Contents lists available at ScienceDirect

Chemical Engineering Research and Design

journal homepage: www.elsevier.com/locate/cherd

Increase in energy and land use by a bio-based chemical industry

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ABSTRACT

About 80% of the chemical products are still based on crude oil. Bio-based materials will increasingly gain importance. As the fraction of oxygen is normally higher in biomass than in crude oil as well as in the derived conventional products, this implies a need to develop new synthesis pathways. Depending on the types of new synthesis pathways, the effects of a complete raw-material change on land and exergy use differ. Here, different synthesis pathways starting from glucose and plant oil to different kinds of end products are evaluated utilizing material and exergy balances. These evaluations are carried out under today's and future conditions and constraints, like yield, demand of organic chemicals and world population. The analysis in this paper shows that the land and energy use can be significantly reduced, if the products are adapted to the chemical structure of their bio-based feedstock.

Keywords: Raw-material change; Biomass; Exergy; Land use; Bio-based synthesis pathways

1. Introduction

In many fields of daily life products of the chemical industry are used. Especially plastics are a part of many applications because of their adaptable properties. The main applications are packaging, building and construction and in the field of automotive (PlasticsEurope, 2012). The global plastics production increased from 1.7 Mio. t in 1950 to 280 Mio. t in 2011. This means an increase of the annual per-capita demand from less than one kilogram to today's value of approximately 40 kg (PlasticsEurope, 2012; United Nations, 2011UN, 2011). The spreading of plastics was supported by the abundant supply of cheap crude oil, which is the main feedstock of the chemical industry.

In the last decade the price of crude oil has increased strongly apart from a few exceptions (EIA, 2013). This may be a sign that the demand exceeds the supply. Therefore, some studies assume that the peak-oil, the date from which on the global production of crude oil will decrease, lies in the near future or has already been passed (de Almeida and Silva, 2009; Bardi, 2009). Additionally, there are international efforts to limit the use of fossil raw materials due to the emissions of carbon dioxide and the associated effects on the global climate (IPCC, 2007). For these reasons, alternative feedstocks gain importance also in chemical industry. An alternative carbon feedstock that is available in sufficient quantities and easily accessible is biomass (i.a. Weusthuis et al., 2011; Bozell and Petersen, 2010; Cherubini, 2010; van Haveren et al., 2008; Corma et al., 2007; Ragauskas et al., 2006; Bender, 2000). Since biomass is obtained from agricultural processes that are generally significantly more land-intensive than conventional crude-oil extraction, land use is a very relevant parameter for evaluation of different biomass options.

In this paper the land-use change and additional energy required for a complete raw-material change toward biomass feedstock is estimated under various constraints and scenarios of future development.

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Received 31 July 2013; Received in revised form 4 December 2013; Accepted 19 December 2013
Available online 28 December 2013
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http://dx.doi.org/10.1016/j.cherd.2013.12.024

List of symbols

a	agricultural land area (ha)
e	annual production volume (t/a)
$\bar{e}$	average yield (t/(ha a))
E	molar exergy (J/kmol)
E_{chem}	molar chemical exergy (J/kmol)
$E_{chem,el,i}$	chemical exergy of an element (J/kmol)
E_{mix}	molar mixing exergy (J/kmol)
E_{phys}	molar physical exergy (J/kmol)
$\Delta_f G^o$	molar Gibbs energy of formation (J/kmol)
$\Delta_R G^o$	molar Gibbs energy of reaction (J/kmol)
H	molar enthalpy (J/kmol)
$m_{feedstock}$	mass of feedstock (kg)
$m_{product}$	mass of product (kg)
N	number of countries (–)
N_c	number of components (–)
N_{el}	number of elements (–)
$n_{el,i}$	amount of element i (mol)
p	pressure (Pa)
S	molar entropy (J/(kmol K))
T	temperature (K)
Δt	time period (a)
a, b, x, y, z	coefficient in chemical equation (–)
$\alpha, \beta, \gamma, \delta, \varepsilon, \varphi$	stoichiometric coefficient (–)
η_{mass}	mass efficiency (–)
ν_i	stoichiometric coefficient (–)
$\sigma_{\bar{e}}$	standard deviation of yield (t/(ha a))

2. Today's and future raw materials and products

The chemical composition of biomass differs significantly from crude oil. Crude oil is a homogeneous mixture mainly consisting of hydrocarbons and aromatic compounds (Banks and King, 1984). The structure of biomass is clearly more heterogeneous. 75% of the 170 billion tons of global annual growth of biomass taken as dry matter are carbohydrates, 20% are lignin and the rest are oils, proteins and other ingredients (Kamm and Kamm, 2007; Eggersdorfer et al., 1992). Carbohydrates are mainly complex biopolymers like cellulose and hemicellulose. By hydrolysis they can be converted to mostly C6- and C5-sugars like glucose or xylose (Hamelinck et al., 2005). Based on these precursors, a biotechnological or chemical conversion is possible. Glucose and xylose differ from crude oil with regard to their higher O:C-ratio. The difference of the O:C:H-ratio by weight is depicted in Fig. 1. The typical bio-based feedstock is depicted in squares and fossil raw materials in triangles. Here and in the following plant oil is calculated as triolein, the triglyceride with three oleic acids as side groups. It has been ensured that the influence of this choice as compared other common fatty acids is marginal. Fossil raw materials contain mainly carbon and hydrogen and essentially no oxygen. The conventional polymers (circles), which are produced from crude oil and represent more than 80% of the European demand for plastics, also have a low oxygen fraction (PlasticsEurope, 2012). Especially the bulk plastics polyethylene, polystyrene, polypropylene, which contribute over 55% of the European market, are almost oxygen-free. In contrast to that, the oxygen content of the biobased carbohydrates cellulose, hemicellulose and glucose ranges up to about half of their mass.

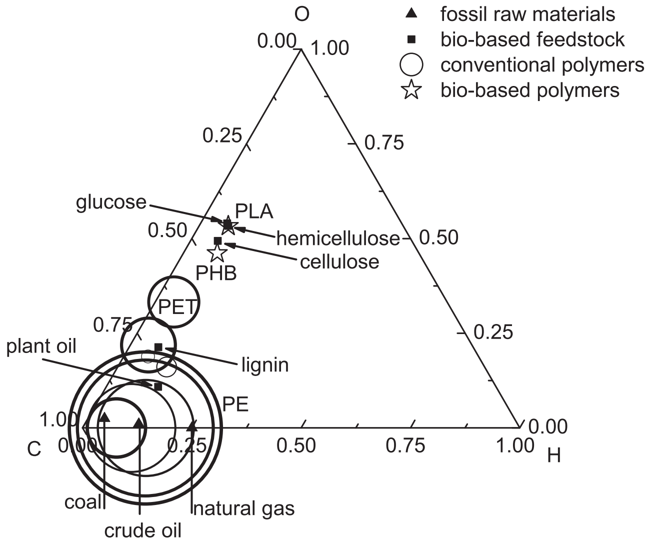

Fig. 1 – O:C:H-ratio by weight of fossil raw materials (triangle), bio-based feedstock (squares), bio-based polymers (stars), and today's polymers (circle). The diameter of the circles is proportional to their annual European production volume.

For the production of conventional products the O:C-ratio needs to be adjusted. The substantial adjustments are smaller if the O:C-ratio of feedstock and products are more similar. In order to minimize the substantial adjustments, there are two options: Either raw materials are used, that do not contain much oxygen. These raw materials are similar to today's end products. Or new products are developed with an oxygen content that is similar to typical bio-based feedstock like glucose.

One approach along the first line is the usage of lignin. Lignin is a bio-polymer responsible for the lignification of biomass. On the one hand, its contribution to the annual global growth of dry matter is relatively large and it is the only renewable source for aromatics (Bugg et al., 2011). On the other hand, the depolymerisation and the selective usage of defined fragments as raw material for further chemical steps is difficult because of its complex structure. Another bio-based feedstock with an oxygen content that is low is plant oil. It has an average oxygen content of approximately 11 wt% and consists mainly of various long-chained triglycerides. Plant oil is already used today in large quantities for the production of bio-diesel by transesterification (Balat and Balat, 2008).

The second approach is a shift of the desired products in the direction as to contain more oxygen. An example frequently used today is polyethylene terephthalate (PET). Two other examples for new bio-based plastics (stars) are polylactic acid (PLA) and polyhydroxybutyrate (PHB).

The substantial adjustments regarding the O:C and H:C-ratio may have effects on the economic potential the synthesis pathways. In order to examine the effects on the economic potential of the synthesis pathways, an indicator is required. The application of energy and material balances does not suffice, because energy balances do not distinguish between the qualities of different energy forms. For example, the economic value of steam and electricity based on energy is usually different. On the other hand own estimations show that the price ranges in the narrow band between 1.4 and 2.0 €-cent/MJ of exergy for energy sources ranging from crude oil to industrial steam on different pressure levels to electricity. Thus, exergy