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Computer Aided Solar Energy Based Sustainability Evaluations in Process Design

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The paper studies the application of emergy analysis into process flowsheeting for sustainability evaluations. Emergy analysis is an energy-focused environmental accounting method that expresses all the process inputs and outputs in solar energy equivalents. Normally the emergy analysis is done separately from flowsheeting but because of growing demand for sustainability evaluations during design, an integrated assessment with flowsheeting would be valuable. Therefore an approach for integrated emergy assessment with process simulation is discussed. The approach is demonstrated by a lignocellulosic ethanol case study.

1. Introduction

Sustainable development and reduction of greenhouse gas emissions are matters of great concern and need to be considered in process development and design. The sustainability of an industrial process can be evaluated by various techniques reflecting different sustainability point of views. Emergy analysis is an energy-based environmental accounting method expressing all process inputs (such as energy, natural resources, services) and outputs (products) in solar energy equivalents. Emergy is defined as the solar energy used directly and indirectly to generate a product or service. Emergy is a measure ('memory') of how much work the biosphere has done to provide a product. Therefore emergy analysis is a method for assessing the performance of the plant on the larger time and space scales of the biosphere; i.e. sustainability (Odum, 1996). The differences to conventional sustainability evaluations are the energy and biosphere point of views. In this approach also the ‘free’ processes such as air for burning is considered since the biosphere needs to work the CO_2 generated back to oxygen. The method has earlier been utilized for various ecological and engineering topics, lately also for energy system analysis (Sha and Hurme, 2012).
Most of the process design is nowadays done by using steady state process simulation (flowsheeting) programs. Also the emergy analysis is much based on the material & energy balance of the process. Still the utilization of process flowsheeting for emergy analysis has not been discussed earlier in the literature. Therefore the aim of this paper is to present a computer based approach for evaluating the emergy based sustainability of processes by utilizing flowsheeting programs.
At the end the paper gives a case study on the application of the technique on a lignocellulosic biofuel process to demonstrate the methodology.

2. Principle of emergy

Emergy analysis considers all systems to be networks of emergy flows and determines the emergy values of the streams involved. It bridges the connections between economic and ecological systems. Emergy analysis presents a unique solar energetic basis for quantification and valuation of ecosystems, goods and services, which is based on the principles of thermodynamics, system theory and ecology. The method counts as solar energy Joules, how much solar energy would be needed to make a service or a product. The benefit of emergy evaluation is that it allows comparison of all resources on the same basis, i.e. solar

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energy Joules (seJ). Since the early 1980s, emergy evaluation has been used widely for analyzing environmental and economic systems but also industrial processes (Odum, 1996).
An important concept in the emergy analysis is transformity, which is defined as the solar energy required for making a unit of product. The transformity is expressed in solar energy Joules; seJ/J, seJ/g and seJ/€. Therefore the solar energy required to make any item can be calculated by multiply the amount by its transformity (Odum, 1996):

$$E = \tau F \qquad (1)$$

where E is the emergy, τ is the transformity and F is the mass, energy or monetary amount.

From analysis point of view the emergy of a product in a process is the unknown. In emergy analysis the emergies of inputs are summed up to calculate the emergies of outputs based on the rules of emergy algebra. The inputs are often divided to renewable, non-renewable and social feedback (service) inputs. The feedback includes e.g. labor and investments required.

Because emergy is a footprint calculation, it does not follow the rules of balance. This means that the sum of emergies of the products is often larger than the sum of inputs. The four rules of emergy algebra can be summarized as follows (Brown and Herendeen, 1996):
1) The output of a unit equals to the inputs serially.
2) The emergy cannot be split for by-products; each by-product from a process or unit has the total emergy assigned to each pathway.
3) When a pathway splits, the emergy is assigned to each 'leg' of the split based on its percent of the total energy flow on the pathway.
4) Double counting is not allowed; Emergy in feedbacks may not be double counted. By-products when reunited cannot be added to equal a sum greater than the source emergy from which they were derived.

These calculation rules are demonstrated by the example calculations for four basic structures (series, parallel, bypass and feedback) presented in Figure 1 (Mu et al., 2012).

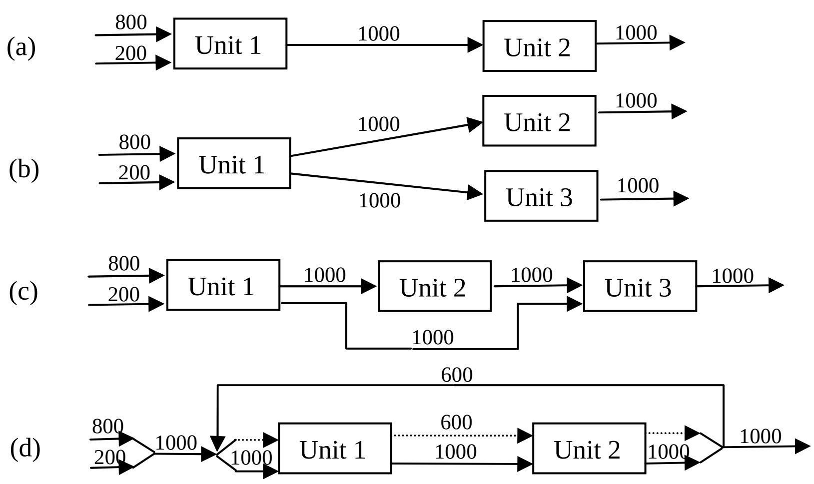

Figure 1: Four basic structures for emergy flow calculation. (a) series; (b) parallel; (c) bypass, (d) feedback. (The unit of numbers is seJ)

Mu et al. (2012) has presented the principle of emergy values calculation for chemical processes with recycle streams. The method uses virtual streams (the dotted stream in Fig.1) to allow the emergy recycle calculations. This method has not a direct connection to process flowsheeting however.

3. Emergy analysis in flowsheeting

Process simulation has been used for decades in process design and development to calculate mass and energy balances. These are also the major contributors in emergy analysis. Therefore the aim of the paper is to discuss, how conventional steady state process simulators (flowsheeting programs) could be utilized and extended for making emergy analyses. Now the emergy analysis is done after the flowsheeting by transferring the input-output information to a spreadsheet program. However since there is a rising demand to incorporate sustainability evaluations more tightly to process design and development, a more integrated and automatic approach for making emergy analyses would be beneficial.

For the emergy analysis of chemical processes the following information is needed:

1. Composition and amount of in-coming and outgoing streams,
2. Utility amounts,
3. Service amounts; i.e. capital and labor costs and other cost factors.

All of these are typically divided into renewable and nonrenewable components and social feedback.

A typical process simulator includes the routines for the material and energy balance calculations. However some aspects required in emergy analysis are lacking in the common process simulators and they need to be supplied by the user (see Table 1):

1) Capital cost estimating (not available in most simulators). The costing can be done based on equipment capital cost correlations and cost share approach, which represents the rest of cost items as percentages of equipment costs.
2) Estimation of some operating cost items such as labor and transportation costs are lacking. Also not all electricity consumptions, except for large main machinery, can be calculated by the simulation programs. They need to be given by the user.

Table 1: Sources of information for the computerized emergy analysis

Sources of information for emergy analysis		
Flowsheeting	Flowsheeting extensions	User input
Mass flows	Conversion to emergy	Electricity demand
Steam,	Emergy allocation	Capital costs
(Electricity demand)		Labor cost
(Capital cost)		Other operating costs
		Emergy allocation

3) Conversion of mass, energy and monetary values to emergy is based on the transformity values. For the purpose a transformity databank is needed. An emergy databank is under development by Tilley et al. (2012). The user however needs to choose a relevant transformity value or modify the value to a certain degree, since the transformities often depend on the manufacturing process and raw materials.

4) Finally an approach for making the emergy calculations of streams based on the input emergies is needed. Special emergy calculation rules are required since emergy does not follow the rules of balance but the emergy algebra as discussed earlier. This applies also to the allocation of emergy to the products, which is affected by the type of side products, if they are inseparable or semi-independent (Cao and Feng, 2007). Since the emergy algebra is not directly applicable as a calculation routine, the following calculation approach is presented:

i) Find out the number of recycle loops in process. (In process flowsheeting they correspond to the number of cut streams.)

ii) If there are no loops, all feeds are summed up till each output to get the emergy of products.

iii) In a recycle area all outputs have the same emergy if no splitting exists. If there is a split of output stream, the split stream emergies are divided correspondingly (see emergy rule 3). For calculation of process inside streams, the inputs are summed sequentially from the beginning up to the output stream. The recycle emergy is not double counted (rule 4).

iv) If there are multiple inside loops, the calculation has to be done separately for each input stream by tracking its way to products. Finally all the input stream derived emergy components are added up for each stream. When there are unions of streams, the streams may not be double counted (compare emergy algebra rule 4).

4. Lignocellulosic ethanol case study

An example on lignocellulosic ethanol process emergy analysis is given to demonstrate the methodology in connection to flowsheeting.

4.1 Process description

Ethanol is produced from a lignocellulosic feedstock in the following way (Hamelinck et al. 2005): Crushed switchgrass feed is contacted with sulphuric acid, steam and water at 215 ºC to hydrolyze cellulose and hemicellulose into hexoses (C6 sugars) and pentoses (C5 sugars). The moisture of feed switchgrass is 13.5% and liquid to wood ratio in the pretreatment is 2. The dilute acid catalyzed steam pretreatment removes the easily hydrolyzed hemicellulose sugars and makes the cellulose part more accessible to subsequent enzymatic hydrolysis. The acid has to be neutralized before fermentation. The prehydrolyzed stream is fed to simultaneous hydrolysis and fermentation, where cellulose is enzymatically hydrolyzed into monomeric sugars consisting mainly of hexoses. The mixture is simultaneously fermented using yeast, which is also capable of fermenting part of the pentoses into ethanol. The enzymes used in the cellulose hydrolysis are produced in an integrated process, which utilizes part of the sugars obtained in the hemicellulose hydrolysis.

Ethanol is separated from the mixture by distillation; 45 % ethanol water is obtained as the top product from the beer column. Subsequently the mixture is further concentrated in the rectifier column. The beer obtained in the first column is sent to a stripper, which removes the remaining part of the ethanol from the fermented liquid. Yeast and the solid residues containing the unhydrolyzed fibers, lignin and yeast are separated from the liquid. The water is recycled to the hydrolysis section except for waste water separated, which is treated before the disposal. The process is presented in Figure 2 as a block diagram and in Figure 3 as an energy system diagram.

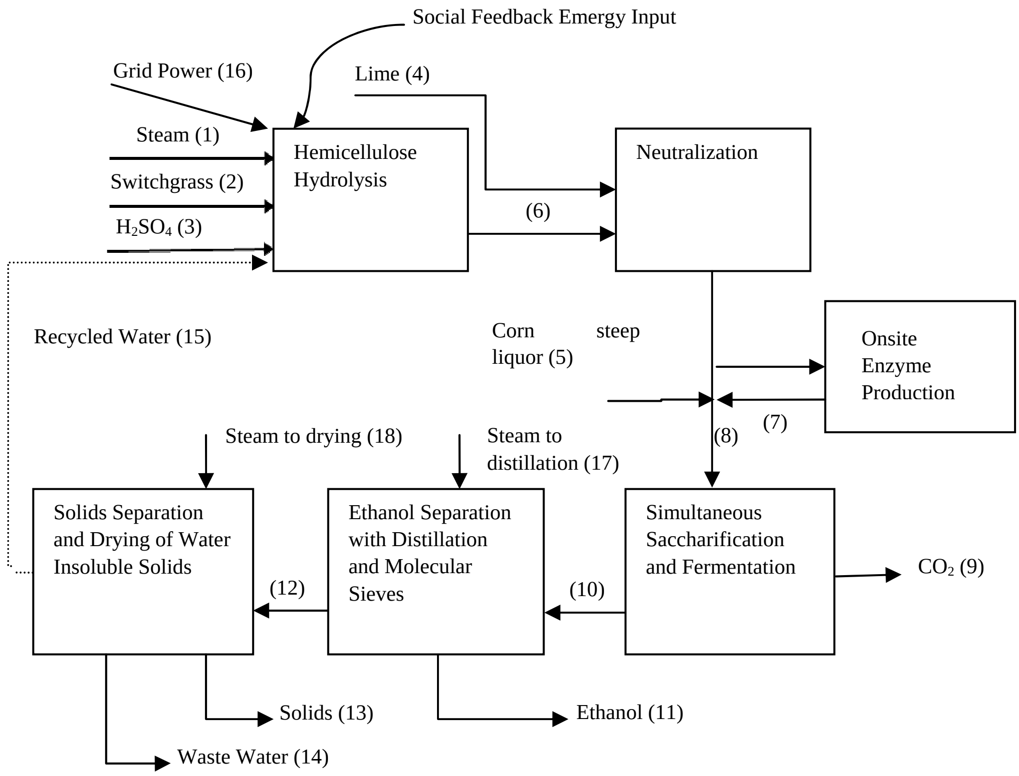

Figure 2. Block diagram of the switchgrass ethanol process (stream numbers refer to Table 2).

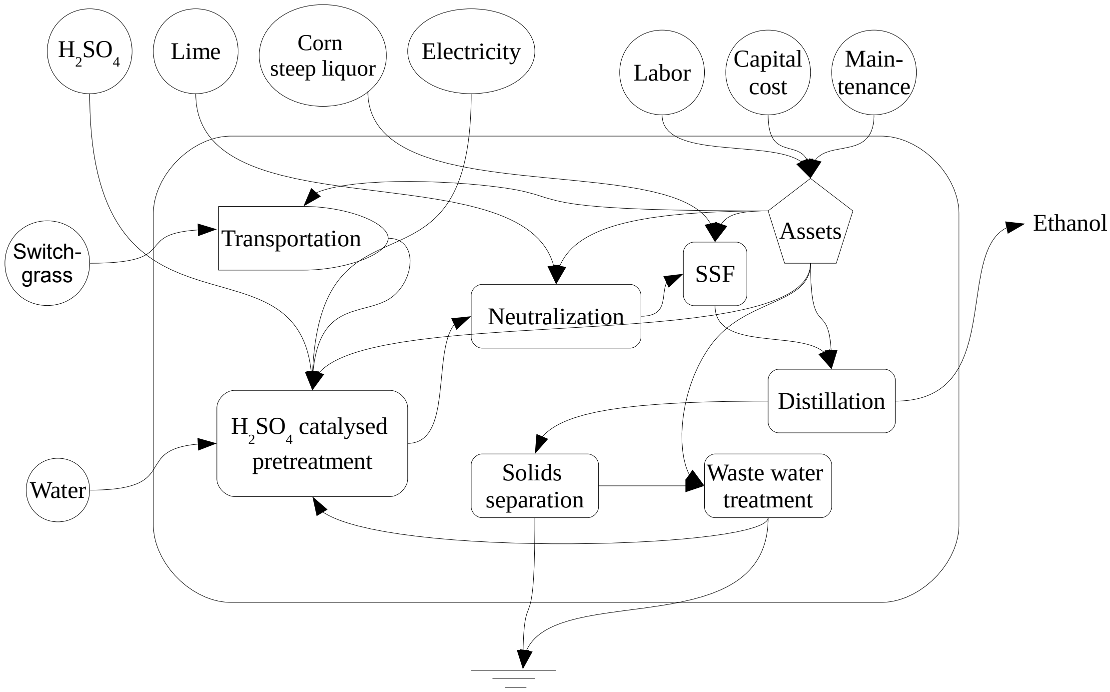

Figure 3. Energy system diagram of the switchgrass ethanol process.

4.2 Emergy simulation of the process

First the process simulation model is built on a flowsheet simulator, for example Aspen Plus. The case study is a recycle process, therefore in the recycle area all the outputs have the same emergies corresponding to the sum of emergy inputs, since there are no split flows (see item iii). The split flows would be recognized in simulation diagram by a divider operation ◄. Next the emergy inputs are calculated: For the simulation input streams transformities are selected from the database. A fully automatic selection is not possible but the selection needs to be confirmed, since there may be different transformities for the same compound depending on its manufacturing process and raw material. Also manual inputs for certain emergy streams, such as services, need to be given (see Table 1). Here the social feedback (services) consists of the biomass raw material transportation, labor costs, investment annuity, ash disposal treatment cost and waste water treatment cost. The sum of these is $1.48 \cdot 10^{16}$ seJ/h). In some simulation programs the investment cost can be estimated, however. In addition the electricity consumption and hydrolysis enzyme cost needs to be given by the user. After this the emergy module can calculate the emergies for the input flows by using Equation 1. The sum of input flow emergies is allocated for each output flow, since this was a single recycle process with no split streams. Inside the recycle all the intermediate flows have also the same emergy, since there are no split streams. The calculated results are shown in Table 2. The transformity of the ethanol produced is $2.43 \cdot 10^{15}$ seJ/t (based on $9.44 \cdot 10^{24}$ seJ/a global baseline). The value represent the solar emergy footprint of the ethanol fuel produced with this process and raw material and can be compared to other manufacturing routes to find out the relative energy sustainability.

Table 2: Values of simulate the emergy connected to process flowsheeting.

Flow Number	1	2	3	4	5	6	7	8	9
Flow rate, t/h	125	289	4.7	1.8	6.87	754.7	8.0 k€/h	763.4	91.9
Transformity, TseJ/t	63.6	209	153	1000	0.33	203	1.43 TseJ/€	200	1664
Emergy PseJ/h	7.95	60.4	0.7	2	0.002	153	11.5	153	153
Flow Number	**10**	**11**	**12**	**13**	**14**	**15**	**16**	**17**	**18**
Flow rate, t/h	671.5	63	608.5	128	144.5	336	55.6 MW	83	346
Transformity, TseJ/t	228	2428	251	1195	1058	455	200 kseJ/J	63.6	63.6
Emergy PseJ/h	153	153	153	153	153	153	40	5.3	22

Note: T = 10^{12}, P = 10^{15}, Stream numbers refer to Figure 2.

5. Conclusions

An emergy analysis approach based on process simulation has been presented. This is needed, because flowsheeting programs have long been used for process design in a routine way. Since there is a need to incorporate sustainability evaluations into process development & design to guide the decisions, a more automatic emergy evaluation would be helpful. This can be achieved by integrating emergy analysis to flowsheeting. A full integration seems however impossible, since some inputs are needed from the user. Even a transformity database would be available, a fully automatic retrieval of transformity values is not feasible, since the values often depend on the manufacturing route of the material. Also all the values needed in emergy analysis are not available from flowsheeting but need to be given. These include e.g. cost items such as salaries. An additional difficulty is brought by the special calculation rules employed by the emergy method (so called emergy algebra). The paper has presented some guidelines which can be used for computerizing the emergy evaluation in the context of process flowsheeting. Care should be taken especially when the flowsheet includes recycle or split streams.

Despite of the challenges in integrating the emergy analysis with process flowsheeting, it would bring benefits by allowing sustainability evaluations to be done early in the process development when the process changes can still be done with a low cost. Therefore the approach will both enhance the sustainability of processes developed and bring cost benefits.

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