Remote Optimization in Petrochemistry

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Abstract: - In order to extend worldwide the *processing business* of the petrochemical plant, its potential business partners can themselves concurrently simulate production plans with high quality technical and economic features. In the simulation process, a large number of divergent goals are under attention. Therefore, the plant computer will use the multi-objective linear programming as a tool for negotiations. The dialog between a partner and the plant computer consists in two steps, namely *processing demand* and *plant response*, performed repeatedly until the business makes sense or it shows unacceptable. In the first case, can be signed the processing contract.

Key-Words: - E-Business, Large Scale Systems, Mathematical Modeling, Web Enabled Optimization, Multi-Objective Linear Programming, Internet Computing.

1 Introduction

As opposed to discrete process plants that can adopt, beside new technology, the reorganization of their internal functions and can better realize the horizontal integration with their business partners, possibly by considering the concept of "extended enterprise", continuous process plants, like petrochemical ones, can only resort, at this stage of technological development, to "reengineering" the business processes [1], [2], [3]. Obviously, the approaching of the business processes reengineering are linked to the development of new software for production control [4], [5], [6]. As it is known, *e-business* is now the most important way to determine changes in the acting manner of businesspersons.

Because of scarcity of raw materials, a consequence of shrinking finance, the plant must process the raw materials belonging to various partners in order to avoid working below its actual capacities. Petrochemical plants yield a good deal of their output under "processing regime". This signifies that the raw materials are not purchased by the plant, but are owned by a business partner whose intention is to squeeze maximum out of their treatment. The drawback in this case is bombarding the plant with lots of processing proposals, not to be finalized ever because of their overrating by business people. In order to negotiate a mutual advantageous business, the solution could be a

dialogue via Internet between potential partners and the plant computer. Once founds that business makes sense, the contract signing can be done. The simulating of optimal plans in these circumstances must be very fast and it must allow the concurrent work for a large number of plant partners. For this purpose, ICI has developed the software named Tele-PROCESSING.

2 Plant mathematical model

The software designed for production planning in petrochemical industry achieves both structural and functional description of the plant [7]. The plant "anatomy" is given by describing the structure directed multi-graph, vertices being the individual production cells (IPCs) and arcs being the pipelines (Ps) between these. The plant "physiology" is given by describing the IPCs and Ps' behavior. From this, it is possible to generate and solve planning problems as Multi-Objective Linear Programming (MOLP) problems.

2.1 Synthetic plant model

The planning model is:

$$\begin{split} f_l(\underline{x}) &= \sum_{i=1}^n c_{i} x_i, \ l \in \overline{1,h} \ , \ g_j(\underline{x}) = \sum_{i=1}^n a_{ji} x_i, j \in \overline{1,m} \ , \\ c_{li}, a_{ii}, b_i &\in \Re \ , \ (\forall) \ l \in \overline{1,o} \ , \ i \in \overline{1,n} \ , \ j \in \overline{1,m} \ . \end{split}$$

In conclusion, there exist: n – decision variables, namely the yields of production system, m – constraints ($m = m_1 + m_2$, m_1 are technological constraints and m_2 are commercial constraints), o – objectives ($o = o_1 + o_2$, o_1 are plant objectives and o_2 are partner objectives).

2.2 Analytical plant model

Let $C = \overset{\circ}{Y} C_k$ be the set of IPCs, decomposed into six classes: 1) system inputs, 2) efficiency-type relations based IPCs, 3) blending-type relations based IPCs, 4) specific consumptions relations based IPCs, 5) flow merging / distribution nodes, 6) system outputs. In the multi-graph terminology all the elements of C are vertices, while for C_1 and C_6 only outgoing and incoming arcs respectively exist, for the remaining $C_k((\forall)k=\overline{2,5})$ both arc types being possible. For a certain vertex c, let id(c) be the indegree and od(c) be the outdegree. Some characteristic features of the model, which represents the industrial complex, can be identified: 1) id(c) = 0 $(\forall)c \in C_1$, od(c) = 0 $(\forall)c \in C_6$,

and
$$1 \le id(c), od(c) \le 20,$$
 $(\forall) c \in \overset{5}{\underset{k-2}{\text{Y}}} C_k$; 2) no

(self)loops are present; 3) all circuits have more than two arcs; 4) dimensions are rather large, the number of vertices, arcs and circuits typically amounts to hundreds, thousands and tens, respectively and so, such a kind of plant is a large-scale system (LSS). Each IPCs class has its own behavior, which is presented in the following:

- For C_1 and $(\forall) c \in \overline{1, c_1}$, outputs O_i^c available AVA^c and quantities Q_{\min}^c , Q_{\max}^c , fulfill:
- $Q_{\min}^c \le AVA^c \le Q_{\max}^c$ (limiting of the available quantity relation) (1)
- $\sum_{i=1}^{od(c)} O_i^c \le AVA^c$ (relation for the distribution of the available quantity) (2)
- For C_2 and $(\forall)c \in \overline{1,c_2}$, inputs I_j^c , outputs O_i^c , capacities CAP_{\min}^c and CAP_{\max}^c , inputs I_j^c in outputs O_i^c efficiency transformation coefficients R_{ij}^c ,

quantities Q_{\min}^c , Q_{\max}^c and weights p_k , q_k for inputs and outputs respectively, fulfill:

-
$$O_i^c = \sum_{j=1}^{id(c)} R_{ij}^c \cdot I_j^c$$
 $i \in (\forall) i \in \overline{1, od(c)}$ (efficiency relations)

where
$$R_{ij}^c$$
 fulfills $\sum_{i=1}^{id(c)} R_{ij}^c = 1 \ (\forall) i \in \overline{1, od(c)} \ (3)$

- $CAP_{\min}^c \le \sum_{j=1}^{id(c)} I_j^c \le CAP_{\max}^c$ (refining capacity relation)
 (4)
- $(\exists)i \in \{1, 2, \dots, od(c)\}$ such that $Q_{\min}^c \leq Q_i^c \leq Q_{\max}^c$ (limitation relations for some inputs)

- (
$$\exists$$
)
$$\begin{cases} ISUB^c \subseteq (\{1,2,...,id(c)\} \setminus \{j\}) \\ p_k \in \mathfrak{R}_+(\forall)k \in ISUB^c \end{cases}$$
 for fixed j such

that
$$I_j^c = \sum_{k \in NUD^c} p_k I_k^c$$
 (6)

&
$$(\exists)$$

$$\begin{cases}
OSUB^c \subseteq (\{1,2,...,od(c)\} \setminus \{i\}) \\
q_k \in \Re_+(\forall) k \in OSUB^c
\end{cases}$$
 for fixed i such

that
$$O_i^c = \sum_{k \in OSU/R^c} q_k O_k^c$$
 (7)

(the inputs and outputs intercondition relation)

• For C_3 and $(\forall) c \in \overline{1, C_3}$, inputs I_j^c , output O^c , capacities CAP_{\min}^c and CAP_{\max}^c , blending coefficients r_j , qualities $QUAL_l^{\min}$, $QUAL_l^{\max}$ of output and qualities $QUAl_{lj}$ which define the contribution of input j to the corresponding quality of the output $QUAL_l$, fulfill:

-
$$O^c = \sum_{j=1}^{id(c)} I_j^c$$
 (free blend relation) (8)

- $I_j^c = r_j \cdot O^c$, $(\forall) j \in \overline{1, id(c)}$ (blending recipe relation) with $0 \le r_j \le 1$ $(\forall) j \in \overline{1, id(c)}$ and $\sum_{j=1}^{id(c)} r_j = 1$ (9)

$$-O^{c} \cdot QUAL_{l}^{\min} \leq \sum_{i=1}^{id(c)} QUAL_{lj} \cdot I_{j}^{c}, (\forall) l \in \overline{1, l(O^{c})}$$

$$(10)$$

&
$$O^c \cdot QUAL_l^{\max} \ge \sum_{j=1}^{id(c)} QUAL_{lj} \cdot I_j^c, (\forall)l \in \overline{1,l(O^c)}$$
 (11)

(quality standards relations)

-
$$CAP_{\min}^c \le O^c \le CAP_{\max}^c$$
 (capacity relation) (12)

• For C_4 and $(\forall)c \in \overline{1,c_4}$ inputs I_j^c , principal / secondary outputs $PRI_-O_{i_p}^c$ and $SEC_-O_{i_s}^c$, capacities CAP_{\min}^c and CAP_{\max}^c , quantities $Q_{i_p \min}^c$, $Q_{i_p \max}^c$, specific consumptions for obtaining the principal outputs $SC_{i_p j}^c$ and the ratios for obtaining the

secondary outputs from the first principal output $RA_{i_s1}^c$, fulfill:

$$-\sum_{j=1}^{id(c)} I_j^c = \sum_{i_p \in PRI_OSUB^c} PRI_O_{i_p}^c + \sum_{i_s \in SEC_OSUB^c} SEC_O_{i_s}^c$$
 (inputs - outputs balance relation) where:

$$\begin{cases} PRI_OSUB^c, SEC_OSUB^c \subset \{1,2,...,od(c)\} \\ PRI_OSUB^c, SEC_OSUB^c \neq \emptyset \\ PRI_OSUB^c \mid SEC_OSUB^c = \emptyset \\ PRI_OSUB^c \mid SEC_OSUB^c = \{1,2,...,od(c)\} \\ card(PRI_OSUB^c) << card(SEC_OSUB^c) \end{cases}$$

-
$$PRI_{-}O_{i_{p}}^{c} = CS_{i_{p}j}^{c} \cdot I_{j}, (\forall) \begin{cases} i_{p} \in PRI_{-}OSUB^{c} \\ j \in 1, id(c) \end{cases}$$
 (specified)

consumptions relations) (14)

-
$$SEC_{-}O_{i_s}^c = RA_{i_s1}^c \cdot PRI_{-}O_1^c$$
, $(\forall)i_s \in SEC_{-}OSUB^c$ (ratio relations) (15)

-
$$CAP_{\min}^c \le \sum_{j=1}^{id(c)} I_j^c \le CAP_{\max}^c$$
 (capacity relation) (16)

-
$$(\exists)i_p \in PRI_OSUB^c$$
 such that $Q_{i_p \min}^c \le Q_{i_p \max}^c \le Q_{i_p \max}^c$ (limitation for principal outputs) (17)

• For C_5 and (\forall) $c \in \overline{1, c_5}$, inputs I_j^c , outputs O_i^c and weights p_k , q_k for inputs and outputs respectively, fulfill:

$$-\sum_{j=1}^{id(c)} I_j^c = \sum_{i=1}^{od(c)} o_i^c \text{ (inputs-outputs balance relation) (18)}$$

$$- (\exists) \begin{cases} \mathit{ISUB}^c \subseteq (\{1,2,..,id(c)\} \setminus \{j\}) \\ p_k \in \mathfrak{R}_+(\forall) k \in \mathit{ISUB}^c \end{cases} \text{ for fixed } j \text{ such that }$$

$$I_j^c = \sum_{k \in SUR^c} p_k I_k^c \tag{19}$$

&(
$$\exists$$
)
$$\begin{cases} OSUB^c \subseteq (\{1,2,...,od(c)\} \setminus \{i\}) \\ q_k \in \mathfrak{R}_+(\forall)k \in OSUB^c \end{cases}$$
 for fixed i such that

$$O_i^c = \sum_{k \in OSUB^c} q_k O_k^c \tag{20}$$

(the inputs and outputs intercondition relations)

- For C_6 and $(\forall)c \in {\tt l}, c_6$, inputs I_j^c , deliverable DEL^c , minimum needed quantity O_{\min}^c and maximum quantity that can be stored / transported $S/T_O_{\max}^c$, fulfill:
- $DEL^c = \sum_{j=1}^{id(c)} I_j^c$ (deliverable quantity accumulation relation) (21)

- $Q_{\min}^c \le DEL^c \le S/T Q_{\max}^c$ (relation that limits the deliverable quantity) (22)

Remarks:

• For the Ps with accumulation buffers, input in accumulation buffer I^c , output from accumulation buffer O^c , capacity CAP_{\max}^c , initial stock I_S^c , final stock F_S^c and quantities before / after the accumulation buffer $A \ Q^c$ and $P \ Q^c$, fulfill:

-
$$A_{\underline{Q}}^c + O^c = P_{\underline{Q}}^c + I^c$$
 (flow balance relation)
(23)

- $I^c + I_S^c = O^c + F_S^c$ (accumulation buffer balance relation) (24)

-
$$I^c + I_S^c \le CAP_{\text{max}}^c$$
, $O^c \le I_S^c$ (accumulation buffer capacity relations) (25) therefore, the links have their own behavior;

• The IPCs belonging to C_2 and C_4 can have several running modes. Thus, the relations (3), (13), (14), (15), (16) and (17) should be written adding a superscript r that denotes the running mode. As a result, the following relations must be added:

$$-\sum_{r=1}^{r(c)} I_j^{cr} = I_j^c, (\forall) j \in \overline{1, id(c)}$$

$$\tag{26}$$

$$-\sum_{r=1}^{r(c)} O_j^{cr} = O_j^c, (\forall)_j \in \overline{1, id(c)}$$
 (27)

- At any given moment, the IPCs belonging to C_3 can function according to only one set of the relations: (8) / (9) / (10) & (11);
- The decision maker can define a set of linear objective functions, denoted by $\underline{f} = (f_1(\underline{x}), f_2(\underline{x}), ...$

..., $f_l(\underline{x})$, where $\underline{x} \in \mathfrak{R}_+^n$. For instance, the value of final products is:

$$-\sum_{c \in C_7} DEL_PRICE^c \cdot DEL^c$$
 (28)

where
$$\begin{cases} C_7 = C_7' Y C_7'' \\ C_7' I C_7'' = \emptyset \end{cases}$$
, C_7' being deliverable outputs and

 $C_7^{"}$ being remaining outputs (side effects).

• The parameters and variables describing the IPCs and Ps' behavior are in \mathfrak{R}_{+} .

2.3 Model Characteristics

In this field, MOLP problems have the following characteristics: huge dimensions (thousands of rows and columns), predominance of equality relations (following from Kirkhoff's first law), emphasized

sparsity, wide differences in the order of magnitude of the various coefficients of the model (leading to scaling), "tight" feasibility (sometimes leading to the absence of a feasible solution). This is true mainly for the technological constraints. Nevertheless, the problem also contains commercial constraints that are usually stated by the business partner. They are limits for the end products. Main objectives included in the plant objectives set are the market value of the end products, the value of the net production, processing costs, labor costs, stocks of end products, on flow stocks, profit and pollution prevention costs. The partner objectives set usually contains profit, crude oil value, shipping costs, ingredients cost, processing cost and end products value.

To generate and solve such kind of problems is a very difficult task by itself. In nowadays, many well-trained teams in production departments of petrochemical plants are designated to simulate diverse variants of production plans using the PIMS software. However, to accomplish this task from remote locations, worldwide situated, by people without a special training, it is a true challenge. In the following, it is shown how this thing is possible.

3 Tele-PROCESSING Software

Like any advanced software working from a plant electronic site, Tele-PROCESSING has two functional blocks. The first block addresses the Production Department in plant, therefore, works on the Intranet and is written in MSVC 6.0. The second block addresses the partners of processing business, therefore, works on the Internet and is written in ASP. An automation block, whose role is to exclude plant specialists' intervention in the simulation process, links these two blocks. It is a supervisor program, developed in the dormant technique that automatically runs, at a given tact, the optimizations / re-optimizations as well as other actions such as optimization data management. Obviously, there can be some exceptions that must be treated by human intervention, the computer breakdowns only!

It is to notice that Tele-PROCESSING works as a shell over the PIMS software whose database, contain crude oils and their characteristics, raw materials, ingredients, on-flow products, end products, capacities, technological data (regarding efficiency transformation coefficients, specific consumptions, blending recipes, inputs / outputs inter-conditions relations, stocking capacities, functioning regime etc.), repairs, system timetable, is available. Ones must consider a processing

demand only for a crude oil that the production system can process it and only for the free capacities in a certain time level (decade, month, quarter, and year). Even for the same time level, in various time horizons. free capacities map can be very different because the regular production plans can differ. Adding, to this back-office, structured information about plant partners (users, companies and their banks) and associated simulated production plans one obtains the information framework for Tele-PROCESSING software well functioning. The supplementary information is managed using SQL Server 7.0 Enterprise Edition. This is the ensemble of information necessary to start simulating the processing business, i.e. defining an optimization planning problem, solving it, reading the result and the associated economic indicators, (repeat the process if is necessary) and deciding on bussines opportunity.

3.1 Partners Registration

Using the "Registration" site section, the potential partners must register in the system. Only thus, they become beneficiaries of the mechanism that is able to make a remote plan simulation and an estimation of the profit that can be obtained in the processing business.

The security is a very serious problem, solved in an elaborate manner. For exterior, there is the PKI component that assures access control. authentication, non-repudiation, integrity of data transfer, digital signature, etc. For interior, a special component manages the database integrity. Every unauthorized access, even those made by programmers directly on the database tables, provoke system blockage until the system automatically regains its integrity. The supervisor also runs this function. Therefore, the partners can trust that they work in an environment characterized by correctness and loyalty. The "trust's problem" was very well solved. The partners' risk is minimized because, from the very beginning, they are not financially involved. The organizer risk involves the competitors' earnestness. The business is based, as always, on partners' honor. The size of the business is not a limitation.

3.2 Processing Proposals

It is now possible to access the *e-processing* site using Microsoft Internet Explorer or Netscape Navigator browsers. As a rule, the mathematical model data are the plant "know-how" and are secret. To protect them, the plant makes public on the Internet only the data referring the ingredients and the end products. For a partner it is normal to give the quantity of crude oil to be processed with its physical-chemical properties, the data levels associated with the desired products and the

processing time horizon. These are the data that the business partners find to be of paramount importance and only they are taken into consideration.

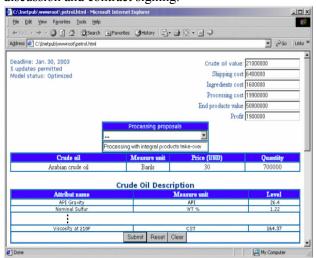
Accessing the site section named "Processing proposals", the business partner can make a "processing demand" by specifying: processing demand's name, crude oil name, measurement unit, price and quantity. To describe the crude oil it is also of outer importance. Ones can do this job by filling up the table containing: attribute name, measurement unit and level for each physical-chemical characteristic. Shipping cost is information of low importance. It is necessary to compute the partner profit (Capture 1). A simple pushing on submitting button triggers the taking over of the processing demand by the Tele-PROCESSING supervisor.

In order to decide whether the crude oil can be processed or not, the supervisor checks the crude oil pattern. If it is technologically unacceptable, the partner is invited to give another crude oil with characteristics that fits to the plant production system. If it is acceptable, the characteristics are frozen, they cannot be afterworlds changed, and the processing proposal is passed, for optimizing, to the scheduling mechanism. This inserts the demand into the waiting queue. The insertion is made according to a priority coefficient computed taking into account the value of the business and the number of the previous optimizations. Even a powerful computer cannot efficiently solve more than five optimizations at the same time. So, the launchings in executions are made gradually in time. The partner is informed about the plant response by consulting the optimization status.

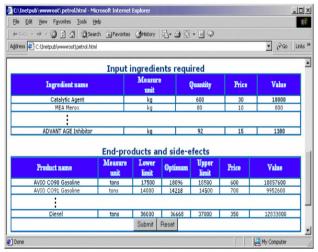
Once the optimization is finished, one offers three categories of information: a) Inputs (ingredient name, measure unit, quantity, price and value); b) Outputs (end product name, measure unit, lower limit, optimal quantity, upper limit, price and value); c) Economic indicators (crude oil value, shipping cost, ingredients cost, processing cost, end products value and profit) (Capture 2). At this moment, the business partner can establish some conditions for the end products, maybe influenced by the market and ask for a new optimization The number of the optimizations, as well as the time allowed for negotiations, is limited. As it is shown before, the business partner analyzes the results of any optimization work, i.e. the end products levels attained through production optimization and the values of objective functions. The partner may consider it necessary that the plant computer must make the iterations of the business optimization for as many times as it takes to reach the best result, or otherwise he may wish to get out of business.

3.2 Best Proposals

Taking into account that a multitude of potential processing partners can concurrently make tempting proposals for the same time level and horizon, Tele-PROCESSING software arranges the proposals, for each time level and horizon, into three classes: big, medium and small businesses. Every business class benefit from a Multi-Attribute Decision Making (MADM) type optimization. If in the MLP problem there exist only ten objectives, in the MADM problem are stated over two hundred attributes, expressed by more than one expert (technologists, economists, bankers, ecologists etc.) in more than one state of nature (economic stability, inflation, deflation etc.) Thus, the plant managers can appreciate on solid basses, which is the best proposal. The practice shows that it is possible to exist one or many winners for every business class. They are invited for a last discussion and contract signing.



Capture 1. Processing proposal



Capture 2. Input and output data of an optimized processing

The production department staff, to whom some IT people will join, will take the responsibility for watching the system and answering to the partners electronic letters. The plant computer automatically solves even the processing demands that present problems, like void feasibility domain, caused by overrating of plant capacities. The function that ensures the man-machine interface on the Intranet is analogous with the function that works on the Internet.

In addition, also a function manages the partners' section of the database. The main goal of this function is to compute, in time, based on statistical data, the partners' allowance.

As ones can see in this paper, the designer preoccupation was the optimization process automation. Only the economic contract signing is out of the system, mainly because of the bureaucracy accepted as necessary in this field. Thus, the plant will be able to improve the quality of the processing business. Extending worldwide the business of a plant is one of the globalization commandments. Another, very important too, is to promote mutual advantageous business. Tele-PROCESING will be capable to support such kind of business. This is possible by making use of advanced simulation and optimization techniques. Web enabled simulation and optimization is a new trend in treating the complex industrial problems. Moreover, the designing team preoccupation is to extend the facilities of treating the concurrent optimizations by using GRID solutions.

4 Conclusion

The Internet created the support for a new range of applications. In our days, *e-applications* undergo a fast development. In the authors' opinion, elaborate *e-business* applications will soon become facts on the IT market.

Tele-PROCESSING software is under final testing; launching it is thought to be a real event and to have a significant impact at level of petrochemical industry. A series of Romanian petrochemical plants have supported testing in real conditions and the conclusions have been encouraging. The software architecture is general for a advanced e-applications but, as Tele-PROCESSING is not business to consumer but business-to-business software and its applicability is with petrochemical plants, some particularities individualizes the manner of doing electronic business with this software. It really contributes to the modernization of the processing business. Its capabilities related to genuine e-business make it

suitable to contribute to the invigoration of the business. With this software, petrochemical plants may become more active on the world market via Internet. The strong point of Tele-PROCESSING software is the fact that the *processing business* is optimal for both the plant and its business partners. Please remark that although the mathematical model shows high complexity, Internet developed interface is a narrow one, because it concerns reasonable demands. Its interface is very "human" because people without a special training in mathematics and informatics can easily use the software.

Tele-PROCESSING delivery conditions and services included are software and documentation on CD, autodemonstration, on-call / on-site assistance in use and short time training course (16 - 40 hours) for initiation in electronic business. Further developments refer to extensions for other continuous process industries. Ones suppose that the Internet modules and the simulation mechanism will be the same, only the Intranet modules and the optimization will change. Therefore, a lot of programming work will be save with good consequences for delivery time and software cost.

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