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Sustainable processes synthesis for renewable resources

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Abstract

Renewable resources pose special challenges to process synthesis. Due to decentral raw material generation, usually low transport densities and the perishable character of most renewable raw materials in combination with their time dependent availability, logistical questions as well as adaptation to regional agricultural structures are necessary. This calls for synthesis of structures not only of single processes but of the whole value chain attached to the utilisation of a certain resource. As most of the innovative technologies proposed to build on a renewable raw material base face stiff economic competition from fossil based processes, economic optimality of the value chain is crucial to their implementation. On top of this widening of the process definition for synthesis, many processes on the base of renewable resources apply technologies (like membrane separations, chromatographic purification steps, etc.) for which the heuristic knowledge is still slim. This reduces the choice of methods for process synthesis, mainly to methods based on combinatorial principles. The paper investigates applicability as well as impact on technology development of process synthesis for renewable raw material utilisation. It takes logistic considerations into account and applies process synthesis to the case study of the *green biorefinery* concept.

The results show the great potential of process synthesis for technology development of renewable resource utilisation. Applied early in the development phase, it can point towards the most promising utilisation pathways, thus guiding the engineering work. On top of that, and even more important, it can help avoid costly development flops as it also clearly indicates “blind alleys” that have to be avoided.

Keywords: Sustainable processes synthesis; P-graph method; Renewable resources; Green biorefinery

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1. Introduction

Synthesis of chemical and petrochemical processes is mostly concerned with developing or optimising processes at a single site. The size of the plant is usually specified in advance, raw materials are considered as standardised commodities at world market prices with no or negligible influence on the structure of the process. Although site-specific boundary conditions (e.g. temporal or spatial availability of utilities, emission restrictions, etc.) can be factored in, the structure of chemical and petrochemical processes is not critically dependent on the location of the site or the regional setting into which the site is to be integrated. Process synthesis then is expected to solve the problem of creating an optimal, integrated and cost efficient structure to convert raw materials to products, more or less ignoring the world outside the factory gate.

The case is, however, dramatically different for processes utilising renewable resources to produce bulk and semi-bulk products. Renewable raw materials are always produced in a specific regional setting and are always restricted in their temporal availability due to the fact that the time for harvesting these raw materials is determined by natural and not economical factors. Besides, in many cases quality of these raw materials varies in a wider range than for petrochemical raw materials and may as well be dependent on regional climatic factors.

Especially if it comes to the production of bulk products renewable raw materials usually have an economical disadvantage, as they are priced higher than fossil or mineral resources, compared to their respective product yield. This is especially true for conventional agricultural products such as cereals or oil seeds, that may on the other hand have preferable technical as well as economical properties like high transport densities, high (or relatively high) content of interesting substances like starch or fats and long shelf life and that are usually traded on an international commodity market, comparable to fossil and mineral resources.

This situation has so far impeded the development of processes based on renewable resources outside conventional sectors like pulp and paper, fat chemistry, food industry and pharmaceutical industry and has contributed to the still undisputed primacy of fossil raw materials as the predominant industrial feedstock. With growing environmental concerns like global warming or increasing waste problems in many countries, but also in the face of expected price increases of crude oil over next 15 years (Schindler and Zittel, 2000) this primacy will however be profoundly challenged. As a result a new set of technologies based on renewable raw materials based on agricultural side products like straw and forestry residues as well as low price crops like grass has been proposed in the course of the last decade. These innovative technologies aim at multi-product plants, thus increasing the efficiency of utilising the available biomass. Using low price or waste materials and utilising these resources to the utmost possible degree, so goes the reasoning, will compensate for the inherent economical disadvantage of renewable resources and allow these technologies to compete with conventional processes on the base of fossil resources.

It is evident that these new crops of technologies pose formidable challenges to technological development in general and the choice of process structures in particular. Raw material production is decentral, transport densities of these raw materials are generally low and shelf life is usually short, factors that put high emphasise on logistics as well as storage technologies. Storage and first processing steps may be located on farms, leading to a new approach for the "site" of production: rather than concentrating process steps in one central unit (which makes sense for processing commodities with standardised properties and high transport densities) the whole region must be seen as "production site", consisting of a mix of decentral and central processing units. Conversely this leads to very different process structures, depending on the natural and agricultural setting of the region but also introducing regional economical factors like storage space availability, costs, prices and availability of energy at different qualities as factors influencing overall process structure.

The paper investigates the possible contribution of process synthesis to the development of this kind of processes. Besides general considerations, process synthesis will be applied to the case study of the concept of a "green biorefinery" in order to exemplify the differences in process structure, that come with changes in regional setting as well as with different regional boundary conditions.

2. The "green biorefinery" concept

In order to investigate the potential of process synthesis in its application to renewable raw materials we will use the case study of the *green biorefinery*, and in order to integrate regional boundary conditions we will use the Austrian situation, which is in some aspects peculiar (e.g. concerning the small size of farms, scattered grassland, high costs in the agricultural sector) but may still be seen as typical for many central European settings.

Let us first have a look at the technological concept of the green biorefinery. The general starting point for this concept is the fact that (at least under European conditions) grassland increasingly becomes a serious surplus problem for agriculture. Conventional use of grassland is as forage for cattle and as basis for milk production. With meat production stagnating (or even declining) and milk production aiming for ever higher productivities per cow (thus substituting green bio mass by concentrated fodder like cereals), the percentage of utilised grassland will decrease considerably over the next decade with grave consequences for farm income as well as landscapes.

The green biorefinery is a concept that utilises green biomass industrially to generate bulk chemicals (especially lactic acid and amino acids), fine chemicals, fibres and fibre products and energy from biogas generation. The idea is that by industrial utilisation of green biomass, farm income and cultural landscapes can be stabilised and new impulses can be generated for a high tech process industry on the base of renewable resources, possibly in regions that are currently disadvantaged due to their peripheral situation and rural structure.

Currently there are a number of technical solutions to this challenge in discussion (Amon et al., 2003; Kromus, 2002). One among them (Kromus, 2002) is the base for the current investigation (see Fig. 1 for a rough flow sheet). The starting point for this technological concept is the (decentral) production of silage on the farms. By starting from silage, two crucial steps are combined: storage (thus enabling the downstream processes to operate continuously) and the conversion of carbohydrates in green biomass to lactic acid. Besides this, silage production also transforms many proteins into amino acids or peptides (Povoden, 2002; Koschuh et al., 2004).

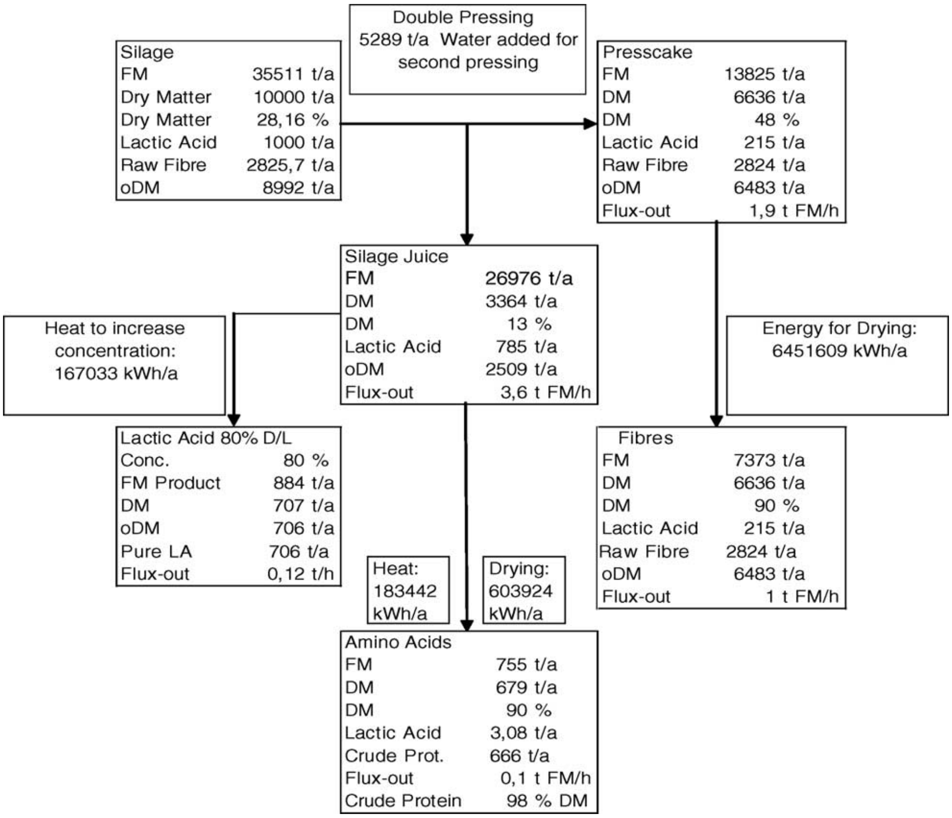

Fig. 1. Flow sheet of a green biorefinery (mass flows and concentrations according to base case).

In a next step silage has to be fractionated by pressing into a solid press cake (containing fibres and still a sizeable amount of amino acids, peptides and carbohydrates) and a liquid juice, containing lactic acid and water soluble amino acids. This step may be intensified by an intermediate washing step after a first press step in order to increase the yield of lactic acid and amino acids for further processing.

The solid press cake can be either further processed to fibres and fibre products. The range of products however is limited, as the fibres from grass usually are relatively brittle. Applications may be seen in insulation materials (especially if noise insulation is required, grass fibres offer excellent properties for this application) or as blending material for insulation and MDF boards. A further way to utilise press cake can be as feedstock for biogas production and generation of electrical (and thermal) energy.

Juice may be processed to yield lactic acid (which is a base chemical for many applications, from food additive to solvents to plastics). Besides lactic acid, a mixture of various amino acids and peptides can be derived from the juice. Technological solutions for these separation steps are generally state of the art, although process optimisation is still necessary in this area. Nevertheless order of magnitude estimates of costs for these steps may easily be derived from a rich volume of experimental data from previous projects (Kromus et al., 2002).

Organic residues from either juice processing or fibre production again may be utilised in biogas units, thus making the technology an example for a sustainable process, that uses renewable resources and derives the maximum of products and services from them.

3. Constructing a base case

For the practical implementation of this concept a number of interesting questions arise. The most pertinent among them are:

- Is there an economically feasible solution for this technology on the regional scale?
  This question especially alludes to the identification of those lines of utilisation of grassland that bring about the highest over all value along the whole production chain. There is simply no use of initiating such a project, if, e.g. utilisation of silage in biogas units proves to be economically advantageous. Green biomass (and silage) being a renewable resource that is produced decentrally by nature, this question can only be answered if transport costs are included into the considerations.
- What (if any) steps in the process should be realised decentrally?
  Given the low transport density (and also the high water content of e.g. silage) transport may play a significant role in devising the right structure of the whole production chain. A number of steps, especially the pressing, but also biogas generation can be done locally as well as centrally. The choice of the right "mix" between local and central production steps may significantly influence the economy of the whole concept.
- What are the sensitivities against prices of key products?
  This question is especially important in order to develop a future oriented process set up. If key prices change, so does the structure of the process chain that will yield maximum value. If these trends can be quantified, a more stable design can be derived.

These questions must be answered relatively early in the development process of the technological concept. Results from this investigation are not only important to convince possible industrial partners. They are also a necessary precondition to guide research and technological development in order to efficiently implement a technological concept.

For the base case the following assumptions were made in terms of raw material availability and the basic setting for logistical considerations for an area of about 1000 km^2 in Austria:

(I) total amount of silage is 35.511 t/year;
(II) the average distance of the local transport is 10 km, tractors are used, maximum load is 5 t, average speed is 20 km/h;
(III) the average distance of the central transport is 60 km, trucks are used, maximum load is 12 t, average speed is 50 km/h;
(IV) time limit for transportation is 2000 h/year for trucks and tractors;
(V) there may be one "central plant" (biogas and biorefineries) that are accessible via "central transport" from the silage silos at the farm;

(VI) there may be up to five “local plants” for biogas generation, accessible via “local transport” from the farms;
(VII) fractionation of silage can be accomplished by a mobile press (that is driven to the farms) or by presses in the “local” or “central” plants.

The economical optimization is based on a payback period of 5 years.

The synthesis method is based on combinatorial acceleration of separable concave programming developed by (Nagy et al., 1998). The method consists two parts, a master part controls the algorithm and the minor part accelerates it. The master part is based on the solution of separable concave programming problem, and the minor part uses the combinatorial technique for accelerating the solution method. These combinatorial techniques had been introduced by Friedler et al. (1992a) and based on the process graph or P-graph representation, on the axioms of the combinatorially feasible process structures and combinatorial algorithms (Friedler et al., 1992b), e.g., maximal structure generator (MSG) (Friedler et al., 1993), solution structure generator (SSG), and decision mapping (Friedler et al., 1995).

The synthesis method necessitates a comprehensive list of raw materials, intermediates and possible products. Note that in this method transport is treated like a processing step that uses trucks (or tractors) as installations and the resources raw material (or juice or press cake) and “available time” in order to derive a realistic logistics pattern. Consequently there must be an “intermediate material flow” that leaves this “process step”, which is the respective material at the plant. This is necessary to understand the list of materials for the base case, see Table 1.

Conversely, the synthesis method needs a list of (possible) process steps. Note that some of these steps listed in Table 2 reflect the necessary logistical handling (e.g. the “local” and “central” converters for various materials).

Table 1
List of materials used in synthesis of base case

Materials	Acronyms	Price (€/t)
Silage, the raw material	S	20.578
Juice, after mobile press	J	–
Cake, after mobile press	C	–
Silage, after central transport	SC	–
Silage, after local transport	SL	–
Cake, after local transport	CL	–
Juice, after local transport	JL	–
Cake, central	CC	–
Juice, central	JC	–
Fibres, potential product	F	153
Rest of fibres, local	RFL	–
Rest of fibres, central	RFC	–
Lactic acid, potential product	LA	1000
Amino acids, potential product	AA	1500
Rest of juice, central	RJC	–
General organic dry matter, local	GODML	–
General organic dry matter, central	GODMC	–
Electricity, potential product	E	€ 145 MWh^{-1}

Table 2
List of process steps used in synthesis of the base case

Operating units	Acronyms
Mobil press	MP
Central press	CP
Local fibres production	LF
Central fibres production	CF
Green biorefinery	GBR
Local biogas	LBG
Central biogas	CBG
Local converter, silage	LCS
Central converter, silage	CCS
Local converter, cake	LCC
Central converter, cake	CCC
Local converter, juice	LCJ
Central converter, juice	CCJ
Local converter, rest of fibres	LCRF
Central converter, rest of fibres	CCRF
Central converter, rest of juice	CCRJ
Local transport, silage	LTrS
Central transport, silage	CTrS
Local transport, cake	LTrC
Central transport, cake	CTrC
Local transport, juice	LTrJ
Central transport, juice	CTrJ
Central transport, rest of fibres	CTrRF

Although the synthesis routine used is easily capable of going into more detail within these process steps, at this stage of development (and also for the sake of the more general purpose of this paper) this has not been applied here.

For the economical optimisation of the value chain (because here we are not any longer concentrating on a single process) some basic cost functions are necessary. These costs are derived from previous studies about the green biorefinery or taken from literature or the result of enquiries of our industrial partners. Figs. 2 and 3 show the investment cost dependency on size as an example for the cases of the press and the biogas unit. For other units comparable information was used. A rough overview over the used parameters is given in Table 3.

Combining all this information we first can generate the maximal structure of the problem, depicting all possible ways to process silage with the given process steps (Fig. 4). Note that in this figure bars depict process steps and nodes stand for materials.

4. Results from synthesis of base case

Using all data as specified above leads to an optimal structure where silage is transported to a central processing unit (by four trucks) that fractionates silage and processes the juice to produce lactic acid and amino acids. The press cake goes to a central biogas unit (optimally at the same site). In the course of this process all silage is utilised, 884 t

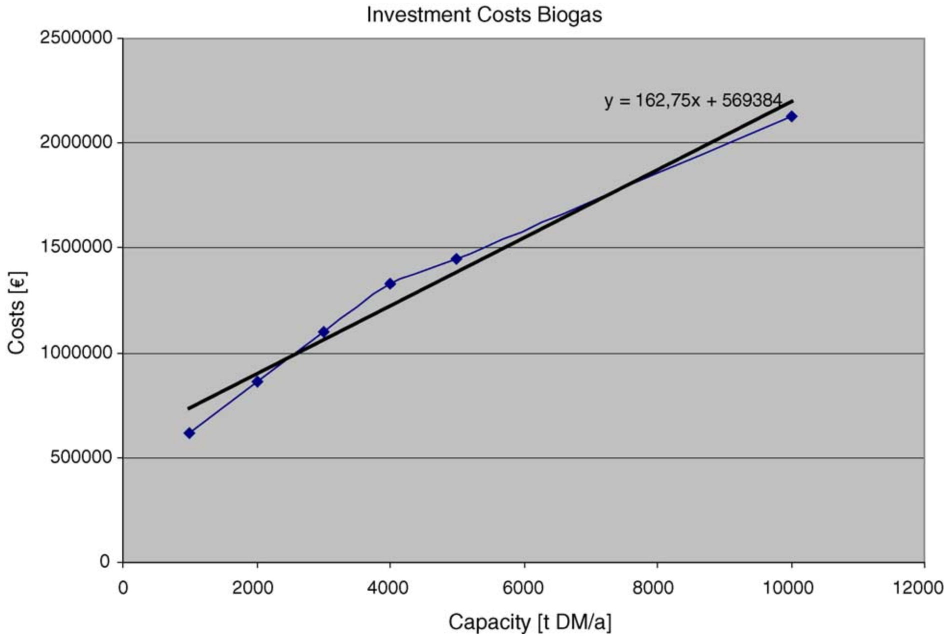

Fig. 2. Investment cost for biogas units dependent on capacity.

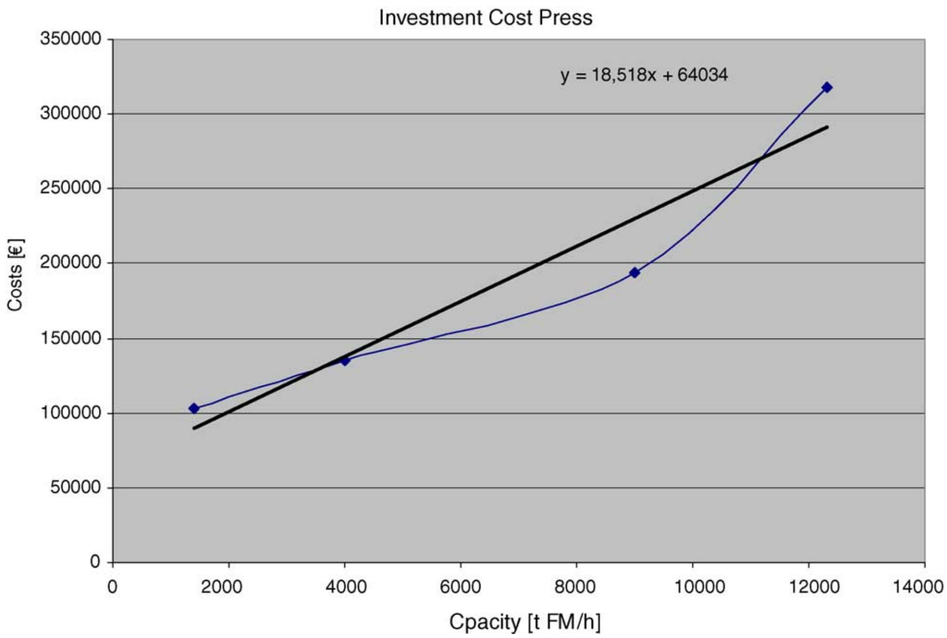

Fig. 3. Investment cost for presses dependent on capacity.

Table 3
Economic parameters for optimisation of the base case

Acronyms	Number of available units	Cost parameters			
		Investment cost		Operating cost	
		Fix (€)	Proportional (€)	Fix (€/year)	Proportional (€/year)
MP	2	192102 for each unit	18.518	0	3
CP	3	64034 for each unit	18.518	0	3
LF	5	0	12.2965642	0	22
CF	1	0	12.2965642	0	22
GBR	1	0	32.25089	0	15
LBG	5	333000 for each unit	112.172	0	107.13719
CBG	2	333000 for each unit	112.172	0	44.640497
LTrS, LTrC, LTrJ	10	0	0	5400 × (number of tractors used)	€ 4.5 turn^{-1}
CTrS, CTrC, CTrJ, CTrRFL	10	0	0	10800 × (number of trucks used)	€ 54 turn^{-1}

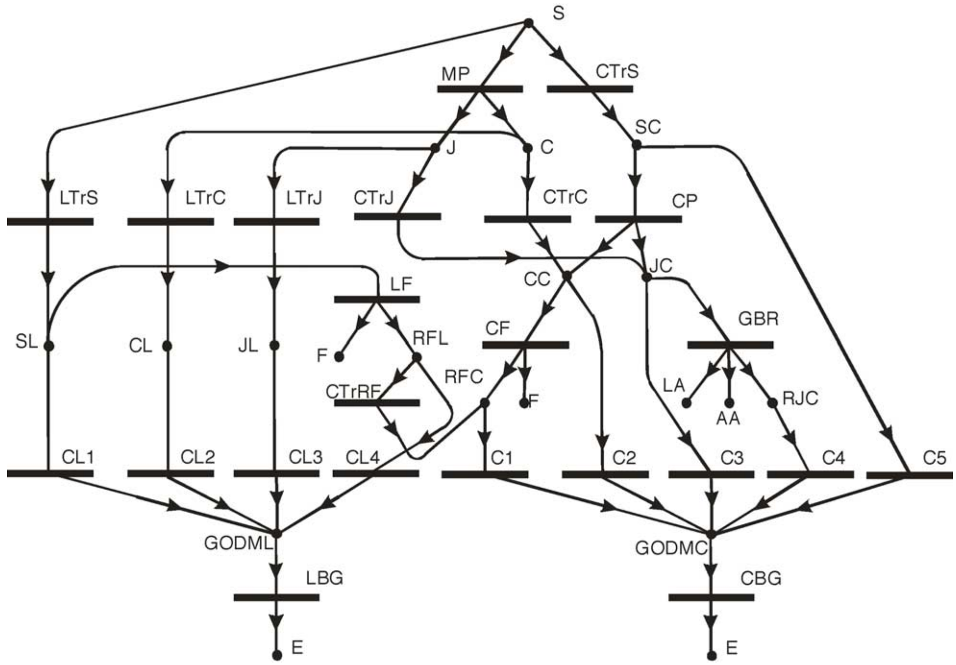

Fig. 4. Maximal structure of base case synthesis.

of LA (lactic acid), 755 t of AA (amino acids and peptides), and 8005 MWh of electricity (E) are produced. The annual profit is a healthy € 653.808. The structure is shown in Fig. 5.

Analysis of these results reveal some interesting insights:

4.1. The profit

Although the synthesis is based on best available information and although within the whole project economic valuation is made at every turn, this estimate may be overly optimistic. As everyone involved in technology development knows from many experiences, profit margins tend to shrink along the path of implementation. On top of this, the pay back period of 5 years clearly only attracts investors who want to be in for the long haul.

Nevertheless, the profit margin at this (already advanced) stage of development shows that the concept has a very good chance to be economically viable. This is corroborated by the generally conservative estimates for prices, at least for lactic acid and amino acids and peptides.

The fact that all silage is utilised in the base case clearly indicates, that as long as the boundary conditions of industrial utilisation remain as they are, green biomass certainly has a future as industrial raw material.

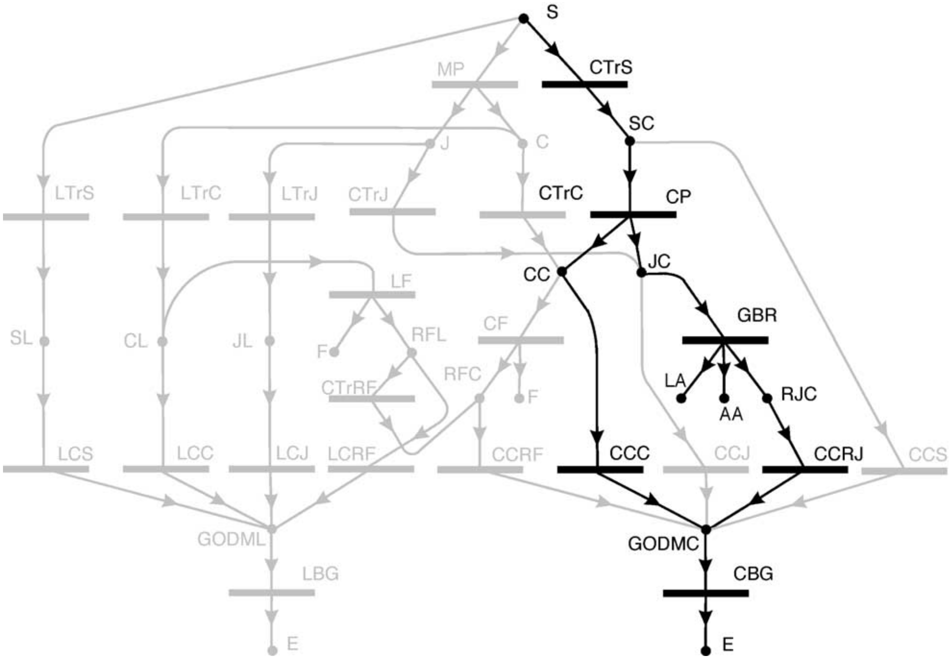

Fig. 5. Optimal structure for base case.

4.2. Central versus local

It is very interesting that the optimal structure clearly gravitates "to the centre". This is somewhat surprising, given the decentral character of the raw materials and their low transport density and high water content. Being in favour of decentral solutions we thoroughly tested this outcome. The solution however remained remarkably stable, even against drastic changes: no amount of investment subsidies will change the pattern (we increased the payback period to infinity without changing the resulting optimal structure!). Even if we decrease the proportional operating cost of local biogas units to the level of the central unit, we had to increase the payback period to (infeasible) 52 years to change the structure to more local pattern. Interestingly enough, even a doubling of transport costs will only lead to a more decentral solution if the payback time is (a still impossible) 24 years.

4.3. Missing fibre production

Results from synthesis clearly favour biogas over fibre production. We therefore wanted to know, how great the "price elasticity" for fibres are to change the process set up. At a price of € 176 t^{-1} fibres, the structure changes in a way that fibres are produced centrally instead of utilising press cake completely in the biogas unit (which now only is fed with the residuals from the central processing of juice and cake). This means that (given a constant electricity price!) fibres need applications with achievable prices in excess of € 180 t^{-1} to be an alternative product. This is an increase of approximately 20% over the prices currently achieved on the market.

5. Sensitivity analysis as a means to improve technology development

However, interesting the synthesis of the base case is, it is always only a good starting point for technology development. It always requires the understanding of the whole system of the value chain, how it reacts to changes and how it adapts to differences in boundary conditions, in order to come to a stable and reliable technological concept worth implementing.

This is especially important when utilising renewable resources. On the one hand, given the competitive disadvantage of relatively high raw material prices, processes based on these resources are especially vulnerable to changing economical conditions. On the other hand, this field is in a very dynamic stage of development, where change is more the rule than the exception.

It goes without mentioning that process synthesis is an extremely valuable tool for this purpose. It allows at a very early stage in the technological development to get a feeling for the systemic reaction of the whole, complex value chain, which a given process (in our case the green biorefinery) is a part of. This information is not only important for technological development itself, pointing to those sub processes that are crucial for the flexibility required by changing boundary conditions. It is also an invaluable tool for the discussion with stake holders for implementation of the technology.

Some of the results of sensitivity considerations, especially in terms of investment conditions for biogas units as well as prices for fibres have already been discussed with the base case. From the many sensitivity runs made for this project, two more will be discussed here, as they showed profound influence not only on parts of the base case, but on the structure of the whole value chain.

6. Variation in biogas-electricity prices

In current European energy markets the prices for “green electricity” and, within this framework, of electricity from specific energy sources is essentially a political price, subject to constant revisions. It is therefore important to know, if changes in this particularly important product price have any influences on the structure of the whole value chain and in consequence on the green biorefinery concept.

We therefore increased the price of electricity continually with no change in the structure until a price of € 0.403 kWh^{-1} was reached. At this price (roughly triple the price of the base case) the structure changes and decentral biogas units become feasible, together with decentral presses. The central biogas unit still remains in the structure, however, it utilises only a small fraction of the available dry matter which come from the residues of the biorefinery installation. The biorefinery structure remains stable, with the central biorefinery still in place (Fig. 6).

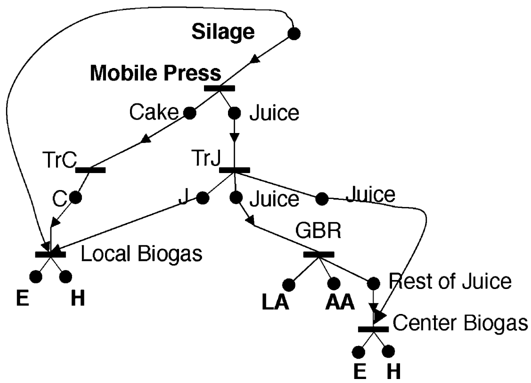

Fig. 6. Optimal structure for high bio-electricity prices.

Although a tripling of the electricity price seems a remote possibility, it is interesting that the general structure of the biorefinery remains stable against even drastic increases in this crucial price. Overall, this adds to the general stability of the concept.

7. Press cake as a product

Process structures discussed so far start from the assumption that there is no conventional use of grass as fodder. However, reality is not as black and white in most cases, meaning that in most regions with surplus grassland, there is still sizeable animal husbandry with grass as a major resource. In a series of sensitivity analysis it has been investigated, if the green biorefinery concept can be viable if there is still demand for fodder from silage. This is a crucial flexibility for implementing this technology, since in most cases it will compete with conventional utilisation of green biomass.

If we introduce a product that is made from press cake and that can be valued according to its nutritional quality (and sold at a price in excess of € $50\,t^{-1}$), the structure immediately changes, favouring decentral pressing and the utilisation of the press cake from these decentral presses. The central green biorefinery still remains in the optimal structure (see Fig. 7), lending additional stability to the concept. This means that the green biorefinery will also be viable in a transition period, where conventional use of press cake (as a fodder from silage with longer shelf life and improved storage and transport properties) is still necessary to sustain stock in regions with high green land portions.

It is interesting, that when the price of fibres increases to levels higher than € $200\,t^{-1}$ we see again a change in the structure. Now we face a split, with a parallel structure of local pressing (for fodder) and central pressing (for fibre production). In general it seems to be a save bet, that if the press cake can be utilised on the farms (or at least close to the farms) decentral pressing units will be part of the structure.

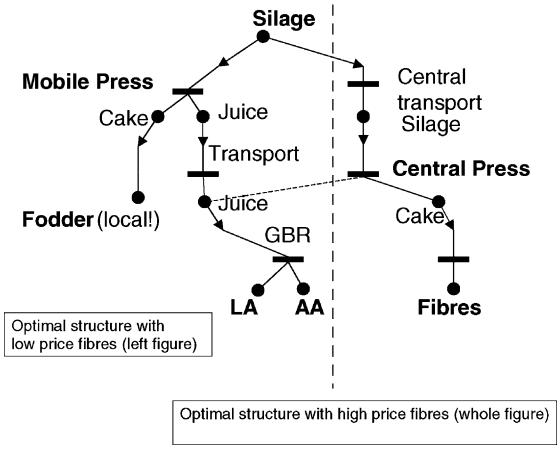

Fig. 7. Optimal structure for press cake utilisation as fodder.

8. Conclusion

The purpose oft the paper was to examine the contribution that process synthesis can offer to the development of processes on the base of renewable resources. As these resources face formidable competition from fossil raw materials and as they are usually produced decentrally, only optimal structures of the whole value chain leading to different products will lead to economically viable processes. In contrast to conventional chemical processes, logistical questions exert influence on the structure of the value chain and must therefore been taken into consideration when developing processes.

The requirements of using process synthesis in this especially challenging application calls for special qualities on the side of the synthesis method itself. The P-graph method, based on combinatorial principles and using a branched and bound optimisation method proved to be extremely efficient and flexible and is optimally suited for this purpose.

The problem investigated in this work concerned the green biorefinery concept. Process synthesis led to a base case that proved to be very resilient against changes in the boundary conditions. Contrary to the line of development pursed so far, process synthesis revealed that only central biorefinery units will lead to economically successful solutions. This is astonishing, given the low transport density and high water content of the raw material, silage. However, this result is an important base for future development strategies, as from now on design of the process will concentrate on units of sufficient size.

One of the major advantages of process synthesis is the possibility to apply sensitivity analysis not only on the process but also on the value chain level. In our case these sensitivities revealed a remarkable stability of the central biorefinery structure, with variations concerning optimal locus for silage fractionation and biogas plants within the value chain, depending on prices of key products like electricity or press cake.

The work on this case study clearly established the usefulness of process synthesis applied to process chains on the base of renewable resources. Not only will process synthesis result in optimal structures for the whole value chain. It will also result in important information concerning the direction of further development work. Given the fact that innovative processes based on renewable resources proceed in many cases in "uncharted waters" both with regard to technology as well as in economic terms, this extra information may amount to the difference between success and failure.

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