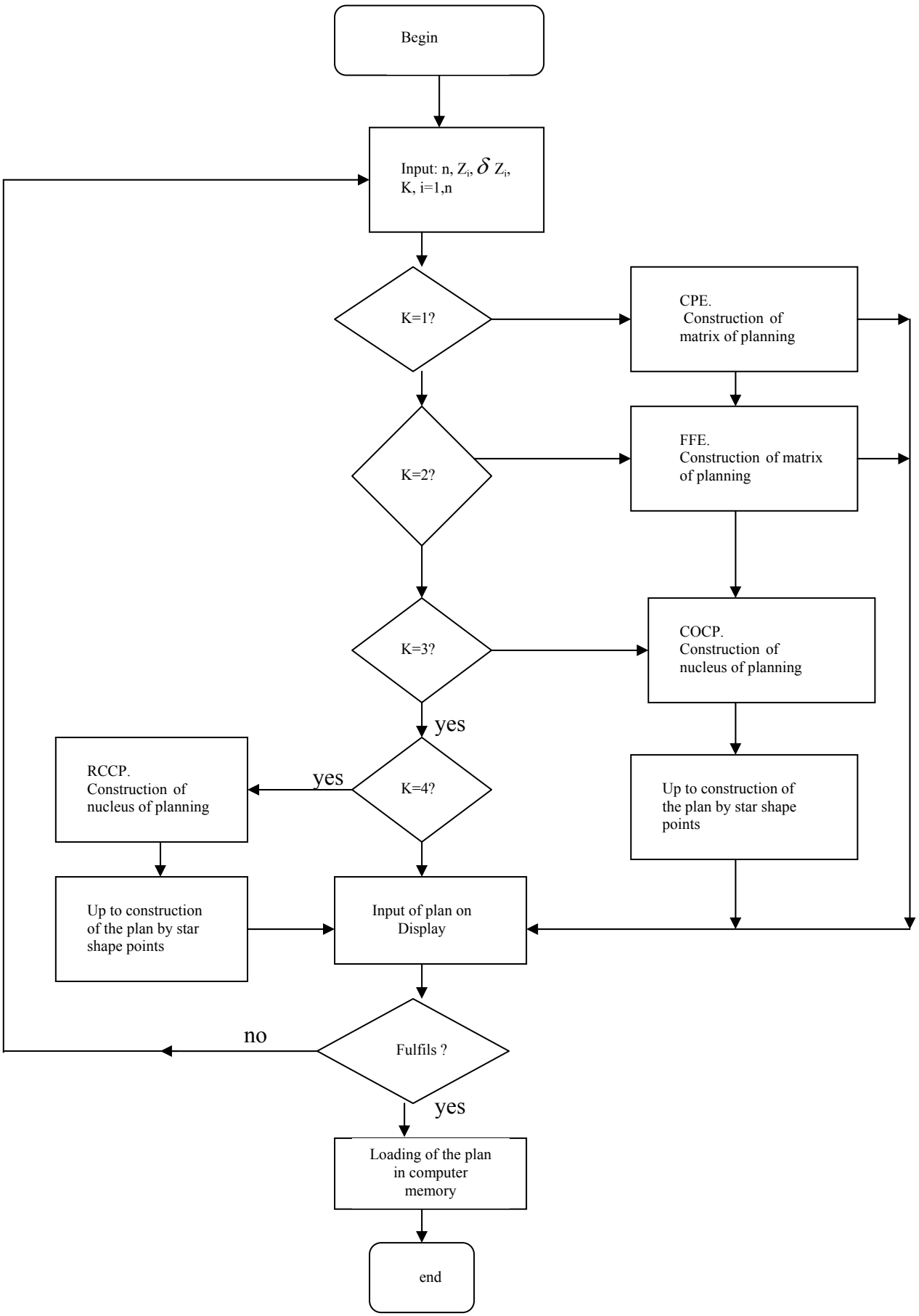
Begin
Input: n, Z_i, δZ_i, K, i=1,n
K=1?
CPE. Construction of matrix of planning
K=2?
FFE. Construction of matrix of planning
K=3?
COCP. Construction of nucleus of planning
yes
K=4?
yes
RCCP. Construction of nucleus of planning
Up to construction of the plan by star shape points
Up to construction of the plan by star shape points
Input of plan on Display
Fulfils ?
no
yes
Loading of the plan in computer memory
end

Fig.1. The block-scheme of the article of the dialogue system at formation on an initial matrix of planning (1 stage);

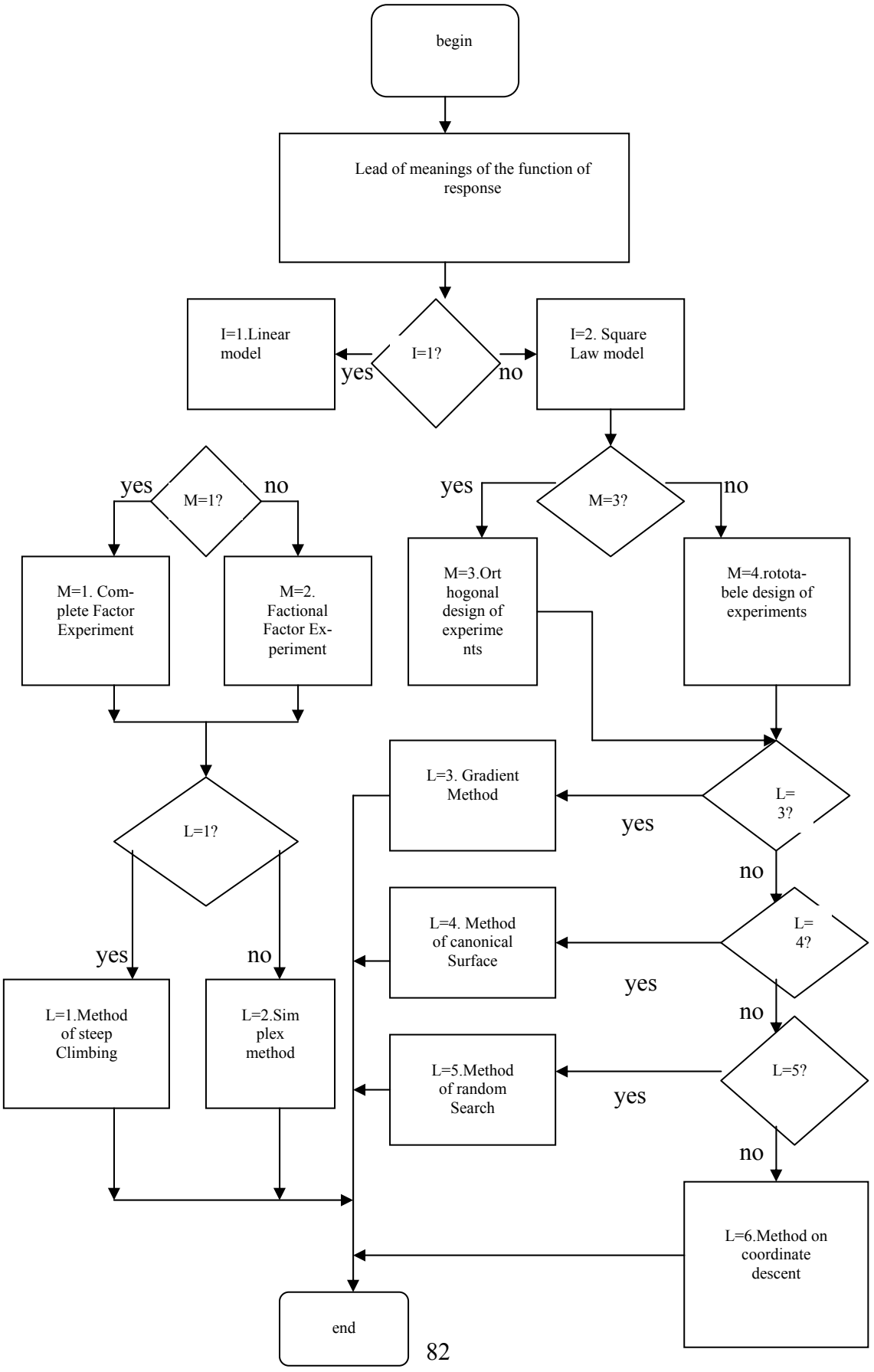

Fig.2. The block-scheme of dialogue system at data processing of an active component (2 stage).

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