7

Perspectives for Further Development of the Concept of Microporous Systems

In this Chapter, we will analyze the perspectives of the further development of the concept of microporosity and microporous materials. We will analyze the principal existing obstacles hindering the fast progress in this concept and provide some recommendations about canceling these obstacles, comprising some initiatives aiming to attract investors to all phases of microporous material elaboration.

Our analysis will be based on methods of the analysis of computer systems. This approach allows the optimization of information systems, maximization of their effectiveness and usefulness.

The illustrations were prepared with using CASE Studio 2 (for DFD and ERD) and Access (for DSD).

I. METHODS OF ANALYSIS USING COMPUTER SYSTEMS

Below, we will use the following methods of analysis using computer systems:

A. Entity-Relationship Diagram (ERD)

This method presents the *entities*—''participants'' (subjects) in the information exchange process, the objects on which the action is performed, and the principal operations allowing their relationship. The *relationship* can be presented as one entity related to one entity (one to one) or one entity related to many entities (one to many). The presentation *one to one* means that there is the single relationship between two different entities (e.g., an

individual and his or her assurance number), while the presentation *one to many* means that there are two or more options of relationships of entity 2 to entity 1 (e.g., first name and individual: the same first name can be found for many individuals, that is the relationship ''one (first name) to many (persons)''). The relationship ''many entities to many entities'' is also possible but, for technical reasons, is presented through intermediate entities as a series or relationships ''one entity to many entities''. An example of the relationship ''many to many'': the same author may write two or more books, but the same book may be written by two or more coauthors, hence, the relationship ''authors-books'' needs an intermediary entity ''author-book'' formed for each situation when a concrete person is one of the coauthors in a concrete book.

The drawback of ERD presentation consists in the absence of a logical relationship between events; such relationship is allowed by ''data flow diagrams'' method.

B. Data Flow Diagrams (DFD)

This method allows understanding of the relationship between objects, databases and events (functions). DFD comprises three types of components:

Subjects: some interested persons or groups actively participating in some events
Events (functions): processes and their results changing the situation for the subjects
Databases: storage of information about some phenomena, technique, persons, etc.

Combined with ERD, DFD allows the presentation of both relationships between the subjects and acted objects, but the system of information storage is not optimal. The optimization of the information storage is allowed due to using of data structure diagrams.

C. Data Structure Diagrams (DSD)

This method allows the optimal systematization and presentation of information databases, comprising the logical relationship between them. That is usually done in the form of tables, including:

The code and the principal characteristics of the object (or subject) described
The codes of principal related objects or subjects
The relationships between different objects and subjects

Combinations of ERD, DFD, and DSD allow the presentation of relationships between the subjects and acted objects, the optimized systems for storage and furnishing information about events related to changes in the considered system.

More detailed information about such methods of computer system analysis as ERD, DFD, and DSD is given in Refs. 1–4.

II. PRINCIPAL PROBLEMS IN THE DESIGN OF NEW MICROPOROUS MATERIALS

The principal problems in the design of new microporous materials are NOT related to the scientific knowledge or talent of explorers but only to the system of their financial support.

The existing system of the financial support of the research of microporosity comprises two principal subsystems working almost independently and related mostly by the publication of results. These subsystems are

The academic system of fundamental theoretical and experimental studies of microporosity in universities, specialized colleges, and governmental institutes. These institutions are supported by governments and/or private philanthropic sponsors, while the relationship with the industry is minor. The researchers working in this subsystem are not very interested in the financial results of their explorations, and their interest is mostly morale (nice to contribute to the science and the perspectives of mankind). They publish many papers and sometimes get patents, but the real output of their efforts is dubious.

Private and some governmental (mostly military) research centers and institutes. They depend much more on the results of their work, and their interest to obtain really important scientific results is minor. They solve the current problems related to materials science, and they are informed about the achievements of their colleagues working in the subsystem above mostly due to scientific publications and conferences. The worst thing is that they are not interested even in forecasting the global and environmental sequences of the realization of their ideas, unless that is imposed by existing laws.

Is the existing system (described above) good enough? In principle, it allows the obtainment of new scientific results and the solution of urgent technical problems—at least, today. However, this system is not optimal of all. The whole previous part of this book (Chapters 1–6) presented the power of the concept of the joint consideration of synthesis, structure and

measurable properties of microporous materials. Nevertheless, all scientific results presented above cannot attract workers in the existing system of the research of microporosity, because

Workers in sponsored institutes, universities, and colleges are not interested in rejecting their previous suggestions and plans without getting the serious financial stimulation.

Workers in private and military research centers are not interested in accepting the risk of the realization of novel organizational ideas, effectiveness of which cannot be approved in few months.

On the other hand, *there are* subjects really interested in the increase of the effectiveness of studies of microporosity—those financing the sponsored sector and investing in the private sector. They are really interested in getting maximum scientific and technical effect per each dollar spent.

Is it possible to suggest any initiatives stimulating the sponsored researchers and reducing the risk of private researchers in the case if they accept the methodology of the joint consideration "synthesis–structure–properties"? The below scheme suggests a way for the solution of this problem.

A. Traditional Scheme of the Elaboration of New Microporous Materials

In the previous chapters, we mentioned sometimes the specificity of the existing system of study of microporosity. Its ERD scheme is presented on Fig. 7.1.

As follows from Fig. 7.1, all begins by the user of material, needing a new material with special properties that are not found for existing materials. The user of material request this new material from the supplier (in principle, the normal situation is: *many* users request materials from *many* suppliers, which is relationship ERD many to many simplified to a pair of relationships one to many through orders of materials). The supplier orders the needed research to the researcher of material (or many suppliers order research to numerous researchers), this one synthesizes the material with the needed properties, forwards the technical information to the supplier, and publishes the scientific results. The patent rights are transferred, in most cases, to the supplier.

Thus, we find in the considered scheme the following subjects:

User of material
Supplier of material
Researcher of material

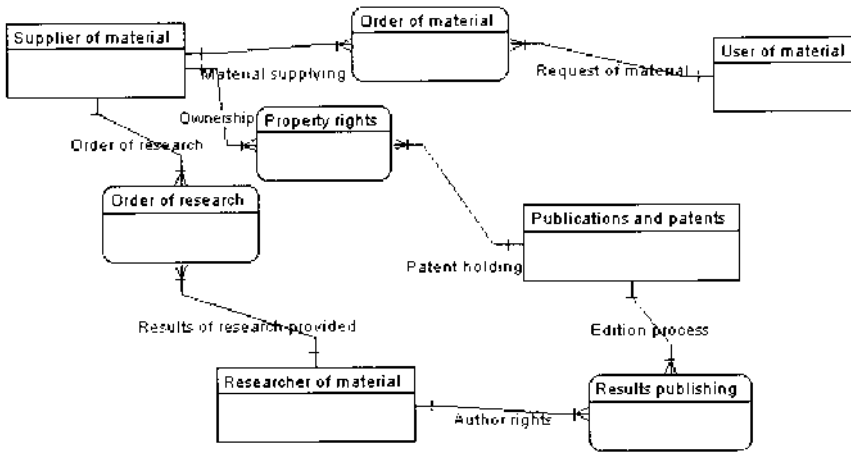

FIG. 7.1 The existing scheme ERD of relationships of subjects in the existing system of studies of microporosity.

Of course, talking about user of material, supplier of material, and researcher of material, we mean not only concrete persons but related collectives, institutes, companies, ministries etc.

Now, let us consider the DFD scheme of the same system. That is presented by Fig. 7.2.

As follows from Fig. 7.2, the most problematic phase of the new material creation is its elaboration by the researcher. First of all, this one tries the existing materials and finds them inappropriate for completing the received order. However, the researcher finds some materials, properties of which get closer to those of the requested material. Based on these materials, the researcher tries some combinations of known materials, modifies them, and, after all, maybe prepares the material with the desirable properties. But—maybe not! The main disease of the existing scheme is the impossibility to forecast whether or not the requested material can be ever prepared—just theoretically! Well, let us assume that the order will be completed, but the resources needed for the solution of the defined problem may be too expensive. After all, the material is synthesized, the supplier and user are satisfied, the novel scientific data are published, the special technical information is patented, and the existing database on microporous materials, their synthesis, structure, and properties is updated.

In addition to the active participants in the traditional scheme (subjects already listed above) we find also the database on microporous materials, touched twice by the material researcher: the first time when he

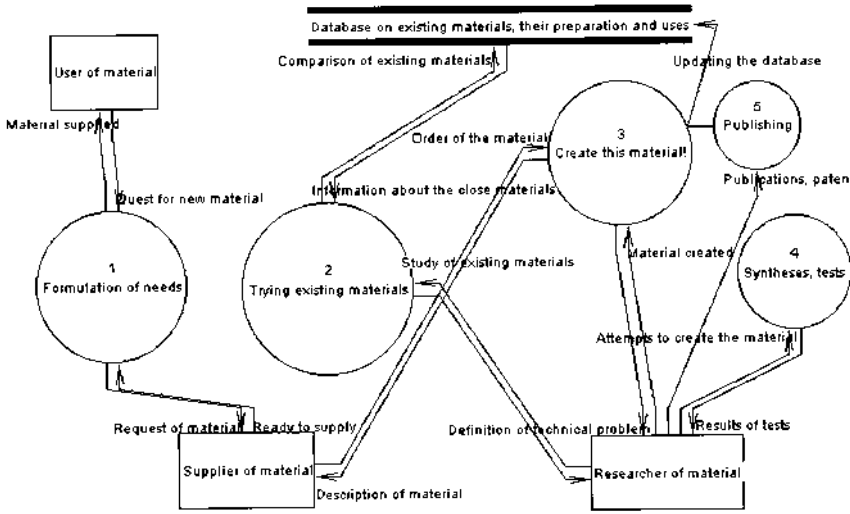

FIG. 7.2 The DFD scheme of the traditional system of microporous material design.

seeks for the appropriate or close materials and the second time when he updates this database with papers and patents and, respectively, enriches the human knowledge about microporosity.

The financial aspect of the traditional scheme of the synthesis of new material with desired properties is illustrated by Table 7.1.

As follows from Table 7.1, the most problematic phase of the creation of the novel material with the desired properties—empirical synthesis by the researcher of material—corresponds to the expenses ($n_{s1} \times \mathrm{COST}_{s1}$). If the number of attempts n_{s1} becomes infinite, that corresponds to one of two regretful options: the initial order of the material is incorrect and requires impossible things, or the researcher of material does not possess the needed resources. In both cases, the result is negative, and the research fails. If the researcher of material belongs to a sponsored institute, his damage is just moral; otherwise, his losses are much more material.

B. Suggested Scheme of the Elaboration of New Microporous Materials

The suggested scheme of the elaboration of new microporous material with desired properties is based on the concept of the joint consideration

TABLE 7.1 Expenses for the Synthesis of Novel Material with Desired Properties by the Traditional Scheme of Study of Microporosity

Operation or event	Performer of the operation	Performer of the payment	Number of the operations	Expenses per one operation
Formulation of order	Material user	Material user	1	$\mathrm{COST}_{\mathrm{or11}}$
Receipt of order	Material supplier	Material supplier	1	0
Order or research	Material supplier	Material supplier	1	$\mathrm{COST}_{\mathrm{or12}}$
Choice of close materials	Researcher	Researcher	1	$\mathrm{COST}_{\mathrm{ch11}}$
Synthesis and tests of new materials	Researcher	Researcher	n_{s1}	COST_{s1}
Comparison with the order	Researcher	Researcher	n_{c1}	$\mathrm{COST}_{\mathrm{com1}}$
Patenting, publishing, report preparation	Researcher	Researcher and/or supplier[a]	1	$\mathrm{COST}_{\mathrm{pub1}}$
Completing of the order	Researcher	Supplier	1	$\mathrm{COST}_{\mathrm{matres11}}$
Supplying material	Supplier	User	1	$\mathrm{COST}_{\mathrm{matsup12}}$
Total costs:				
Total11	—	User	—	$\mathrm{COST}_{\mathrm{or11}} + \mathrm{COST}_{\mathrm{matsup12}}$
Total12	—	Supplier	—	$\mathrm{COST}_{\mathrm{or12}} + \mathrm{COST}_{\mathrm{matres11}}$
Total13	—	Researcher	—	$\mathrm{COST}_{\mathrm{ch11}} + (n_{s1} \times \mathrm{COST}_{s1}) + (n_{c1} \times \mathrm{COST}_{\mathrm{com1}})$

[a]We assume that in any case these expenses are paid by the supplier.

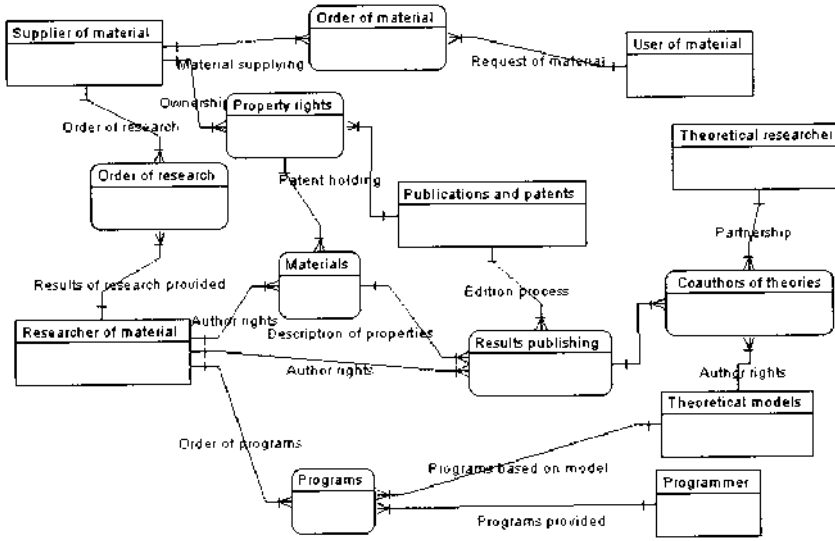

FIG. 7.3 The suggested scheme ERD of relationships of subjects in the system of studies of microporosity.

of synthesis, structure, and properties. Its ERD illustration is presented by Fig. 7.3.

As follows from Fig. 7.3, the suggested scheme of the relationships between the participants in the novel material elaboration is more complex than the traditional system. That includes not only user of material, supplier of material, and researcher of material, but also programmer and theoretical researcher, whose results are necessary for the realization of the joint concept. Also they are interested in the protection of their rights, especially in the case if the elaboration of the new material succeeds and results in a financial profit.

Now, let us consider the DFD scheme of the suggested system, which is presented by Fig. 7.4.

As follows from Fig. 7.4, there are no significant changes in the events related to the required microporous material synthesis, until the design itself is begun by the researcher of material. In the proposed scheme, the researcher of material, instead trying all close materials, first of all estimate the needed structure able to bring the required properties. This estimation is done on the base of computer calculations, using, as semiempirical parameters, experimental data from the database on existing microporous materials. The previously mentioned problematic phase of the new material

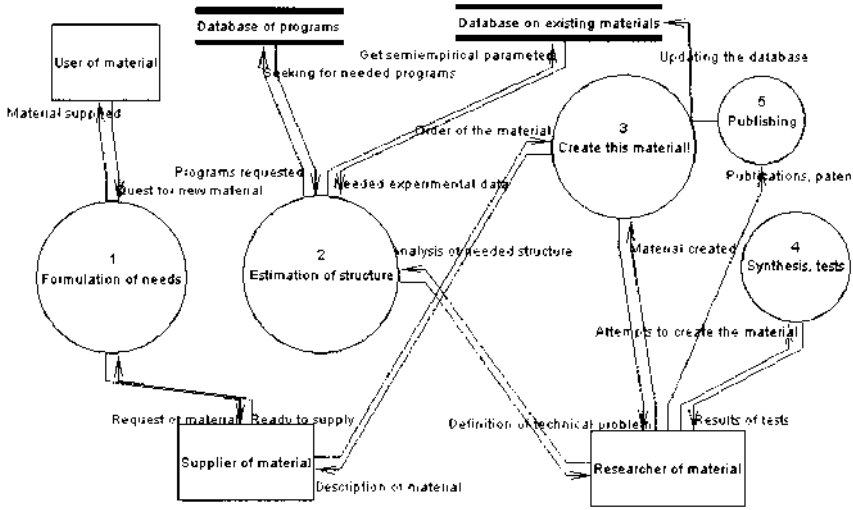

FIG. 7.4 The DFD scheme of the suggested system of microporous material design.

creation by the traditional scheme is cancelled already on the stage of the estimation of the structure: just after executing the calculating program, the researcher of material immediately knows whether the problem received from the user (through the supplier) is defined correctly. If not, the researcher of material informs the supplier that the problem has no solution or the needed resources are not available; then, the supplier decides what to do: ask the user to soften the requirements, or provide the needed resources to the researcher of material, or anything else. In any case, the researcher of material economizes efforts, time, and money.

In the case if the computer calculations do not bring any warning result about the chances of the solution of the defined problem, the researcher of material just takes the recommendations about the structure he needs to obtain and the preparation conditions he needs to assure. The synthesis is accomplished, in the normal situation, once only (unless the results of calculations are not enough clear).

In addition to the database on existing microporous materials, the proposed scheme comprises also the database on computer programs for estimating the structure allowing several (desired) measurable properties, and the parameters of the synthesis process for the preparation of the needed structure. During the realization of the proposed scheme, this database gets no change.

The theoretical researcher does not still appear in the suggested scheme, because he is not directly related to the researcher of material and the attempts to create the novel microporous material with the required properties.

Let us note also another difference of the proposed scheme from the traditional one: the database on the existing materials is used not for finding the closer materials but mostly for finding semiempirical parameters for the input in the program to run. The really obtained material with the desired properties may differ very much from "closer" materials! In the traditional scheme, such result cannot be ever obtained.

The financial aspect of the traditional scheme of the synthesis of new material with desired properties is illustrated by Table 7.2.

As follows from Table 7.2, the main financial effect of the realization of the proposed scheme consists in the fantastic reduction of the expenses for the stage of the synthesis and the tests. In the case if the calculating program is not expensive and its running does not require any expensive technique, $\mathrm{COST}_{\mathrm{est}} < \mathrm{COST}_{sl}$ and the economy is assured almost always. The profit obtained due to the realization of the proposed concept can be used by the researcher of material in two ways (probably both):

Increase of revenues

Reduction of the price of supplying the results of the research to the supplier of material ($\mathrm{COST}_{\mathrm{matres21}} < \mathrm{COST}_{\mathrm{matres11}}$)

In the second case, also supplier of material gets an additional profit due to the use of the proposed scheme.

The profit obtained due to the realization of the proposed concept can be used by the supplier of material in two ways (compare to researcher of material):

Increase of revenues

Reduction of the price of supplying the results of the research to the user of material ($\mathrm{COST}_{\mathrm{matres22}} < \mathrm{COST}_{\mathrm{matres12}}$)

In the second case, also user of material gets an additional profit due to the use of the proposed scheme.

C. Suggested Scheme of the Elaboration of New Programs for Simulations of Structure and Properties of Microporous Materials

The suggested scheme of the elaboration of new microporous material with desired properties works okay in condition that the price required by the program owner does not ask too high price for the software. Otherwise, the

TABLE 7.2 Expenses for the Synthesis of Novel Material with Desired Properties by the Suggested Scheme of Study of Microporosity

Operation or event	Performer of the operation	Performer of the payment	Number of the operations	Expenses per one operation
Formulation of order	Material user	Material user	1	$COST_{or21} = COST_{or11}$
Receipt of order	Material supplier	Material supplier	1	0
Order or research	Material supplier	Material supplier	1	$COST_{or22} = COST_{or12}$
Estimation of needed structure, parameters of synthesis	Researcher	Researcher	1	$COST_{est}$
Synthesis and tests of the new material	Researcher	Researcher	1	$COST_{s2} = COST_{s1}$
Comparison with the order	Researcher	Researcher	2	$COST_{com2} = 2 \times COST_{com1}$
Patenting, publishing, report preparation	Researcher	Researcher and/or supplier[a]	1	$COST_{pub2} = COST_{pub1}$
Completing of the order	Researcher	Supplier	1	$COST_{matres21} \leq COST_{matres11}$
Supplying material	Supplier	User	1	$COST_{matres22} \leq COST_{matres12}$
Total costs:				
Total21	—	User	—	$COST_{or11} + COST_{matsup22}$
Total22	—	Supplier	—	$COST_{or12} + COST_{matres21}$
Total13	—	Researcher	—	$COST_{est} + COST_{s1} + 2 \times COST_{com1}$

[a]We assume that in any case these expenses are paid by the supplier.

condition $\mathrm{COST}_{\mathrm{est}} < \mathrm{COST}_{s1}$ is not completed, and researcher of material is not interested in the novel way to material synthesis. However, in such case the program owner also loses the profit; hence, he is not interested in overestimating the real value of the programs.

Let us consider the process of the creation of novel computer program for modeling structure and properties of microporous material. DFD of this process is given in Fig. 7.5.

As follows from Fig. 7.5, the process of designing a program for simulating microporous materials is very similar to that for designing novel materials according to the proposed general scheme. This time, the role of the user is played by the researcher of material, and the order completing is performed by the programmer. This DFD includes two databases: database on programs (that is checked by program owner before ordering the new program writing, and later, when the program is ready, this database is updated) and database on theoretical models, among which the programmer finds the most appropriate mathematical tools allowing him to write the ordered program.

The resulting expenses for the program design are determined by two principal factors:

The price of licensing the appropriate theoretical model

The salary of the programmer

The theoretical researcher appears in this scheme indirectly, through the database on theoretical models.

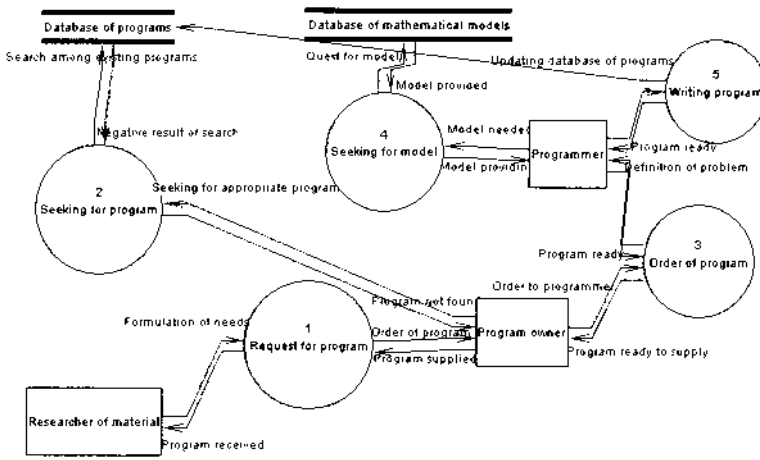

FIG. 7.5 The DFD scheme of the suggested system of design of computer programs for simulating structure and properties of microporous material.

The financial aspect of the traditional scheme of the synthesis of new material with desired properties is illustrated by Table 7.3.

As follows from Table 7.3, the condition of the financial reasonability of the design of a novel program is given by: $\mathrm{COST}_{\mathrm{reqmod31}} + \mathrm{COST}_{\mathrm{wrpr31}} < \mathrm{COST}_{\mathrm{prog31}}$, $\mathrm{COST}_{\mathrm{prog31}} < \mathrm{COST}_{\mathrm{prog32}}$; hence, too high price for licensing the needed theoretical model can destroy all financial interest: not only for the programmer and the program owner but also for the researcher of material and owner of material.

Today, everyone can take an existing theoretical model for free and write a related computer program, but, as we noted above, this system destroys all interest in theoretical studies and investments in theories; below we suggest some ways to compromise between the interests of programmers to get the theoretical models for minimal price and the interests of theoretical researchers in maximal royalties.

In the case if licensing the theoretical model is not expensive, $\mathrm{COST}_{\mathrm{reqmod31}} + \mathrm{COST}_{\mathrm{wrpr31}} < \mathrm{COST}_{\mathrm{prog31}}$, and the profit is obtained by both programmer and program owner. As in the case of material synthesis, the profit obtained by the programmer in two ways (probably both):

Increase of revenues

Reduction of the price of supplying the results of the research to the program supplier $[(\mathrm{COST}_{\mathrm{reqpr32}} + \mathrm{COST}_{\mathrm{reqpr33}} + \mathrm{COST}_{\mathrm{prog31}}) < \mathrm{COST}_{\mathrm{prog32}}]$.

In the second case, also program supplier gets an additional profit due to the use of the proposed scheme.

If program supplier gets an additional profit due to the reduction of price by the programmer, that one can use his profit material in two ways (compare to the programmer and the supplier of material):

Increase of his revenues, and/or

Reduction of the price of supplying the results of the research to the researcher of material (reduction of $\mathrm{COST}_{\mathrm{prog32}}$).

In the second case, also the researcher of material gets an additional profit due to the use of the proposed scheme.

Now, let us consider the proposed scheme for the theoretical researcher.

D. Suggested Scheme of the Joint Elaboration of Novel Theories, Models, Computer Programs, and Materials

As we noted earlier, the existing scheme of the financial support of theoretical researchers does not stimulate all of them. Independently of

TABLE 7.3 Expenses for the Design of Computer Program for Simulating the Structure of Novel Material with Desired Properties

Operation or event	Performer of the operation	Performer of the payment	Number of the operations	Expenses per one operation
Request of program	Researcher	Researcher	1	$\mathrm{COST}_{\mathrm{reqpr31}}$
Query for the program	Program owner	Program owner	1	$\mathrm{COST}_{\mathrm{reqpr32}}$
Order of the novel program	Program owner	Program owner	1	$\mathrm{COST}_{\mathrm{reqpr33}}$
Quest for the model	Programmer	Programmer	1	$\mathrm{COST}_{\mathrm{reqmod31}}$
Writing program	Programmer	Programmer	1	$\mathrm{COST}_{\mathrm{wrpr31}}$
Order completing	Programmer	Program owner	1	$\mathrm{COST}_{\mathrm{prog31}}$
Program supplying	Program owner	Researcher of material	1	$\mathrm{COST}_{\mathrm{prog32}}$
Total costs:				
Total31	—	Researcher of material	—	$\mathrm{COST}_{\mathrm{reqpr31}} + \mathrm{COST}_{\mathrm{prog32}}$
Total32	—	Programmer	—	$\mathrm{COST}_{\mathrm{reqmod31}} + \mathrm{COST}_{\mathrm{wrpr31}}$
Total13	—	Program owner	—	$\mathrm{COST}_{\mathrm{reqpr32}} + \mathrm{COST}_{\mathrm{reqpr33}} + \mathrm{COST}_{\mathrm{prog31}}$

the novelty and level of proposed theories and models, their correctness and capability to treat the maximum of experimental data with minimum of fitted parameters, the theoretical researchers get some specified salary—or do not get anything. Their results can be used by everyone, just if copyright is not violated. There exists no system of protection of propriety rights of theoretical researchers or institutions paying them salary.

The system proposed above makes sense only on the condition that propriety rights of theoretical researchers and their employers will be respected in the same manner as the rights of patent holders. The organizational aspect of this problem will be considered below. Now, let us consider only the DFD and financial aspect of theoretical research, assuming that the proposed system makes impossible the traditional use for free of the original and effective theoretical tools. We also introduce the notion of owner of theoretical model (university, college, academy, private research company, etc.), meaning the employer of the theoretical researcher, defining the general problem for the theoretical research and possessing all propriety rights onto the obtained results.

The above-suggested scheme of the elaboration of new microporous material with desired properties and related computer programs works okay if the price required by the owner of theoretical propriety, while offering some significant profit, is not too high for the theoretical models he possesses. Otherwise, the programmer and the researcher of material are not interested in the novel way to material synthesis. However, in such case the owner of theoretical models also loses the profit and, hence, is not interested in overestimating the real value of the models.

Let us consider the process of the creation of novel theory and related models allowing the solution of particular problems in microporosity. DFD of this process is given below on Fig. 7.6.

As follows from Fig. 7.6, the process of designing a new theory of the synthesis, structure, or measurable properties of microporous materials is similar to that for designing novel materials and related computer program according to the proposed general scheme. This time, the role of the user is played by the programmer, and the order completing is performed by the theoretical researcher. This DFD includes two databases: database on existing microporous materials (that is treated by the theoretical researcher on all stages of creating theory and later, when mathematical models are applied to known experimental data to estimate the correlation between theoretical models and the experimental data) and database on theoretical models, to which the new theory is compared (aiming to estimate its novelty and place in the hierarchy of theoretical concepts of microporosity).

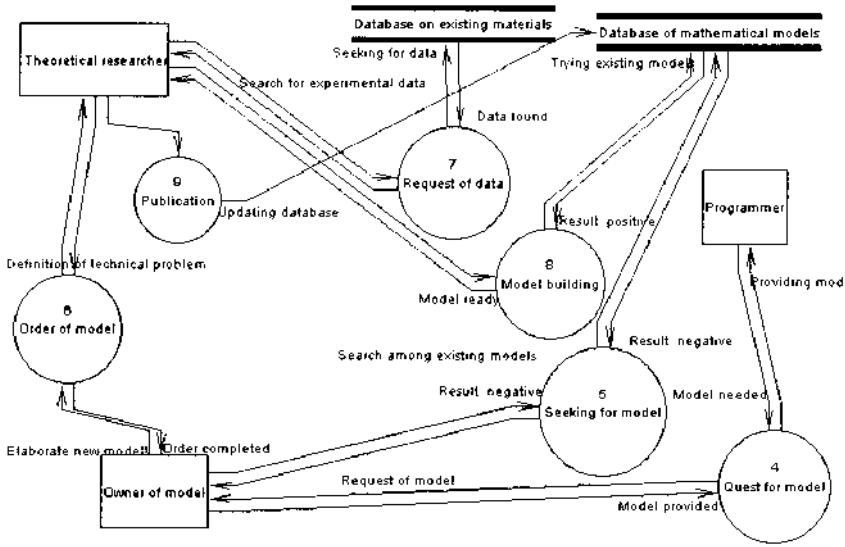

FIG. 7.6 The DFD scheme of the suggested system of design of theories and theoretical models of microporous materials.

After the receipt of the model order from the owner of theoretical model, the theoretical researcher:

1. Requests access into the database of existing theories and models.
2. Analyzes the existing theories—their advantages, principal assumptions and drawbacks.
3. Concludes about the necessary changes of the assumptions, in order to improve the theoretical base.
4. Builds novel theoretical models based on the "fresh" theoretical concept, using the appropriate mathematical tools applicable to various particular problems in microporosity science.
5. Compares the fresh models to these existing in the database; estimates their advantages and shortcomings.
6. Applies the fresh models to the treatment of real experimental data.
7. Concludes about the effectiveness of the proposed models.
8. Forwards the results to the owner of theoretical model.
9. Decides together with the owner of theoretical model about the relevant publications and protection of the created intellectual propriety.

The resulting expenses for the program design are determined by two principal factors:

The price of access into the database of theoretical models
The salary of the theoretical researcher

The financial aspect of the traditional scheme of the synthesis of new material with desired properties is illustrated by Table 7.4.

As follows from Table 7.4, the condition of the financial reasonability of the design of a novel theoretical concept is given by

$$\begin{aligned} &\mathrm{COST}_{\mathrm{theoran41}} + \mathrm{COST}_{\mathrm{theoran42}} + \mathrm{COST}_{\mathrm{theorimp41}} \\ &\quad + \mathrm{COST}_{\mathrm{newmod41}} + \mathrm{COST}_{\mathrm{compmod41}} + \mathrm{COST}_{\mathrm{compmod42}} \\ &\qquad < \mathrm{COST}_{\mathrm{matmod41}} \end{aligned} \tag{7.1}$$

and

$$\mathrm{COST}_{\mathrm{matmod41}} < \mathrm{COST}_{\mathrm{matmod42}} \tag{7.2}$$

Let us note that

The theoretical researcher may need writing computer programs on the base of the models, aiming to apply them to known experimental data but should do it without any assistance of the programmer (to avoid a sharp increase of the expenses), and the costs of writing such temporary programs are counted in $\mathrm{COST}_{\mathrm{compmod42}}$;

Since the theoretical researcher needs the database on existing theoretical models, the theoretical researcher is not interested in the increase of the price of the access to this database, which also limits profit;

Since the theoretical researcher needs the database on existing materials, the interest is in the collaboration with the researcher of material, aiming to maintain the prices of the access to all databases in limits allowing both of them to get a significant profit but preventing too sharp an increase of expenses.

III. REGISTRATION AND PROTECTION OF INTELLECTUAL PROPRIETY

As we noted above, one of the principal causes of the loss in the effectiveness of studies of microporosity is the absence of such protection of

TABLE 7.4 Expenses for the Design of Theoretical Models of Microporous Materials—Their Synthesis, Structure, and Properties

Operation or event	Performer of the operation	Performer of the payment	Number of the operations	Expenses per one operation
Request of new model	Programmer	Programmer	1	$COST_{reqmod41}$
Query for the new model	Owner of model	Owner of model	1	$COST_{reqmod42}$
Order of the novel model	Owner of model	Owner of model	1	$COST_{reqpr41}$
Access to database of models	Theoretical researcher	Theoretical researcher	1	$COST_{theoran41}$
Analysis of existing theories	Theoretical researcher	Theoretical researcher	1	$COST_{theoran42}$
Improving assumptions	Theoretical researcher	Theoretical researcher	1	$COST_{theorimp41}$
Building new models	Theoretical researcher	Theoretical researcher	1	$COST_{newmod41}$
Comparison of new models with existing ones	Theoretical researcher	Theoretical researcher	1	$COST_{compmod41}$
Application of new models to experimental data	Theoretical researcher	Theoretical researcher	1	$COST_{compmod42}$
Completing the order	Theoretical researcher	Owner of model	1	$COST_{matmod41}$
Completing the request	Owner of model	Programmer	1	$COST_{matmod42}$
Total costs:				
Total41	—	Programmer	—	$COST_{matmod42} + COST_{reqmod41}$
Total42	—	Owner of model	—	$COST_{reqmod42} + COST_{reqpr41} + COST_{matmod41}$
Total13	—	Theoretical researcher	—	$COST_{theoran41} + COST_{theoran42} + COST_{theorimp41} + COST_{newmod41} + COST_{compmod41} + COST_{compmod42}$

interests of the theoretical researcher that would allow him a good profit in the case of building an effective theory, solving classical problems of microporosity and applicable to numerous experimental data. This problem may have a solution due to the registration of novel theories, theoretical models, computer programs, and novel materials (even having no patent novelty) by some registering institutions. These institutions can be

International scientific or technological committees, centers, associations (e.g., UNESCO, IUPAC, NACE)
Governmental institutions (e.g., U. S. Department of Energy)
National institutions or associations (e.g., American Chemical Society, U. K. Royal societies)
Regional institutions or organizations (comprising universities)

The procedure of the registration should be automated, simple, and fast. The registration fees should be minimal (e.g., below U.S. $100 in the United States). The registration must officially assure

Author rights and owner rights
Limiting the similarity between different intellectual solutions of the same kind
The unification of the form of the presentation of different intellectual solutions of the same kind
Making easier the solution of possible conflict situations

The list of the data appearing in the registration forms for intellectual solutions (theories, theoretical models, computer programs, and microporous materials) is given in Table 7.5.

The simplest database system for storing information, allowing the automated regulation of the proposed scheme, is given on Fig. 7.7 as DSD relationship.

As follows from Fig. 7.7, the data structure for researcher of material and theoretical researcher is the same: of course, they are colleagues, and they differ only in the research experience and the profile of job!

All relationships on Fig. 7.7 are given through the codes only; such form allows the minimization of repeating data, which is typical for DSD.

However, the most important detail on Fig. 7.7 is the absence of any divergences between owners of materials, programs, models and theories. That means that the main function of owners is not the research itself but the financial support and control of research. Moreover, the same juridical person is allowed to be owner of materials, programs, and theoretical models. That is a very important aspect related to investments in studies of microporosity.

TABLE 7.5 Information in the Registration Forms for Intellectual Propriety Related to Studies of Microporosity

Data	Theory	Theoretical model	Computer program	Microporous material
Code	Code of theory	Code of model	Code of program	Code of material
Author(s)	Code(s) of theoretical researcher	Code(s) of theoretical researcher	Code(s) of programmer	Code(s) of researcher of material
Owner	Code of owner of model	Code of owner of model	Code of program owner	Code of owner of material
Name	Theory name	Model name	Program name	Material name
Designation	Sphere of applicability	Problems available to solve	Output available	Technical uses
Specificity	Assumptions	Equations	Language, algorithm	Most important properties
Information needed for use	—	Fitted parameters	Input	Restrictions
Hierarchic position	Class of theories	Initial theory (code)	Similar programs (codes)	Similar materials (codes)
Priority date	Date of first publication	Date of first publication	Date of registration	Date of registration, first publication, or patent
Publications available before the registration	Publications (codes)	Publications (codes)	—	Publications (codes)
Base	—	Theory code	Model code	Program code(s)

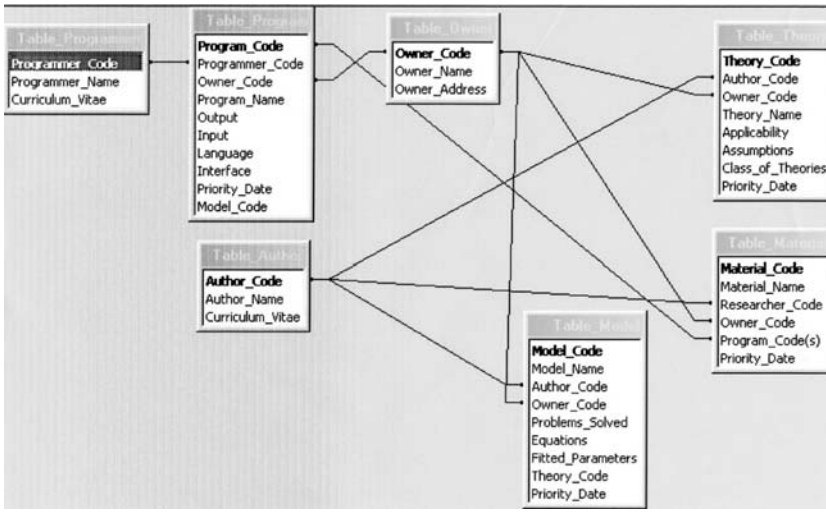

FIG. 7.7 DSD scheme for database on registered theories, theoretical models, computer programs, and new materials in the field of microporosity.

IV. INVESTMENTS IN STUDIES OF MICROPOROSITY

Some aspects of the investments in the existing system of studies of microporosity were considered above: nonprofit sponsorship by government or private philanthropic foundations and private investments aiming to get money back with the maximal profit as soon as possible. Of course, the scheme of investments in the proposed system of joint studies of materials, programs, and theory should be absolutely different.

First of all, all stages of study of microporosity can be realized on the profit base. Money can be invested not only in material synthesis and tests (as in the existing system) or programs but even in "pure" theory, because this becomes a product in the form of information from database. Moreover, investments in theoretical studies may have serious advantages: the expenses are related mostly to the salary of researchers that can return to the investor very fast (see Table 7.6: the expenses by the traditional scheme are compared with those by elements of the suggested scheme).

As follows from Table 7.6, the expenses for the suggested scheme are always much less than those for the traditional scheme; hence, in the aspect of costs the suggested scheme is definitely preferable for investments.

However, not only costs determine the effectiveness of systems. Let us compare the proposed system to the traditional system in various aspects

TABLE 7.6 Structure of Expenses in Different Studies of Microporosity

Item	Equipment amortization, energy consumption	Salary	Chemicals	Intellectual property (use of databases)
Researcher of material (by Table 7.1)	+++[a]	++[b]	+++	+[c]
Researcher of material (by Table 7.2)	+	++	+	++
Programmer (by Table 7.3)	+	++	−[d]	++
Theoretical researcher (by Table 7.4)	+	++	−	++

[a] +++ expenses are very high.
[b] ++ expenses are high.
[c] + expenses are moderate.
[d] − expenses are negligible.

TABLE 7.7 Various Aspects of Investments in Studies of Microporosity According to Different Schemes

Factor of comparison	Traditional scheme of research	Suggested scheme: only material study	Suggested scheme: only programming	Suggested scheme: only theory	Suggested scheme: all
Costs	Very large	Large	Minor	Minor	Large
Product to sale	Materials	Materials	Programs	Models	All
Relationship with material user	Direct	Direct	Indirect	Indirect	Direct
Dependence on partners	No	Yes	Yes	Yes	No

related to investments. We will consider three options for investments (see Table 7.7):

1. Investments in studies of microporosity according to the traditional scheme
2. Investments in theoretical research *or* programming *or* material synthesis
3. Investment in theoretical research *and* programming *and* material synthesis according to the suggested scheme

As follows from Table 7.7, only investing in all elements of microporosity studies can compete with the traditional scheme in all factors of comparison! Investing in theory and programming, although it seems

very attractive financially, is too risky if the partners (for theoretician, programmer only; for programmer, both theoretician and material researcher; while for material researcher, programmer only) change the prices for their products. Moreover: theoretical researcher depends also on colleagues, whose intellectual products determine the prices in the database of theories and models, so necessary also for the theoretical study! The indirect relationship with the final consumer (material user) makes the additional risk for both theoretician and programmer.

Thus, the most effective in the aspect of the complex of characteristics of investing policy are investments in material synthesis, programming, and theoretical study together. Note that such investments are preferable also in the aspect of minimization of tax payments, because the products of theoretician and programmer are not always supplied to exterior consumers but first of all used inside the system.

V. CONCLUSIONS

1. The existing system of studies of microporosity does not stimulate the fundamental, especially theoretical research because theoretical results can be used by everyone without paying any fees to the author and/or investor in the fundamental research.
2. One of the sequences of the low efficiency of the existing system of studies of microporosity consists in the impossibility of forecasting whether a novel material with desired properties can be synthesized with the available resources.
3. The suggested system of studies of microporosity comprises the following:
   a. The protection of the propriety rights of owners of theoretical models of microporosity, with the registration of theories and models by competent organizations and/or institutions
   b. The registration of computer programs for forecasting properties of hypothetical materials in the same organizations and/or institutions
   c. The registration of novel materials not only in patent offices but also in the same organizations and/or institutions that register the novel theories, models, and computer programs on microporosity
4. The realization of the suggested system of studies of microporosity will allow:
   a. The financial stimulation of all aspects of studies of microporosity, comprising the elaboration of novel materials with

forecasted properties, writing computer programs for forecasting properties of new materials, and the creation of novel theories and theoretical models

b. The stimulation of investments not only in the elaboration of novel materials but also in new theories and computing programs linking theories to material synthesis
c. The increase of the effect of investments in studies of microporosity

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