EuroBioRef

Project acronym:	
Project Title:	EUROpean multilevel integrated BIOREFinery design for sustainable biomass processing
Instrument:	Large Scale Collaborative Project
Thematic Priority:	FP7-ENERGY.2009.3.3.1
Grant Agreement:	241718
Start Date of Project:	01/03/10
Duration:	48 Months

SP7 – Conceptual Process Design and Integration of the Whole Process Chain/Grid into a Biorefinery
WP7.1 – Conceptual Process Design for Each Process to be Integrated

Deliverable report

Due Date of Deliverable: M36 - 28/02/2013
Actual Submission Date: M36 - 20/02/2013

Deliverable Identification	
Deliverable Number:	D7.1.11
Deliverable Title:	Conceptual process design for sub-processes to be integrated into a biorefinery
Responsible Beneficiary:	PDC
Contributing Beneficiaries:	PDC
To be Submitted to the EC:	Yes

History			
Version	**Author**	**Modification**	**Date**
V1	Raf ROELANT	First version	15/02/2013

Approval				
	Name	**Organization**	**Date**	**Visa**
Deliverable Responsible	Raf ROELANT	PDC	15/02/2013	OK
Work Package Leader	Wei Zhao	PDC	18/02/2013	OK
Sub-Project Leader	Wei Zhao	PDC	18/02/2013	OK
Coordinator	Franck DUMEIGNIL	CNRS-UCCS	19/02/2013	OK

Dissemination level		
PU	Public	X
PP	Restricted to other programme participants (including the Commission Services)	
RE	Restricted to a group specified by the consortium (including the Commission Services)	
CO	Confidential, only for members of the consortium (including the Commission Services)	

* In case of dissemination level of PP/RE, the persons (or group of persons) agreed to have an access to the document are: Non applicable

Content

Executive summary

Description of the deliverable objective and content

The objective of this Deliverable is to describe the methodology applied by PDC to perform the conceptual design of the individual EuroBioRef processes. These processes are being integrated into value chains, but that integration is beyond the scope of this Deliverable.
As this document is to be made publically available, it does not contain any confidential details. For the individual processes, refer to the confidential Deliverables of WP7.1.

Deviation from objectives and corrective actions

There are no deviations from the objectives stated in the Description of Work.

Impact of the results

This Deliverable provides insight into PDC's methodology and draws attention to some methods which are specifically suited for the nonconventional bio-derived chemistries typical to EuroBioRef. This is useful for the partners of the Consortium, but also for current and future other projects on the production of bio-derived fuels or chemicals.

Related IPR

The contents of this report are not patentable.

Publishable information

The contents of this report will be presented at the 9th European Congress of Chemical Engineering, to be held in The Hague, The Netherlands, April 21-25, 2013. The title of the presentation will be "Heuristic-numeric process synthesis for bio-based chemistries". PDC does not pursue a written publication.

Conclusion

PDC performs its conceptual design in a structured way through its proprietary expert system PROSYN®. The core of this expert system is a collection of heuristic rules which power the user with the knowledge of experts from various branches of chemical engineering. The system guides the user through the relevant design questions, avoiding the collection of unnecessary information. PROSYN® contains more than heuristic rules. Through the use of numerical procedures, in particular to calculate physical properties, it assists the user in providing the right input. PROSYN® can be applied to specific unit operations or whole processes.
In order to judge the technical feasibility of a process, the most challenging unit operations need simulation through specialized software. In view of the many unconventional and polar components in EuroBioRef, the necessary attention has to be paid to the physical property methods applied. In any case, simulation has to be applied parsimoniously in order to save design time.
Mass balances can be quickly obtained for flow sheets by approximating (part of) the unit operations by linear functions. By a rough design of the heat exchanger network or a pinch analysis, the mass balances can be supplemented with estimated consumptions of utilities.
The economic evaluation of a process concept starts with the estimation of the main dimensions of the unit operations. PDC's Cookbook, part of PROSYN®, allows to estimate the capital costs for these unit operations based on these dimension estimates. The total capital cost and the operating costs, which mostly follow from the mass and energy balances, allow predicting the production cost of the main product and the profit related to the process.

ANNEX I – Technical content

Aims in EuroBioRef

The aim of applying conceptual process design in EuroBioRef is threefold:

1. To design technically and economically feasible process flow diagrams, if such proves possible. Structural conceptual design bridges the gap between experiments and industrial implementation. Conceptual design is particularly suited at an early stage of R&D, which applies to most of the bio-conversion routes studied in EuroBioRef. This allows the concentration of the limited resources available for R&D on the most promising reaction routes.
2. To provide guidance to the catalyst developers. This feed-back stems from our observations during process design. Our analysis could show, for example, that the production of a certain by-product is the most important evaluation criterion in catalyst design from the point of view of industrial implementation. It could also show that the activity of the catalyst needs to be enhanced.
3. To generate novel intellectual property in the form of patented combinations of catalysts and processes.

A need for structuring conceptual process design

Ulrich & Vasudevan (2004) present conceptual process design as the following sequence of steps[1]:

1. Conception and definition,
2. Flow sheet development,
3. Design of equipment,
4. Economic analysis,
5. Optimization.

(1)

The Description of Work of EuroBioRef mentions a similar sequence of steps:

1. Setting up a reliable basic data set (chemical reaction data and physical properties),
2. Conceptual design of the reaction steps,
3. Generating flow sheet alternatives for the separation sequence,
4. Integration of reaction and separation options,
5. Cost optimization of the flow sheet alternatives.

(2)

These work sequences certainly have their merit as ways to structure conceptual design and indeed represent usual orders in which design tasks are performed. However, sequences such as (1) and (2) should not be imperative. For example, before a flow sheet has been developed, it makes sense to perform a black-box economic analysis where only the product revenue and the raw materials cost is taken into account (and perhaps a preliminary estimate of the utilities cost and capital cost contributions). As another example, if the success of an idea depends on a key separation step, then the designer may want to evaluate the technical feasibility of this separation by simulation before a flow sheet has been generated.

In its most general form, a design can be seen as an alternation of questions and answers, as illustrated in Figure 1. The process starts with an initial collection of information: for instance a small experimental data set collected in response to an idea from the market research department. Analysis of this information will allow the creation of one or several very poorly defined process concepts or perhaps even a black-box model. This prompts an analysis of the newly defined concept(s) and possibly the gathering of more information: process simulation results, more experimental data, economic information, etc. In the worst case information has to be reasonably assumed. In any case the information gathered allows the creation, rejection, elaboration and/or modification of process concepts, which will again trigger an analysis round, etc. Eventually the design will be stopped if one or several process designs are obtained which are believed to be near-optimal, or if it is concluded that no viable design exists. This can already happen very early. This would be the case, for example, if a black-box model has shown that the revenue to be expected from the product(s) cannot cover the cost of the raw materials needed. Another possibility is that a rough design with a lot of best-case assumptions already entails too high a capital cost to allow an economical process.

[1] The last step mentioned by Ulrich & Vasudevan (2004), « Reporting », is not mentioned here.

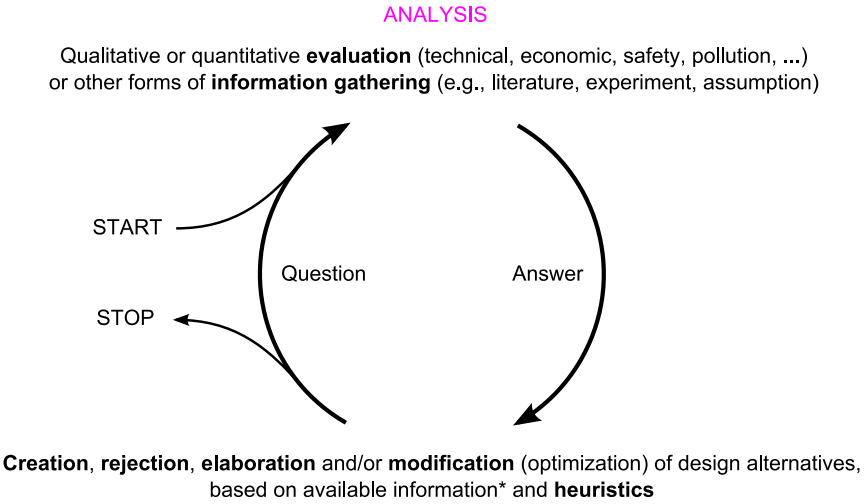


Figure 1. Conceptual design cycle.

The translation of information into process decisions and new information queries relies on the knowledge and wit of the design team. Even if the information is numeric, the design decision usually remains a qualitative process, based on heuristic rules ("rules of thumb"). More experienced engineers rely on larger heuristic rule bases and therefore generally make more successful designers. Unfortunately the personal aspects of the decision making cause design work to be non-reproducible. One design team may have a vast experience in extraction, while another may have a large expertise in crystallization. In this case it is likely that both teams would conclude to different design solutions.

Process synthesis

In the form of its proprietary software PROSYN® (PROcess SYNthesis) and through about 300 man-years of work, PDC has been collecting and implementing a vast collection of heuristic rules to support the decision making in conceptual process design (Schembecker & Simmrock, 1996). This probably makes the expert system the most extensive collection of process synthesis heuristics in existence. Its origin is to be placed in the advent of artificial intelligence, which has reached the field of conceptual process design in the 1980s. PROSYN® offers design engineers a possibility to apply knowledge recorded from experts in various fields (e.g., solvent selection, reactor design, crystallization, reactive distillation, …).
As an example, let us consider a rule on the backmixing characteristics of a reactor:

The backmixing characteristic of the reaction phase of the main reaction X is 'total backmixing', if

1. *The reaction phase is investigated. AND*
2. *The concentration level of the reactants of the reaction phase have to be kept on a medium concentration level. AND*
3. *The list of reactants on a medium level is not empty. AND*
4. *The residence time distribution of the reaction X is 'without influence'. AND*
5. *The goal for reactor selection is 'selectivity'.*

Clause 1, "The reaction phase is investigated", will cause the user to be asked about the reaction phase if such information has not already been supplied before. Evaluation of the Clauses 2 and 3 will invoke rules which investigate the reaction mechanism and corresponding kinetics. These clauses reflect that backmixing (either through mechanical mixing or through non-selective recycling) is recommended if the concentration level of the reactants is to be tempered. Indeed the reactants would be strongly diluted by the products present in the reactor. Tempering the concentration of reactants is desirable for the following reaction mechanism, for example,

$$\begin{aligned} A + B &\rightarrow C, \\ 2\,A &\rightarrow D, \end{aligned} \tag{3}$$

where C is the main product and D is an undesired by-product. Tempering the concentration of A, which is possible by back-mixing the reaction mixture, will suppress the undesired second reaction if

the second reaction is higher order in A than the first one, which is what can be expected from the stoichiometry. Clause 4 ensures that the widening of the residence time distribution caused by back-mixing does not have any negative consequences, which is established by different rules. Clause 5 expresses that the aim of the reactor design is to obtain a high selectivity. There are alternative rules if the aim has been specified by the user as having a high conversion or yield.

The design heuristics are implemented in a logic programming language. As a consequence, the heuristic rules can be introduced without the need to manually structure them in a decision tree. Indeed the compiler performs the linkage of the rules automatically, each time causing an appropriate rule to be invoked based on the outcome of the previously applied rules and all the information gathered as a side-effect. This shows how PROSYN is the result of structuring conceptual process design without predefining a work sequence such as (1) or (2). The invocation of a rule generally involves a request of new information from the user. This incremental way of acquiring information avoids that the user collects information which later remains unused. If the designer were to follow the rigid work sequence (2), for example, the user may collect enthalpies of fusion during step (1), while crystallization could have been discarded a priori. The user often has a chance to provide several alternative answers if he/she cannot reasonably acquire enough information (from literature, experiments, experience, …) to distinguish among them. All information entered by the user is recorded in a knowledge database, which avoids that the user is asked to provide the same information several times. Based on all the information available in the knowledge database, the system proposes one or multiple partial decisions. The user is always offered an opportunity to overrule these suggestions.

From this description it is clear that the application of Prosyn proceeds as a dialogue between the user and the expert system. The whole "conversation" is being recorded, which allows an automatized documentation of the design decisions and why they were made. Moreover, it offers the user a chance to revert certain input provided before. For that matter, this option has been automated.

Besides the design heuristics and the knowledge database, PROSYN® offers numerical procedures to support the user in providing the correct input. As such PROSYN® is not exclusively active in the DECISION part of Figure 1 (through its heuristics), but also in the ANALYSIS part. The largest collection of numerical procedures is a set of models to calculate physical properties of components, e.g., the composition and boiling point of azeotropes.

PROSYN® also contains rules on energy integration and an interface enabling the communication with external programs. The total structure of the expert system is schematically represented in Figure 2. The PROSYN® Manager guides the user through the design of a whole process, invoking the different specific expert systems when the need arises.

In summary, the advantages of applying PROSYN® during conceptual design are that

1. The success rate of designs is increased by making available a vast collection of expert knowledge. This is especially important for those design teams having a narrow field of expertise.
2. The design process is accelerated by
    a. guiding the user through the procedure in a case dependent order,
    b. asking the user for relevant information only,
    c. helping him/her to do so by offering supportive automatic calculation procedures,
    d. taking over the laborious and therefore often neglected task of documenting the design decisions and the underlying reasoning.

PROSYN® has been applied for most conceptual process designs performed in the framework of EuroBioRef. However, in order not to infringe confidentiality, we cannot give examples here.

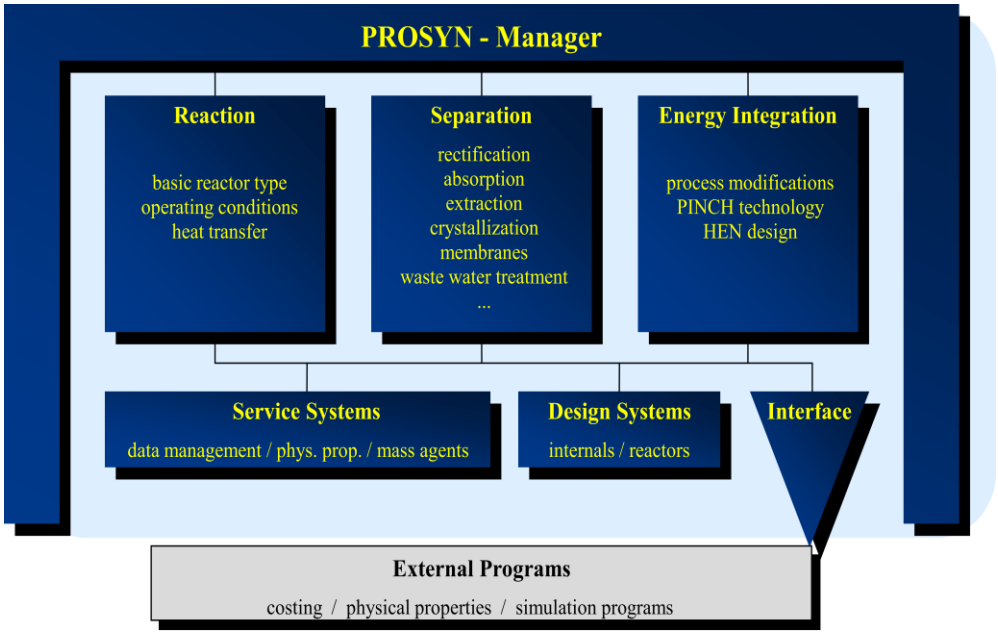


Figure 2. The structure of PROSYN®. HEN stands for "Heat Exchanger Network".

Technical evaluation

Individual unit operations

PROSYN® alone is not enough to conclude a conceptual design. Indeed, to the extent possible, process solutions have to be validated by evaluating their technical feasibility. EuroBioRef offers the possibility of performing pilot tests to do this. However, obviously, the time and resources available do not permit all proposed unit operations to be tested this way. Luckily, we have the powerful tool of simulation at our disposal. PDC performs its simulations in AspenPlus. In order to obtain plausible simulation results, one has to ensure that proper physical property sets and models are selected.

The EuroBioRef project contains a lot of unconventional bio-derived components. Pure component data are not always present in the Aspen databases or in the specialized public literature. For the less conventional components, we indeed have to apply estimates. These are usually obtained through procedures available in Aspen. However, in order to estimate enthalpies of vaporization, boiling points, critical temperatures and pressures, we often apply Marrero-Gani estimates, which are not available in Aspen (Marrero & Gani, 2001). In their turn, boiling points, critical temperatures and pressures can be used to estimate Antoine coefficients describing vapour pressures as a function of temperature. This is possible through the Riedel equation or its modification by Vetere (Vetere, 2006).

Interactions between polar components are non-ideal. It is therefore important to apply phase equilibrium models which describe this departure from ideality as well as possible. For low operating pressures (up to about 10 bar) we apply activity coefficient methods such as NRTL or UNIQUAC. If key binary interaction parameters are important but missing in the Aspen database, they can be estimated from their molecular structure by the group contribution methods UNIFAC or its Dortmund modification. One has to ensure, however, that the estimated parameters are valid in a sufficiently wide temperature range. Non-condensables such as hydrogen have to be defined as Henry coefficients. Otherwise their solubility in liquids is usually overestimated. If vapour-phase association is suspected, which is typical for molecules with carboxyl groups, Hayden-O'Connell corrections are in order.

At high operating pressures (higher than about 10 bar), it is more appropriate to apply equation-of-state models such as Peng-Robinson and Redlich-Kwong-Soave. We have to be aware that these property models do not provide an adequate description of non-ideal interactions in the liquid phase. In order to overcome this, one can apply the predictive Soave-Redlich-Kwong method which uses UNIFAC group contributions.

Rigorous simulations take quite a lot of time, so they are to be applied parsimoniously. For example, it is usually not really necessary to prove the technical feasibility of stripping off organics from a water stream. In this case relevant parameters such as the top vapour composition and the number of theoretical plates can be reasonably 'guesstimated'.

Mass and heat balances of the process

First approximations of mass and heat balances pertaining to a process flow sheet can often be obtained by applying linear models[2] to each reaction or separation block. In this case there is always a unique solution, which can be found readily (sometimes even analytically). Unit operations which have a strongly nonlinear behaviour (for example a reactor of which the outlet approaches an equilibrium) have to be modelled by rigorous, nonlinear models, at least if they appear in a cycle[3]. Usually such nonlinear models require the assumption of a physical properties method as discussed in Section 0. It is often appropriate to apply different property methods to different parts of a process. Obtaining the mass balance of a process is a part of the evaluation of its technical feasibility. Indeed, negative or very high numbers would indicate technical problems such as the build-up of a component in a loop. Such problems need an adaptation of the design.

The heat balances can be translated into utility consumptions after a parsimonious heat exchange design. In any case a detailed design of a heat exchanger network is not wise since this requires information about the whole value chain ("biorefinery") to which the process under study pertains. It can indeed prove effective to transfer significant flows of heat across process boundaries. As an alternative to a preliminary, parsimonious heat exchange design, it is possible to perform a pinch analysis. This yields the minimum net heating and cooling duties of the process. The real duties can be roughly estimated from these by adding an equal quantity to both in order to account for the expected non-perfectness of the heat exchange.

Economic evaluation

For its economic estimates and the shortcut design which precedes it, PDC applies the Cookbook which is a part of PROSYN®. The Cookbook is a partly automated collection of guidelines and correlations collected over the years.

Shortcut design of equipment

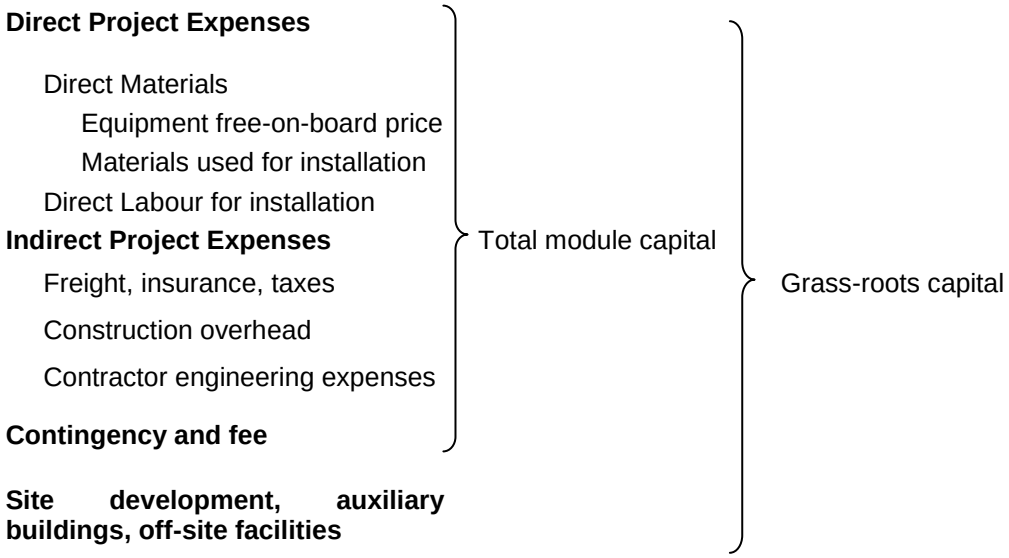
In order to be able to estimate the cost of equipment, one first has to estimate its main dimensions. For a pressure vessel, for example, the diameter, height and orientation (vertical or horizontal) or needed. For a membrane unit, the surface area of the membrane is needed. The rough estimation of such dimensions amounts to a shortcut design of the equipment. For a vapour/liquid separation vessel, for example, the dimensions are determined by a limit on the vapour superficial velocity in order to prevent liquid entrainment and an acceptable liquid surge time. The dimensions of unit operations (typically distillation columns) which have been rigorously simulated in Aspen, see Section 0, can often be estimated in Aspen itself.

Capital expenses

The depreciation of capital expenses represents a particularly important contribution to the total production expenses, especially for the processes in value chains aimed at the production of fuels, which generally have a lower value than chemicals. A breakdown of the capital expenses can be found in Table 1. A distinction has to be made between the case where the process can be installed within the walls of on an existing plant and the case where the site has to be developed from scratch on a greenfield. The basis of the estimation of all capital cost contributions is the equipment free-on-board price, which, in turn, can be estimated through correlations as a function of the equipment dimensions following from their shortcut design, see Section 0.

[2] By linear models, we mean that the effluent streams are linear combinations of the feed streams.
[3] This means that a significant part of the effluent is in some form recycled to the inlet of the concerned unit operation.

Table 1. A breakdown of capital expenses for a new process.



Total production expenses

The mass and heat balances and the preliminary heat integration yields the production of products and by-products and the consumption of raw materials and external heating or cooling utilities (in the form of steam, fuel, cooling water, electricity, …), see Section 0. The cost and revenue corresponding to these streams can be estimated roughly, even though there is quite a lot of uncertainty associated with them. This is due to two factors:

1. The size of the net heating and cooling duties are uncertain due to the preliminary nature of the heat integration, see Section 0.
2. The price of the raw materials and products is abstract as far as they are transferred with other processes in the same value chain. In this case they do not represent net incoming or outgoing streams at the value chain level. Market prices for such streams are not available if these intermediate products are unconventional or impure. It is therefore at best possible to make a rough assumption of the associated costs and revenues and/or a sensitivity study as a function of the uncertain prices.

The difference of the expected stream related revenues and costs gives an impression of the potential of the process, which is useful in an early round of design. The total annual expenses, however, contain many more contributions than those related to the raw materials and utilities, see Table 2. In order to estimate the different contributions, correlations are available which take the capital estimates, see Section 0, the stream related costs, as well as some information from shortcut design of the equipment (e.g. catalyst costs), see Section 0, as input. Deducting the total expenses from the revenue from sales gives the annual profit before taxes. This number summarizes the economic evaluation.

Table 2. Contributions to the total annual expenses related to a process (Ulrich & Vasudevan, 2004).

Manufacturing expenses
Direct
Raw materials, chemical solvents
Catalysts
Operating labour
Supervisory and clerical labour
Utilities
Maintenance and repairs
Operating supplies
Laboratory charges
Patents and royalties
Indirect
Overhead, packing, storage
Local taxes
Insurance
General expenses
Administrative costs
Distribution and selling
Research and development
Depreciation

References

Marrero, J., Gani, R., 2001. Group-contribution based estimation of pure component properties. Fluid Phase Equilibria 183–184, 183–208.

Schembecker, G., Simmrock, K.H., 1996. Heuristic-numeric process synthesis with Prosyn. AIChE Symposium Series No. 312 Vol. 92, 275–278.

Ulrich, G.D., Vasudevan, P.T., 2004. Chemical Engineering – Process Design and Economics – A Practical Guide, 2nd ed. Process Publishing, Durham, New Hampshire, USA.

Vetere, A., 2006. Again the Riedel equation. Fluid Phase Equilibria 240, 155–160.