Information System for Phosphorus-Containing Compounds Production
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Information System for Phosphorus-Containing Compounds Production

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Abstract

Sustainable development of the society requires that phosphorus industry significantly boosts its environmental performance which needs radical technological improvements. Those requirements are addressed by an EC supported FP6 ECOPHOS Project (www.ecophos.org). The project focuses on new technologies for (a) the production of useful phosphorous salts (fodder, food and pharmaceutical phosphates), phosphorous acid and phosphates in a cost efficient and ecologically sustainable way, (b) the improvement of existing methods in the phosphoric acid production for the drastic minimisation of waste, (c) the utilisation and processing of industrial solid waste from the production of phosphoric acid and (d) the production of a new generation of phosphoric fertilizers.

One of the key aspects of the work is the development of an integrated toolbox for the production of the wide class of phosphorus-containing products with information and data on waste minimising processes, process safety, resource and energy saving processing techniques and exchange of information about advanced production technologies.

The toolbox has a multilevel structure (three-level architecture) that consists of the following components: database server, application server and client application. The main core of the toolbox is based on mathematical models relevant to the production

processes that are incorporated into the mathematical model library of the toolbox. These toolbox models will mainly support the training capabilities of the system.

Keywords: information system, information technologies, databases, phosphorus-containing compounds, mathematical modelling

1. Introduction

New research and innovation strategy for the waste minimisation and utilisation in the phosphoric acid industry is being developed within the EC supported FP6 ECOPHOS Project. The research aims to develop ecologically sustainable, environmentally friendly, resource- and energy-saving industrial process technology for the production of a wide-class of phosphorus-containing substances. The research focuses on new technologies for

- Production of useful phosphorous salts (fodder, food and pharmaceutical phosphates), phosphorous acid and phosphates in a cost efficient and ecologically sustainable way,
- Improvement of existing methods in the phosphoric acid production for the drastic minimisation of waste,
- Utilisation and processing of industrial solid waste from the production of phosphoric acid and
- Production of a new generation of phosphoric fertilizers.

Mathematical models and computer-aided process engineering tools are being developed to provide efficient and sustainable operation of the production systems with key focus on reduction of cost, waste and energy.

The present day technology of waste minimisation and utilisation in phosphorus chemical industries is outdated and unable to face the environmental problems (Klemeš et al, 2006). The work combines the best practice in the field of phosphorus chemistry with the latest advances in computer-aided tools for resource-saving process synthesis, design and optimisation to lead to new technologies in the production of new useful products from phosphoric acid production waste. The wide class of new sustainable production technologies will bring significant changes in the environmental impact of relevant industries and furthermore increase their competitiveness.

One of the key aspects of the work is the development of an integrated toolbox for production of the wide class of phosphorus-containing products with information and data on waste minimising processes, process safety, resource and energy saving processing techniques and exchange of information about advanced technologies of these chemical productions. The advanced processes developed during the work include (i) sodium phosphite production, (ii) phosphorous acid production, (iii) dibasic lead phosphite production, (iv upgraded dihydrate method for phosphoric acid production, (v) dihydrate-semihydrate method, semihydrate method, and (vi) ortho-phosphoric acid purification. These will constitute the core of the open-type advanced

technologies toolbox. The toolbox will be based on mathematical models of those processes which will be incorporated into a mathematical model blocks of the toolbox.

The toolbox will also contain detailed data for a number of technologies (including process flowsheets and relevant data) for waste minimisation by utilisation such as: (i) phosphogypsum utilisation, (ii) cadmium containing phosphate ores processing, (iii) production of food and pharmaceutical quality phosphates and (iv) production of prolonged and aqua-accumulating fertilizers

Databases within the integrated toolbox will include:

- Advanced technologies of phosphorus-containing products manufacturing.
- Phosphogypsum disposal and its impact on the environment.
- Phosphogypsum processing technologies.
- Producers of phosphorus-containing products.
- Substance physicochemical properties.
- Raw materials and their producers.
- Equipment and its manufacturers.
- Expert system knowledge.
- Models for phosphorus-containing substance production.
- Phosphorus-containing products production flow sheets.
- Some other auxiliary databases.

2. Overall Structure of the developed ECOPHOS IS (Information System)

The structure of the ECOPHOS IS (Information system) comprises three basic components (Figure 1):

1. Client application.
2. Application server
3. Databases for Database server.

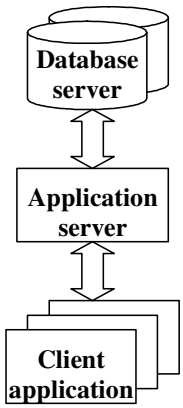

Figure 1. The structure of the ECOPHOS IS

Exchange of information for Production of Phosphorus-Containing Compounds is organized according to the following scheme (Figure 2).

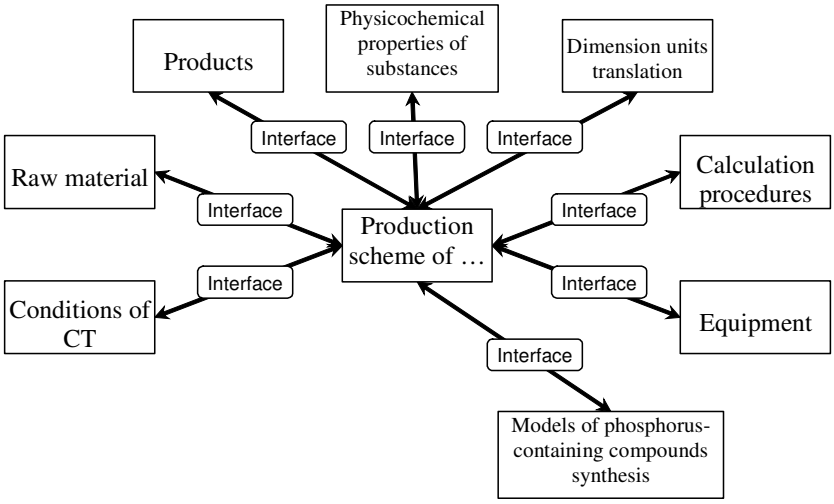

Figure 2. Exchange of information within ECOPHOS IS («interface» means interface of information exchange, allocated on the Application server)

The exchange of information in the system as a whole is represented in Figure 3.

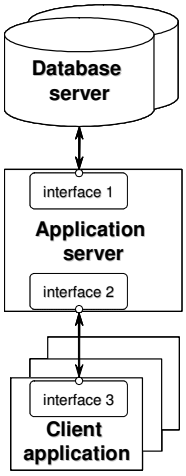

Figure 3. Exchange of information within the ECOPHOS IS

The information exchange is controlled by the Application Server on the basis of requested and submitted information from the Client Application. The control is carried out through interfaces of information exchange. So the Application Server has the interface of information exchange both with Database Server, and the Client

Application. The Client Application has the interface of information exchange only with the Application Server.

3. Client Application

The work has been recently focused on Client Server since the client application is the most important part for the end user.

This part represents the client application of the ECOPHOS IS. It is the part of Information system which the final user directly contacts with: inputs the information for data query or inputs new data, receives the reports and modelling results or results of other ECOPHOS IS sections.

The overall structure of Client Application is shown in Figure 4. The basic idea underlying the Client Application is that the end user should have all the information and data at hand for the development of a phosphorus related production flowsheet. Unlike existing process simulators, the ECOPHOS IS provides the user with full range of the information, including expert advice, real equipment parameters, related documentation and papers, etc.

The user can choose to model a phosphorus (phosphorus containing product) manufacturing flowsheet, seek for an expert advice using an internal expert system, can browse through equipment selection. Selecting the database section of the Client Application, the user can either browse the information or (having some administrative authority) add new or edit existing data. Client Application also provides a wide and flexible choice of reporting templates regarding the flowsheet modelling, expert advice and database information. The user can also change settings within the IS.

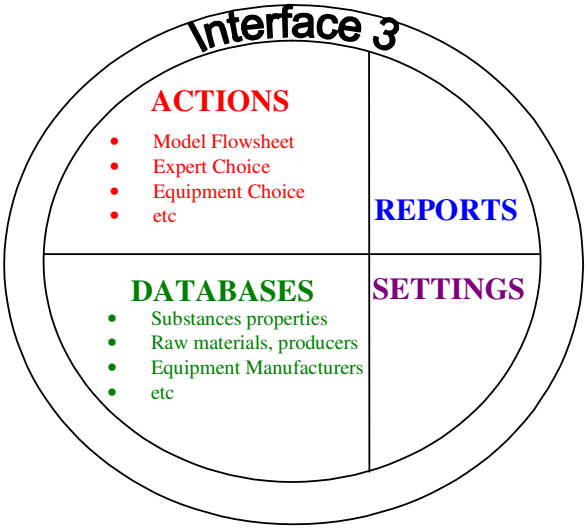

Figure 4. Overall structure of ECOPHOS IS Client Application

The IS openes with the screen with the main menu and the speed button toolbar. The user connects to the server by executing 'Connect' action (to press the speed button  or menu File → Connect). System will ask the user name and password. The main window of Client ECOPHOS IS will then change to work mode (Figure 5).

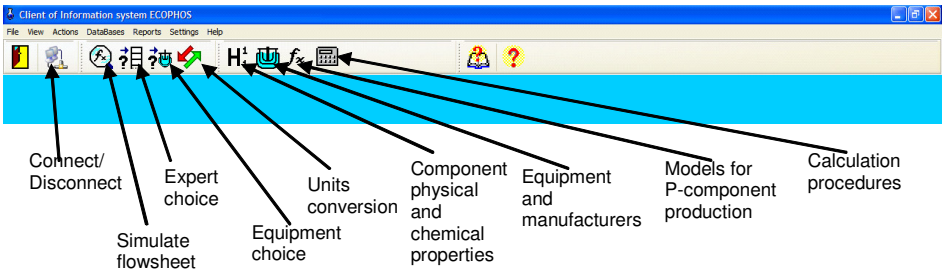

Figure 5 . Connection to the server activates the menu commands

After connection to the server, the first level of the menu commands includes File, View, Actions, Databases, Reports, Settings and Help items (Figure 6).

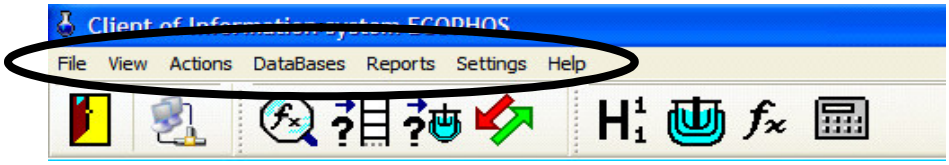

Figure 6. First level of menu commands

3.1. Actions Section

The Actions section is presented by Actions submenu (Figure 7) and Actions toolbar (Figure 8)

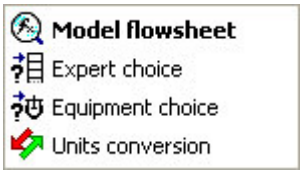

Figure 7. Actions submenu

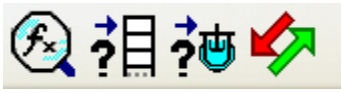

Figure 8. Actions toolbar

a. Model flowsheet implies modelling of the process flowsheet. Represents a window that allows modelling, through a series of actions, of a certain process flowsheet or its components. Envisages standard interface modules as well as more flexible attachment of calculation subroutines.
   Models that will be included in the system:
   - Modelling of the dihydrate process for extraction phosphoric acid production.
   - Modelling of sodium hypophosphite production process.
   - Modelling of sodium phosphite synthesis from phosphorus sludge.
   - Modelling of dibasic lead phosphite crystallization.
   - Modelling of phosphoric acid production process.

b. Expert Choice. Represents a window that allows making an expert choice of some aspects concerned with phosphorus-containing product technology (for example, expert choice of appropriate process flowsheet for production of a certain material, equipment type choice etc).
c. Equipment Choice – implies Choice of equipment. Represents a window that allows selecting the process equipment from the Equipment and its Manufacturers database. The selection is supported by a search of equipment according to various parameters.
d. Units Conversion.

3.2. Database Section

The Database section is presented in Database submenu (Figure 9) and database toolbar (Figure 10)

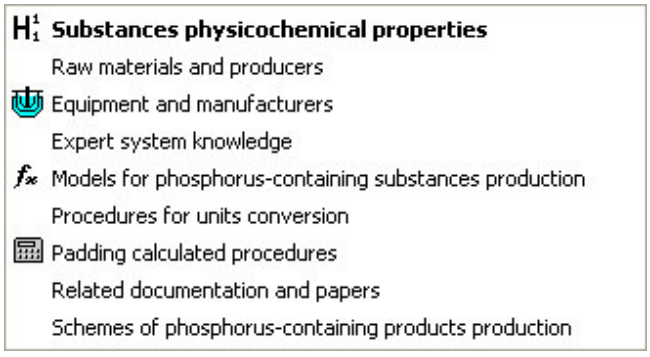

Figure 9 Database submenu

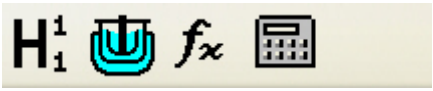

Figure 10. Databases toolbar

a. Editor of substance physicochemical properties is a screen that allows search, viewing, input of new and editing of already existing physicochemical characteristics of chemical substances. The Editor of component physical and chemical properties (Figure 11) enables to search, edit existing, and enter new properties of components.

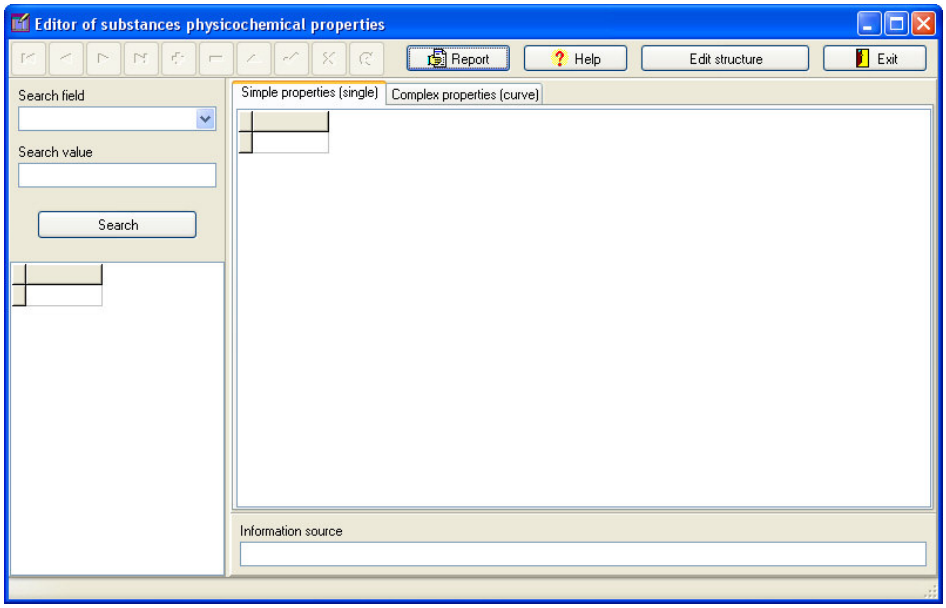

Figure 11 Editor of component physical and chemical properties

As an example, main characteristics are given below (the list can be added if this function is needed, will be provided in the system):

- Constitutional formula of the compound
- Name of the compound.
- Molar mass of the compound.
- Crystal density (if exists in solid phase under normal conditions).
- Heat capacity (coefficients) of crystals.
- Molar volume of dissolved substance.
- Latent crystallization heat.
- Temperature dependence of solubility.

b. Editor of raw materials and producers is a screen that allows search, viewing, and input of new and editing of already existing raw materials for phosphorus-

containing products technology as well as information on raw material suppliers. The data are being stored as for the phosphorus-containing products as well for other substances (supplementary or accompanying the process).
It has been continuously extended by including technical information on raw materials, contact information on the suppliers, volumes and possible delivery forms. This includes raw materials and suppliers from Russia as well as from the other CIS countries, Europe, and several other countries worlwide.

c. Editor of equipment and manufacturers is a screen that allows search, viewing, and input of new and editing of already existing equipment of different types for phosphorus-containing products technology as well as information on equipment suppliers. The data have been stored for the main type of equipment (reaction apparatuses, heating/cooling apparatuses, separation columns etc.) as well as for supplementary equipment (stirrers, pumps and so on). Editor of equipment and its manufacturers (Figure 12) enables to search, edit existing, and enter new equipment for P-containing products, and equipment manufactures.

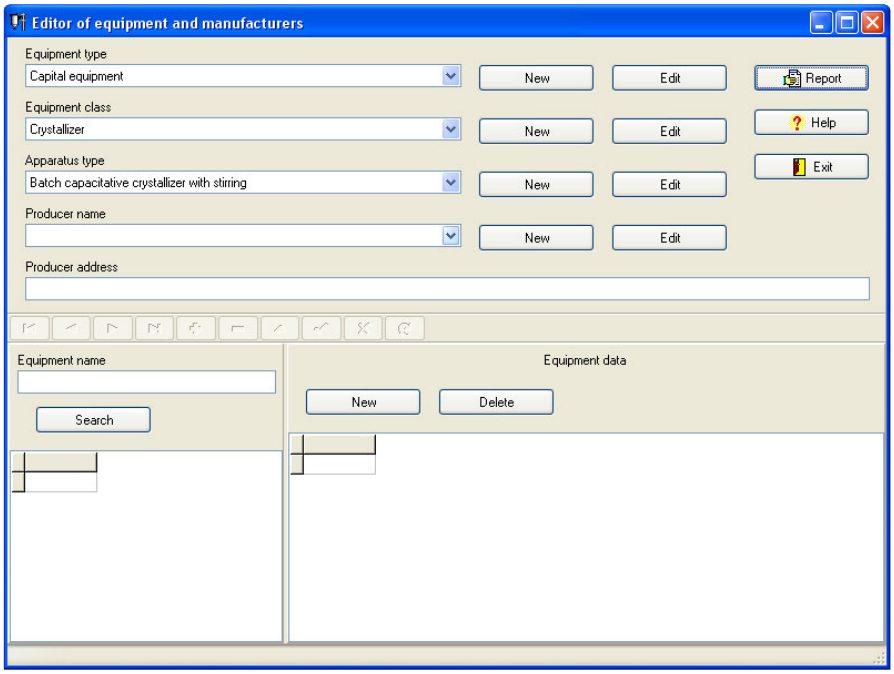

Figure 12. Editor of equipment and its manufacturers

d. Editor of expert system knowledge is an option that enables search, viewing, and input of new and editing of already existing expert system knowledge. For example, expert choice of suitable process flowsheet for different products, crystallization equipment type adjustment, and so forth.
e. Editor of models for phosphorus-containing substances is a screen to create, add and edit models for phosphorus-containing substance production. Represents a window that allows search, viewing, and input of new and editing

of already existing models for phosphorus-containing substances production, their parameters, and also adjustment of auxiliary parameters intended for model functioning in framework of information system.

f. Editor of procedures for unit conversion – is a screen that allows search, viewing, and input of new and editing of already existing unit conversion procedures.
g. Editor of padding calculated procedures is a screen that allows search, viewing, and input of new and editing of already existing auxiliary calculation procedures. Data have been stored for various supplementary computational operations (for example, curve approximation).
h. Editor of related documentation and papers is a screen that allows search, viewing, input of new and editing of already existing specialized documentation and papers. Data relevant to scientific papers concerned with phosphorus-containing substance production; process regulations and other supplementary documentation are stored. It is a separate database which enables the storage as text files as well as complete documents of various formats.
i. Editor of schemes of phosphorus-containing product production is a window that allows search, viewing, and input of new and editing of already existing flowsheets phosphorus-containing product technology.

Examples of process flowsheets for phosphorus-containing products:

- Process flowsheet for sodium hypophosphite production.
- Process flowsheet for sodium phosphite production.
- Process flowsheet for dibasic lead phosphite production.
- Flexible process flowsheet for production of sodium hypophosphite, sodium phosphite, dibasic lead phosphite.

3.3. 3. Reports Section

The Reports menu is shown in Figure 13. Planned is the output of reports is envisaged in Word, Excel and other formats. Where possible, output of Process flowsheet reports will be accompanied also with graphic document formats (CorelDraw, AutoCAD vector graphics documents etc.). Along with this, the «universal» report (report master) for database reports output may be included. For Expert choice supplementary report output with expert choice results will be included as well as progression of expert system questions and user answers respectively.

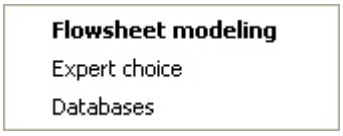

Figure 13 .Reports menu

a. Reports on flowsheet modelling are presented in a screen for viewing and printing ready reports (with data) and editing of already existing templates for reports of flowsheet modelling.
b. Reports on expert choice are presented in a screen for viewing and printing of ready reports (with data) and editing of already existing templates for reports of expert choice.
c. Reports on databases are presented in a screen for viewing and printing of ready reports (containing data) and editing of already existing templates for reports of databases (possible is a variant of developing universal templates or dialogs for forming reports of databases).

4. Database Server and Application Server

4.1. Database server

The Database server represents the Data manager for the storage of information needed for operation of the Information system ECOPHOS IS. Databases are constructed on the basis of relational data model. Work with Data manager is conducted with SQL (structured query language).

The Database server has been built and it its final version will consist of the following databases:

- The database of substances physical-chemical properties;
- The database of phosphorus-containing substances and raw material producers;
- The database on equipment and its producers;
- The database of expert system knowledge;
- The database of models for phosphorus-containing substances synthesis;
- The database of procedures for dimension units translation;
- The database of calculation procedures (approximations etc.);
- The database of users and managers access authorities to information system;
- The database of specialized documentation and papers;
- The database of schemes of phosphorus-containing products production;
- The database on simulation of chemical-technological processes

4.2. Application server

Represents a specialised application (the ECOPHOS project development) based on the DataSnap technology (developed by CodeGear) and COM technology (developed by Microsoft) and designed for functioning as an intermediate member between the Client application (IS ECOPHOS client) and Database server. The function of the Application server aims at ensuring data communication between the Application server itself and, generally, remote database server through Internet. In addition, it provides data exchange between ECOPHOS IS Client and the Application server and the ECOPHOS IS Clients. In their turn, many application servers are able to exchange

data with various database servers. Such an organisation scheme possesses good scalability and high capacity.

The Application Server can further provide ECOPHOS IS Clients with supplementary services such as eg MathLab, MathCad, AspenPlus. At the same time, the Application Server provides computational processing of modelling processes and processing of the main tasks of the Information system. Results of such services are finally supplied to the users in convenient formats (dialogs, reports, popular format documents and so forth).

5. Conclusions and Future Work

- The ECOPHOS IS has a multilevel structure (three-level architecture). The system consists of the following components: database server, application server and client application. So far the work has been focused on Client Application development.
- The information available from various sources will be fed into the toolbox, including the data from projects such as CAPE-OPEN (1997-1999), GLOBAL CAPE-OPEN and CO-LaN 2001-2004 (www.colan.org) for the chemical industry and will follow the standards established in these projects. Thus particular emphasis will be placed in order to promote the use and the development of the CAPE-OPEN standard in Computer-Aided Process Engineering (CAPE) software, and more generally to encourage all actions aiming at facilitating the use of CAPE software tools in industry, administration and academia.
- Future development has been focused on Application Server and Database Server development with subsequent filling in the databases and testing the Information System as a whole.

6. Acknowledgement

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