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INVENTION TO INNOVATION BRIDGE – HEURISTIC RULES

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1. Introduction

The term of innovation has multiple interpretations and formulations (more than hundred could be found in literature) in scientific interpretation as well as in practical engineering. These are very different depending on functional aspects to which the term is related. Here are few examples of definitions.:

a) in terms of driving force of innovativeness the product, process and diffusion innovations are specified (Schumpeter 1939)

b) in terms of field of application the innovations are classified as horizontal (from field to field) or vertical (from invention to manufacturing), (Jantsch 1967)

c) in terms of market impact the innovations are classified as improvements, incremental innovations, major innovations and break through innovations (Largrish 1972)

d) in terms of location in the field of introduction there are process, product, application and system innovations (Bwonder and Myake 1993) achieved trough core competence, horizontal transfer, competence fusion, and technology fusion as instruments [1].

However, the most practical is consideration of two categories of innovations:

a) intrinsic and

b) extrinsic

Intrinsic innovation is related to product as itself and its application, process, manufacturing system and extrinsic innovation is related to marketing, pricing, sales and all remaining market relations of the product with consumer.

Intrinsic innovation procedures transform the invention (or R&D know-how) into practical manufacturing system . The procedures and their efficiency have decisive influence on competitiveness of the product. The review has shown that only about 5% of inventions (or R&D know-how) are finding the way to the market. It means that investigation of parameters of intrinsic competitiveness are including the bulk of information which leads to the rejection of the majority of invention as not meeting the required market parameters. Only when the intrinsic character of the innovation is tested and confirmed than the extrinsic innovative procedures should be searched to place the product on the market. This logic is leading to the search of parameterization of the innovation as quick as possible after invention has occurred. The mile stones on the way are well known: 1) idea characterized by the newness of the approach to the R&D problem, 2) concept characterized by scientific positive assessment of the idea and 3) R&D and design : a) process functions design b) process structure design c) process valuation

The streamlining of the efforts of the industry towards growth and efficiency depends on the patterns of the innovative process inside the company.

The Council for Chemical Research (CCR) reports that in year 2000 US chemical industry product was of value USD 419 billion, what is 10% of all manufacturing, 2% of GDP and10% of exports . Every USD invested in R&D to-day produces 2 USD of operating income over 6 years showing 17% rate of return after taxes. [1]

Table 1 R&D expenditures of major US companies [2]

Expenditure *\	1990 USD million	1995 USD million	2000 USD million
Capital spending	8,338	8,324	7,958
R&D Chemical companies	3,493	3,079	4,013
R&D Life Science Companies	6,477	12,216	20,766

*\ current USD

Published data are giving some idea in regard the R&D expenditures:[3]

Rohm &Haas is spending 261 USD million intending to increase by 37,2% . The strategy is „the lab is a place to validate commercial advances and not a just place to make a discovery research.” (D.C. Bonner)

Dow Chemicals is confining 75% of R&D expenditures for new products in existing applications. For that purpose uses molecular modeling, combinatorial chemistry etc. Particular efficiency has been reproted by Cabot Co. whereabout is dropping about 80% of ideas (inventions) pursuing 20% for commercialization and 14% are winners three times more efficient than industry average.

Lehman Brothers companies are keeping their % of R& D expenditures in relation to sales but previously 2/3 went for process improvement and now 2/3 is going to break-through ideas for new products.

The world top 30 chemical companies expenditures in 1999 were 15,9 USD billion denoting growth 3% over previous year giving the 5,2% over the sales and 15,000 USD per employee. The portfolio of R&D intensive companies has grown quicker than twice in relation to FTSE between 1994-1999 [4].

Table N2 New products as related to the R&D effort [5]

Industry	Total R&D expenditures as % of sales	Percentage of total annual sales represented by new and improved products commercialized within past five years
Wood, paper and allied products	1,3	13
Industrial inorganic materials	3,7	20
Plastic materials and synthetics	4,4	18
Drugs and pharmaceuticals	11,2	25
Soap, cleaners and toiletries	3,4	28
Industrial organic chemicals	3,1	10
Agricultural chemicals	9,1	23

Miscellaneous chemical products	5,1	12
Median	2,8	23

Table N 3 .Europe, Japan in USA in research [6]

Comparative parameter	Europe	USA	Japan
Number of researchers per thousand of inhabitants	4,7	7,4	8,0
Share of publications % 1993	32	36	8
Total R&D spending Euro mln 1994.	121 882	142 047	104 009
Total R&D a % of GDP 1995	1,91	2,45	2,95
Expenditures per capita Euro 1994	329	545	833
Number of researchers 1993	774 071	962 700	526 501
Patents 1995-1996	40 069 -informatics 19,5% -biotechnology 29,7 -farmacology 25,8%	109 646 -informatics 67,4% -biotechnology 57,1% -farmacology 59,8%	215 100

2. Macroeconomic aspects of the innovative process

The shortly presented above data show importance of the innovation in modern economy. Observation of the research development and its direction orientation to the technology development and quick industrial application and amount of financial resources invested in the technology development show that there is some relation between the information value and growth parameters. This is interesting to remark that technology as a soft component of the industrial development is created by the information stock expansion. The development of technology requires respective projections of the future market demand; it means there is need to understand what would be necessary for further social and economic development: new pharmaceuticals and new methods of communication allowing increase of the economic efficiency. This view or projection is not created by labor or capital in classic sense. This is created in the human brain by the logic analysis and evaluation of numerous options. Obviously not always the selection is adequate to the trend of development, but in macroeconomic terms it is the fuel for successes. Other element of the research is the search for new application of existing products, of the new products and of the new methods of production. This is made again by the human brain and respective instrumentation of research. However, even the most advanced and sophisticated instrumentation could not ensure the successful invention that is again the information parameter. This parameter has been present always in the development process as a condition of use of capital and labor. However, its influence has been distributed over much longer period of time and therefore it was difficult to observe its influence on the basis of statistical research which were always the basis for the economy parametrization and obviously accuracy of these observation is limited.

Therefore considering these remarks as the initial observation requiring the proof accordingly to the mathematical instrumentation of the problem the hypothesis is proposed that the growth equation should be expanded by the third parameter: information. The classic Cobb-Douglas equation relating the production to the labor and capital, later improved by numerous researchers e.g Solow [4] or Johnson [5] reviewed by Stoleru [6] by introduction so called technical progress coefficient into original Cobb-Douglas equation could not be fully proved statistically and at present time it is less chance to prove them now. It must be also observed that previously large influence of the labour in the equation is not more valid. The growing labor productivity and continuous relative decrease of labor forces should be a reason to review of its mathematical format in the production equation. Therefore continuing the research based on the classic econometric theory the information element should be introduced as a crucial factor of growth, exchanging the place in Solow equation with labor. Than the equation in its simplest form may look like:

$$Y= L_o e^{bt} I^{1-a} K^{a}$$

where: L_o - initial labor component of the production function

b - coefficient of the dynamics of the labor productivity

t - time considered for review

I - information parameter of the production function

K - capital parameter of the production function

a - transformation coefficient of value 0-1

The transformation of the equation to the format allowing statistical evaluation requires advanced mathematical treatment and development of new methods.

However, at the moment it is not important to produce elegant equation but to identify in which way the information would value, it means which parameter may be considered as engine of development. In other words what is a value of new technology. The possibilities of evaluation are very limited:

a) one possibility is to consider the expenditures of the country (government and industry) to the R&D. This would be passive parameter because spending does not mean positive results. But consideration in further analysis could not omit this factor. It must be observed also that to this parameter the expenditures of purchasing new technology by country should be included. Many countries (like Japan during last 50 years) preferred to purchase new technology and later develop it omitting the basic research expenditures and many of costs of defining the future demand (from the physical point of view). This could be statistically collected and introduced into equation.

Taking into consideration established fact that in chemical industry the new technologies or their improvements are pushing the change of the products in the 20 years it may be expected that this parameter would show influence in the equation when statistics would be tested.

b) the other possibility is to evaluate this parameter from the stock exchange values. Assuming the standard ratio for average economy for the parameters like profits over sales or over the capital invested (it means the old economy) it could be calculated how much of stock exchange value of the company or how much profits originate from the technology impact. The ratio of two equations(one without technology and other with it) would give us non dimensional parameter of the influence of information on the growth. Obviously into primary equation some information parameter i(o) must be introduced and its level could be assumed that capital and labor without information does not bring the growth. Obviously this is only artificial assumption to allow better comparison but not necessary reflection the old economy development process. The difficulty of this approach is a fact that stock exchange value and all derivative parameters are changeable and even in the very short term but is one would consider the trend for adequate number of companies the statistical result could be satisfactory.

c) the third possibility is to evaluate the information impact by the cost of all operational technologies. This could be made by the standard (however not accepted universally methods) by the profitability of the process operated. It must be stressed that under process we understand not only production in classic sense but also the services provided by the different processes. This is almost a must in communication area of activities.

The collection of information in this regard is the most difficult because the prices fluctuations are changing very often the real picture of technology value and this prices are not only reflecting value for the society of the product or service but also the competition in the field and possibility to establish the prices not accordingly to the microeconomics principles (budgets), lowering the prices often under not only profitability level but also under the operation cost *(excluding depreciation from the cost).

3. Definition of area of interest

The impact of the innovative process on the world economy is changing and at present new features and its patterns are observed. The globalization of the chemical market is introducing new challenges to the R&D process in particular in Europe [7]:

1) research should be viewed in the world context

2) cost of research with 5% of yield is beyond the means of majority of individual small/medium companies

3) the practical exploitation of results requires large scale investments and enormous marketing efforts.

The main R&D problem facing Europe life-science companies is lack of „incubator” companies capable of developing good research ideas and bridging the gap between the research and commercialization..

At present in the R&D procedures two specific features are observed:

1) Application of the modern instruments of screening of the product (e.g. new catalysts). The results of research using these instruments allow identification of the promising molecule and furthermore the possible ways of its synthesis. Very often well established methods of molecule identification now are used in planning new catalysts. Above that new instruments belonging to wide range of the molecular modeling as well as combinatorial chemistry are implemented to speed up R&D process and increase the number of successful programs.

2) However, the sequence of the process units must be established and their capacity calculated. Here the Computer Aided Design is widely used. The unit processes design based on chemical engineering science is a key to evaluation of the technological process starting from early 30-ties of XX century. However, this was not an answer to the design of efficient technological units and recently after the early 50-ties the concept of the process engineering expanding the ideas of the chemical engineering has been introduced to the research and practice of design. The difference was obvious: the process engineering has been searching for the optimum of the structural and functional properties of the technological unit but chemical engineering was aiming optimization of the process units irrelevant of further relations.

Starting form early 70-ties the sophisticated computerized programs developing the idea of the technological systems synthesis later called 'flowsheeting' have been developed [8].

At early stages they were basing on chemical engineering of the process units modules and by trial and error composed into technological unit. The specific deficiency of this approach is need for multiple approximations in case of one or more recycling flows. Parallel to this approach the equation – oriented process simulation has been researched.

The basic difference from previous approach was the dynamic simulation of the unified networks of the process units basing on linearization of equations as well as including the extended mathematical Newtonian or quasi-Newtonian (gradient based) methods of optimization search. Both approaches at that time were limited to the computer capacities (memory and speed) therefore it is no wonder that they are very much compatible presently and much more useful than in early 80-ties.

The general deficiency of all approaches and inaccuracy of gradient estimate is leading to the conclusion that only investigation of all variations of potential solutions (giving results in the frames of initial data and functions) is not possible. Even to-day when computation capability is exponentially higher than in early 80-ties this is not feasible considering need for step by step search for efficiency at different stages of R&D process.

Table N 4 Number of the theoretical functional equivalent structures in the case of

heat exchange system [9]

Number of warm and cool flows	Number of theoretical structures
4	$4x\ 10^{3}$
5	$3x\ 10^{6}$
6	10^{11}
7	10^{18}

Table N 5 Number of the theoretical functional equivalent structures in case of

distillation columns system [9]

Number of components	Number of theoretical structures
2	1
3	2
4	5
5	14
8	429
10	4862
15	2 674 440

Therefore, the new R&D instruments are not excluding the structuralization of the process and evaluation of the potential structure or structures. Again, either very expensive evaluation instruments would be applied or stepwise application of heuristic rules.

3) Domination of the biochemistry research orientation. From 573,469 abstracts denoted worldwide in the year 2000, 42% were oriented toward biochemistry, only 20% to applied research, and 26% to other chemistry orientations. From over 42,000 patents assigned in year 2000 in USA the more than 8,000 were oriented toward the biotechnology. The most advanced part of the biochemistry and biotechnology is the genetic engineering. The R&D in a typical biotechnology process using fermentation or similar reproduction processes is subdued to similar instrumentation tests as well as evaluation procedures. The genetic engineering is based mainly on the process of introduction of specific gene into cell of other species. At present it is difficult to speak about heuristic rules in this area of research, due to the confidential character of the R&D methodology, however use of the specific viruses seams to be dominating as way to break the cell barrier. This are requires further research in assessment of the R&D instrumentation.

The problem posed at this forum is the way to the innovation. Obviously the starting point to innovation is as defined above the invention covered by patent or by the specific know-how.

a) Invention as a part of innovative product or process.

Requirement to obtain patent is to prove the efficiency of the new process solution either usefulness of the product or its substitutive character. However, the invention very rare covers the whole process or the further processing needs or costly components of the product may deplete integrity of the product, therefore efficiency of the invention. This means that after invention will be accepted for inclusion into company R&D program it is necessary to find out the answer to the complete efficiency of the new product or process and control it during the whole life of the project.

Here starts the problem of efficient instruments of economic evaluation of the new product or process and sequence of respective R&D steps (pilot plant, basic engineering, market active research etc.) before the investment decision. These instruments may be based on very costly procedures or using to the certain step of the project advancement empirical, heuristic rules. These rules are oriented towards selection of the sequence of process units providing the information allowing assessing the process or product conditions of acceptance by the market and will be discussed later.

b) Procedure of transformation of the invention into innovation

The transformation of inventions into innovative product or process as stated above is an activity of very low yield. Accordingly to the different research sources maximum 5% of the inventions find the way to the market. It means that it is impossible to carry out R&D process through all stages of development process (from idea to the product/process) for all inventions available. Therefore, every R&D institution (decision making body) must have a screening system allowing at certain stages of the R&D process to abandon part of research goal which is not meeting the established criteria. The screening system has to be established in specific way ensuring equal judgment of the results. Companies at large have their own evaluation system, some are subcontracting this task to a specialized companies under specific terms of agreement. Whatever are the modalities of evaluation they must be based on similar or even exactly same level of information as well as using similar evaluation instruments. In practice the following elements of screening system are considered obligatory :

a) Technological flowsheet characterized by parameters of consumption of all inputs and algorithm of transformation of these inputs into uniform value

b) Estimate of structural elements cost and algorithm of transformation of this costs into investment cost

c) Select the integrated system of evaluation and evaluate results in strictly comparative modality

d) Control evaluation of the exogamic elements of the system through statistical analysis or prognostic statement

Mentioned above shows that at majority of the research periods the design problem is a fuzzy problem, considering that average chemical process is defined by dozens of thousands of variables, constraints and parameters estimated with different accuracy (at the beginning very low and growing only after expensive research efforts e.g. after establishment of the pilot plant) established by technology itself as well as by the potential technical applicability.

The fascination of the growing capacity of computers as well as availability of more and more sophisticated (but less controlled) software in many cases is acting against the possibility of choosing the optimum design for innovation (innovative process).

The some of deficiencies are as follows:

- the different approach to the periodic and continuous processes
- the number of options surpass the acceptable evaluation costs
- the doubtful origin of the dynamic functions of the variables or parameters
- the differences between the results of functions parametrization and available structure
- the non-uniform approach to the valuation at different stages of R&D process

The design theory and practice of engineering rules application allows to diminish the impact of the deficiencies and provide the instruments for transformation of the invention into innovative process.

4. Elements of the design theory applied to the processing industry

5.1 Problem identification.

Transformation of flows depend on structural properties of the elements belonging to the system and in general is defined by the Cartesian equation:

$$E= R*P$$

Where: E – Cartesian multiple

R – set of relations r (i) e R between elements valorized in binary system (yes, no)

P - set of transformations p(i) e P specific for each element of system which

is function applied in the format of the continuous class C(n).

Relations are components of the set of elements and are belonging to the real numbers system and transformations are defined by element properties and belong also to the real numbers system.

G

(i) G (i)

F(Xo, Yo,...Zo) F (Xk, Yk,...Zk)

Fig. 1 Model of the flow system

Each of elementary structural units has defined functional properties which are transforming flow G(i) variables from the values F (Xo,Yo,…….Zo) to the F (Xi,Yi,…….Zi)

$$P(i)= ?\ (F)$$

where X, Y, Z are parameters or variables defining properties of the flow before and after transformation in element "e (i)" and „p (i)" is a functional of transformation. Functional p(i) is time dependent and related to the intensity of the flow g(i). The functional p(i) has negentropic character; therefore change of each of variables requires exogamic input of information, mass and energy.

4.2 Process functions

In chemical processes technology there are only several functions performed over the flow:

1) Mixing or separation of the flows or their components

2) Reaction of the flows or their components

3) Change of the potential of the flows or their components to achieve parameters required by previous functions

4) Change of the size of the composition

5) Linking functions like transportation or storage

However, the modality of the function transformation is very differentiated and depends on properties of transformation element and potential to operate on the functional properties over the flow is a specific feature of each elementary unit and is defined by its function of structural parameters f (Mi,Ni,Oi….Qi). although, the limited number of functions does not determine limited options of technological structures.

4.3 Structure of functions

Functional and structural properties of the structural element are defined in the separate systems of valorization.

There are two classes of the structural units:

a) Of stationary structural function properties

$$f\ (Mi,Ni,Oi,...Qi)=\ G\ (const).$$

Those are represented by all man-made operational systems i.a. material transformation systems

b) Of expanding (developing) structural function properties

Those are represented by dynamic structures being in the process of development as a result of aimed human activity e.g. construction or erection (structure established by other structure to achieve final structural and functional properties).

$$f\ (Mi,Ni,Oi,Ni,\ldots.Qi)= G(t)$$

To this class of structural units belong also self-developing structures like living species and artificial intelligence species.

Establishment of the structural unit is also negentropic process requiring exogamic information, mass and energy to ensure its transformation properties.

The design problem of the stationary structure is to establish relations between the structural units of required properties ensuring the achievement the potential p(i) of each element and P of the whole system.

$$G > P \text{ or } G = P$$

However, there are a large number of structures fulfilling this equation.

This is a result of possibility to achieve required level of the functional properties by different structural units as well by different relations between structural elements.   Therefore, there must be used as a goal function another variable exogamic to both functional and structural properties and valorized in uniform parameter allowing use of additive algorithms for structural and functional flows of information, mass and energy.

This goal function has to fulfill the function of efficiency either being the difference between the values of inputs of information, mass, energy, structural charges and value of the final output flow or only sum of values of inputs. In the first case the design problem is solved at maximum of this function and in latter case at its minimum.

However, achievement of the required maximum or minimum (which is presented in literature as an optimum solution) for goal functions is hardly to be achieved from several reasons:

1) The properties determining functions of parameters and variables in each elementary unit are result of approximation function with variations of several to a dozen of percents.

2) The structural properties are not continuous functions and must meet the limits of standardization

3) The number of structural options potentially feasible from the relations point of view is very large and is growing exponentially in relation to the number of components of the flow, therefore testing of all options becomes cumbersome and inefficient.

4) The final valuation parameter (monetary units) are fluctuating from two main fully exogamic to the designed system reasons:

- the monetary policy of the dominating currency.

- the demand/supply balance of the inputs and outputs related to the designed structure and related to this balance unit value of inputs and output.

Therefore, to transform invention into innovation, in particular at early stages of the product/process development above the developed sophisticated instruments of evaluation requiring large scale set of information and expensive instrumentation some specific instruments are necessary to ensure competitiveness and timely exposure of the product to the market.

Those are heuristic rules of design.

5.Patterns of the heuristic rules at different stages of the innovative process

5.1 Evaluation at early stage of development process

The goals at this stage are:

- increase the statistical value of the success from 5% to higher value

- decrease the time of implementation from 10 years to shorter time

This stage of evaluation is one of the most difficult and responsible from the point of view of the efficiency of the R&D process. The basic necessary information originating from R&D and exogenic sources (market assessment) assuming that there are not enough data to prepare basic engineering is as follows:

- yield of the product

- price of the raw material

- expected price of the product

- statistical data on investment cost

- company cost structure

There is a few information available in regard of large scale companies test values. DuPont is focusing on the businesses promising growth more than 6% per year and giving the more than 20% of the return, however is not specified if those limit are related to the full investment costs of only R&D costs.

The evaluation is often made by the results obtained by the company in a macroeconomic terms. The Bank of America has parameters of evaluation of the specialty chemicals companies:

Table N 6 Limiting parameters of innovative process continuation [12]

Parameter	Advanced company	Average company
R&D expenditures in relation to sales	7%	4%
R&D expenditures in relation to profit	14%	9%
% of the sales from products introduced in the last five years	35%	25%
Volume growth in relation to GDP growth	2,5	1,8

If this is transformed into values e.g. for Degussa company which has business in specialty chemicals about USD 8 billion, that shows importance of the needs for proper evaluation of the R&D programs.

The positive results of the test are allowing further consideration of the process implementation and continuation of the R&D as well as basic engineering preparation. Here one remark is necessary. It was a tradition to carry out laboratory research (even pilot plant research) without participation of the design and evaluation group. The result of this artificial division of innovative process between the research and design is very painful. Because the industrial installation is not a direct reproduction of the laboratory structure or even pilot plant the results of the research must be adjusted to the design questionnaires and when the stages are separated new research time and effort is necessary.

Whatever were the costs of the laboratory research the next step which is basic engineering preparation is exponentially more expensive, because in many cases laboratory research does not have possibility to consider some specific issues of the process e.g. the recycles.

Table N7 Evaluation of early stage of innovation implementation [11]

Parameter/variable	Origin of the assessed value	Assessed value limits	Decision
Yield of the product	R&D best performance	Less than 40%	Secondary priority
Value of the raw material in the product price	Market trend evaluation	0ver 70%	Abandon proposed process
Expected price of the product	Statistics of the average price of the product group	Less than 130% of the raw materials cost	Abandon proposed process
Investment cost	Statistics of the average unit investment cost in the group of products	Depreciation over 30% of the product price	Abandon proposed process
Overhead costs	Company statistical data	Over the 30% of the product price	Abandon proposed process

Few words of explanation should be given in regard of the mentioned groups pricing /costing.

The idea behind the statistical evaluation of the future price of invented product is based on the supposition that specific groups of the products have a market limit price. This is specifically true in case of direct substitution, however in case of completely new product has also validity. The price could not be exaggerate higher over the group price because on the real market competition will propose existing or new product as a substitute e.g. in group of engineering plastics. This is also true for completely new products in pharmaceutical industry e.g. Viagra has been substituted in less than 18 months because of very high price.

Whatever were the costs of the laboratory research the next step which is basic engineering preparation is exponentially more expensive, because in many cases laboratory research does not have possibility to consider some specific issues of the process e.g. the recycles.

5.2 Process structure establishment

5.2.1 Continuous versus periodic

Mentioned above shows that at majority of the research periods the design problem is a fuzzy problem, considering that average chemical process is defined by dozens of thousands of variables, constraints and parameters estimated with different accuracy (at the beginning very low and growing only after expensive research efforts e.g. after establishment of the pilot plant).

Before starting screening process some basics must be established through first steps of R&D process (after invention occurred):

a) reaction (or reactions sequence) its parameters (kinetic and thermodynamic) and yields

b) components of the inputs and outputs and their basic properties.

The screening of the processes are made several times during the innovative process, and at the very beginning two crucial design problems have to be decided:

1) the modality of the process implementation: periodic or continuous system

2) the capacity of the designed process

3) the reaction system (isothermic, adiabatic reactors)

Neither chemical engineering, nor any computerized system could not provide answer to this questions. Here we have first time to look after heuristic rules of decision making in process engineering.

Table N8 The heuristic preferences of the process modality [11]

Preference	Mono product capacity	Multipurpose capacity
Periodic	450 t/year	1500 t/year
Continuous	>4500 t/year	>15000 t/year
No preference	450-4500 t/year	1500-15000 t/year

As concerns the capacity of the design usual heuristic rule is to start with maximum feasible capacity. There are many reasons for this decision but the most important are as follows:

- the minimum limit of depreciation will be established
- the design will consider by-products and environmentally dangerous substances processing
- the maximum size of one line production will be established
- the possibility of the process transformation into periodic at lower capacity would be possible to analyze
- the operational time will be established

More than one thousand processes is described in detailed form available in the literature or could be provided by consulting companies. Establishing the sequence of the process units it is necessary to investigate the existing processes. The tested by practice at the large scale the unit processes sequence could be useful indication to resolve new process and implement innovation into operational stage.

The preliminary selection of the reaction system and capacity allows the heuristic evaluation of the invention for purpose of further research or abandoning the project.

5.2.2 Heuristic rules at the functions selection [10]

Before entering the discussion of the relations between algorithms of design and heuristic rules (concepts) of design the following considerations have to be taken into account:

a) The advanced chemistry using specialized computerized systems in many cases could design molecule with desired properties as well as reactions sequence of the total synthesis. The discussed below process design system is not related to the design of molecules but processes of their production.

b) The exogamic matters like market of the product, its application, potential substitution as well as marketing instruments introducing product to the market are not a part of the process design system

Design theory which elements have been discussed in Annex I could be applied to any system of relations between the elements of specific actions changing the parameters of flow. In our case we are interested in the area of the chemistry and process of transformation of the invention in pure chemistry into innovative technological process. To analyze the option of application of the heuristic rules to the design of the processing function P it is necessary to define the elements of the system. For purpose of this exercise we are considering the following definitions:

c) The technological process is a set of processing elements interconnected by the specific relations between

them (sequential, parallel, etc). The final output of the technological process is well defined product.

d) The processing unit is a structural unit having the isogamic properties f (Mi, Ni, Oi,…Pi) originating from

the possession of the processing elements ability to change the properties of the flow from the level p(o) to p(i). The output from process units is a defined flow g(i) characterized by specific combination of parameters F (Xi, Yi, ….Zi).

e) The processing element is a physical component allowing establishment of the processing unit. The output

of the processing element is specific property of structural element Mi, Ni….Oi.

The number of functions is limited and their chain defines the process. Functions represent the thermodynamically defined potential of the process at every step of transformation. Further selection of the structure for each function defines the operation capability of the process.

The functions of the process unit and direction of changes through the process are given in the following table.

Table N9 Chemical engineering process functions

Function	Direction of change	Direction of change
Energy level Temperature	Increase	Decrease
Energy level Pressure	Increase	Decrease
Reaction	Synthesis	Decomposition
Composition	Mixing	Separation
Sizing	Reduction	Enlargement
Linking functions	Transportation	Storage

When the new process or product is developed than the result of invention is possibly reaction defined by inputs as well as the thermodynamically parameters. At this stage of research the sequence of functions must be determined to provide information on unresolved process problems. Obviously it does not exist an algorithm for selection of sequence of functions and stochastic search is also not applicable. Therefore it remains only rationale approach derivative of the empirical, heuristic knowledge.

The algorithms of the calculation of the size of the structure of each process unit are well known and permanently improved to reach optimum values. However, the standardization process as well as the possibility of the establishment operational unit requires always the adoption of the heuristic rules.

Table N 10 Examples of models for process functions and structures

Process function	Process Unit	Model of function estimate f(X,Y,...Z)	Model of structure estimate ρ (M.,N,...O,)
Reaction	Isothermic plug flow reactor	$(G/\gamma) \ln (1-x_a)/k$	$(n \pi D^2 L)/4$
Intensification of the flow	Heat exchanger	$G c_p (t_k - t_o)$	n €π D L ΔT k
Separation of mix	Distillation column	{4L (R+1)}{f(R+1)N}/π γ w	πD^2 , H

Obviously the models given in the table are simplified only for illustration purpose.

The design problem of the technological unit is divided into two stages:

- process synthesis
- process units adjustment

The goal of the process synthesis is to establish sequence of process units performing functions over the flow from input values F (Xo,Yo,…..Zo) to output values F (Xk,Yk,….Zk).

The goal of the process units adjustment is to select process units fulfilling conditions established F (Xi,Yi,…Zi) by the process synthesis but using the f(Mi, Ni,….Oi) effectively available in the shopping list.

The first stage of the process development is establishment of the sequence of functions. At the early stage of process development very limited information is available to assess the risk of further research. Here the heuristic rules are very helpful in avoiding expensive modalities of the process evaluation. As mentioned before the process is composed from the functional process units. Every process unit represents specific function and may be implemented in multiple structures.

The next stage is to establish structure of the functional process units

The algorithms of the calculation of the size of the structure of each process unit are well known and permanently improved to reach optimum values. However, the standardization process as well as the possibility of the establishment operational unit requires always the adoption of the heuristic rules.

The initial heuristic step to the establishment of the technological process is to select the sequence of functions. The standard structure is the first assumption:

SàTPAàRàTPAàVSSàSàLSSàSàSSSàTPAàS

where:

S   - storage

TPA - temperature, pressure adjustment

R   - reaction

VSS - vapor (gas) fractions separation

LSS - liquid fractions separation

SSS - solid fractions separation

This structure is statistically dominating in the chemical industry. Obviously the thermodynamic and kinetic parameters of the reaction are established by calculations and experiment as basis of invention.

1) TPA process units selection

Table N 11 Process units at the entrance to the reactor

TPA	Temperature adjustment	Pressure adjustment
Process units	Heat exchangers	Compressors, pumps

The functional size of the process units is calculated by the any of available CAD system.

The functional size is not yet implementable due to the lack of number of data and is later corrected at the structural size determination.

2) Reactor selection

From the point of view of the thermodynamics two options of reactors are available:

Isothermal reactor (IR)

Adiabatic reactor (AR)

From the point of view of kinetics other two options are available:

Plug Flow Reactor- PFR

Continuous Stirred Tank Reactor - CSTR

The selection is not obvious and depends on many specific modalities of the reaction, however the primery rules are allowing to omit not desirable solutions.

Table N 12 Selection of the type of reactor

Reaction	Heat load MJ/h	Reactor isothermal	Reactor adiabatic *\
Exothermic	6,3 - 8,4	PF	PF
Endothermic	6,3 - 8,4	PF	CSTR or CSTR+ PF
Exothermic	>8,4 MJ/h	Not applicable	PF **\
Endothermic	< 6,3 MJ/h	CSTR	PF with heat carrier

*\ at DT between the entrance and outlet <15%

**\ with limited conversion

Regeneration of the catalyst can be made periodically or in continuous reactor-regenerator system where catalyst in adiabatic reactor is playing role of the heat carrier.

The selection of the type of reactor allows the functional size calculation by CAD system.

3) Flows stabilization

The flows through the reactor system are defining the size of the plant which could be much larger then its capacity. That depends on the volume of the recycle of the raw material.

Table N 13 Recycling principles

Conversion	Yield	Flow system
High	High	One-through
High	Low	Change the catalyst or parameters
Low	High	Recycle
Low	Low	Recycle or change the catalyst or parameters

The case High/Low is producing substantial quantities of by-products increasing the size of basic installation as well as make longer the basic functional sequence of the process units.

The case Low/Low is increasing size of installation in case of recycle and also expanding the functional sequence of the technological process.

4) Separation and purification of the products

The next TPA depends on the composition of the outlets from the reactor and general parameters of the reaction. Therefore below are given selections of the separation processes in order of structural enlargement.

Table N14 Order of selection of separation processes

Products	G	L/G	L	S/L
Unit processes	Transformation into liquid Absorption Adsorption PSA Other	Flash Absorption Adsorption	Flash Evaporation Distillation Extraction Azeotropic distillation Extractive distillation	Crystallization Filtration Drying Leaching Sublimation

Products of reaction: G- gaseous, L/G -liquid/gaseous, L-liquid, SL- solid/liquid

The sequence of search to select process units after reactor are related to the phase status of the products.

In case of gaseous products we apply the VSS steps;

a) cooling to the 35oC

b) pressurizing to the 0,5 MPa with cooling

c) flash separation

d) deep cooling (propylene condense)

In principle in all cases the L/G mixtures are obtained from which gaseous fraction is further treated by absorption or adsorption at the condition that it contains no more than 5% of liquids

The separation of the light components from the liquid phase may be organized in specific process unit of distillation character but specifically organizing the flows of light components. Those options are;

a) partial condensation

b) pasteurization

c) stabilizing

The typical and most common process of liquids separation is the distillation. The condition of applying distillation as a separation method is the value of relative volatility $a_1/a_2 > 1{,}1$.

The number of optional distillation schemes is growing exponentially in regard to the number of components and sequential calculations of the mixtures over four are not practical and heuristic methods are applied with very small difference from feasible optimum.

In case of higher number of components the following rules are applied [13]:

a) select the sequence in order of decreasing volatility

b) select the sequence where components' flows are equal

c) as key components select the neighbor relative volatility

d) preference is given to the high level of separation accuracy

e) the most difficult separation should remain last

In practice about 40 rules are applied in logical sequence eliminating the costly schemes.

They are divided in four groups of rules:

A) Related to the composition of the mixture (concentrations of components0

B) Related to the separation parameters e.g. relative volatility

C) Related to the process conditions (design modalities)

D) Related to the system operation parameters (e.g. recycles)

Below is given example of application of heuristic rules in case of six components (42 theoretical options) [14]

The six components of the following mixture are to be distilled:

Table N 15 Mixture to be separated by distillation

Component	Flow kmol/h	Relative volatility

		a
A	9,1	
B	6,8	a_{AB} = 3,5
C	9,1	a_{BC} = 1,2
D	6,8	a_{CD}. = 2,7
E	6,8	a_{DE} = 1,21
F	6,8	a_{EF} = 3,00

The distillation structures selected accordingly to the heuristic rules are as follows;

Table N 16 Optional distillation schemes

Structure	Column 1	Column 2	Column3	Column 4	Column5	Relative cost
Rule (a)	A/BCDEF	B/CDEF	C/DEF	D/EF	E/F	136,7 %
Rule (e)	A/BCDEF	BCDE/F	BC/DE	B/C	D/E	113,84 %
Rule (b) and (e)	ABC/DEF	A/BC	B/C	DE/F	D/E	106,36 %
Optimal scheme	ABC/DEF	A/BC	B/C	D/EF	E/F	100,00%

Other separation systems

When distillation is not feasible or not possible there is a sequence of other L/L separation processes:

a) extraction solving one of components

b) azeotropic distillation introducing the third component to impose deviation (negative or positive) from the Raoult's law.

c) extractive distillation to alter relative volatility of the components

These systems have always a deficiency by introduction of the third component which must be separated in additional separation system.

5..2.3 Heuristic rules at the structure selection

The functional structure of the chemical process is not yet giving the possibility to make evaluation of its profitability after all necessary research has been carried out and process scheme has been designed.

In many countries there exists standards of the process elements entering the structure of the process unit and in all cases the machinery industry has their own prescriptions included in the catalogues of company.

Below are given tables of the most common parameters of the process elements.

a) intermediary vessels (about 20 parameters)

Table N 17 Structural parameters of the intermediary vessels

Parameter	Value
L/D	2,5 - 5
Holdup	60 min at 90% of volume
Thickness of wall 2MPa	9 mm

All parameters are later calculated accordingly to the engineering standards

b) columns (about 30 parameters)

Table N 18 Structural parameters of the columns

Parameter	Value
Maximum height	50m.
L/D	20-30
Thickness of the wall P.=0,12MPa	8 mm
Height of column	3-5 m. over the plates/filling
Plates used at the diameter	over 1m.

All parameters are later calculated accordingly to the engineering standards

c) continuous stirred tank reactors (about 15 parameters)

Table N 19 Structural parameters of the stirred tanks

Parameter	Value
H/D	1,0-1,5
Power requirement	0,3 kW/m3
Power requirement with internal heating/cooling	1kW/m3
Power requirement with reaction	2 kW/m3

CSTR cascade of 5	Equivalent to PF reactor
Diameter of the propeller	0,3 D

All parameters are later calculated accordingly to the engineering standards

d) heat exchangers - tube -shell (about 40 parameters)

Table N 20 Structural parameters of the heat exchangers

Parameter	Value
Condensing components	Shell side
Linear speed of component in tubes	Higher
Length of the tube	Max. 6 m. (stepwise every 0,5 m.)
Tube diameter	15 mm stepwise every 5 mm
Tube distribution	Hexagonal with t=26-32 mm
Maximum HE surface (mounted)	4650 m2
Maximum HE surface (dismounted)	920 m2

All parameters are later calculated accordingly to the engineering standards

For purpose of preliminary evaluation of the heat exchanger surface the following heat transfer coefficients could be used:

Table N 21 Assumed heat transfer coefficients

Cooled component	Heated component	K [W/m2 oK
Water	Water	1420-2480
Water solutions	Water solutions	1420-2480
Light organic	Light organic	230-430
Medium organic	Medium organic	110-340
Heavy organic	Heavy organic	60-230
Light organic	Heavy organic	170-340
Heavy organic	light organic	60-230

Although, to-day CAD packages are giving quick calculation of heat transfer coefficient however are requiring quite large number of physical data of flows.

Special packages are provided for optimization of the heat usage by special design of the heat exchangers system, but this is possible after general structure of heat exchange would be established.

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