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Methodology and data

Table S1. Technical substitution potential[1)] and eligibility for green premium and implementability for bio-based chemicals replacing non-identical petrochemicals (for years 2010 to 2050)

Bio-based chemical	Petrochemical	Technical substitution potential	Green premium	Implementation
PHA	PE	25%	Green premium	Difficult
PTT	Nylon 6	100%	Green premium	Easy
PLA	PET	90%	Green premium	Difficult
PLA	PS	100%	Green premium	Difficult
Ethyl lactate	Ethyl acetate	100%	Without	Difficult
Succinic acid	Maleic anhydride	85%	Without	Difficult

[1)] Typically, a reference petrochemical is used for a broad variety of applications for which the bio-based alternative is more or less suitable. Due to a lack of detailed information on product properties, it is difficult to determine the technical substitution potential exactly for each application and to aggregate these values to a total substitution potential. Instead we use overall estimates of expert on the suitability of bio-based chemicals for the substitution of reference petrochemicals. These estimates were made by experts participating in the BREW project. For those cases where the bio-based and the petrochemical product are chemically identical the technical substitution potential is 100% (not shown).

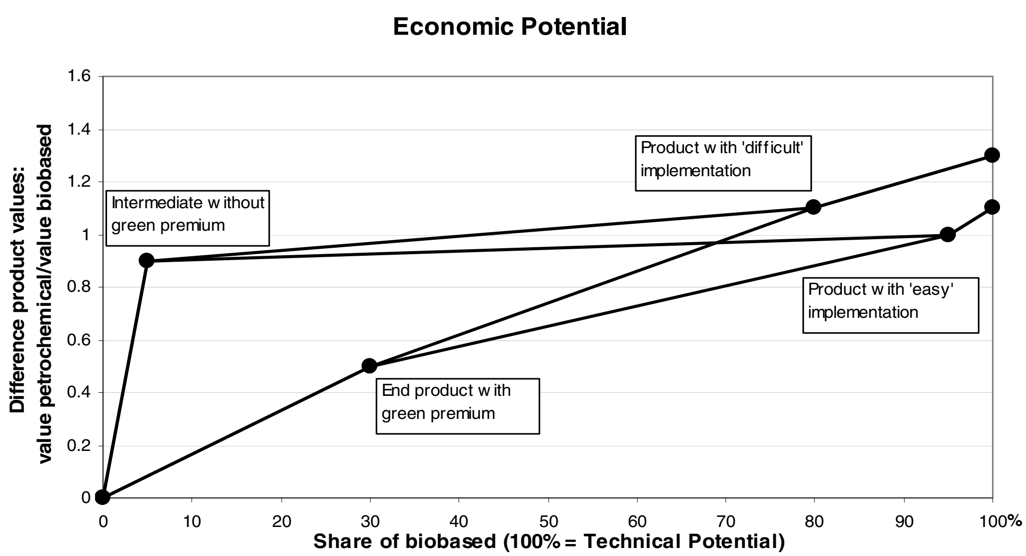

Figure S1. Economic market potentials depending on the difference of product values of a bio-based chemical and a reference petrochemical including green premium and ease of implementation

Table S2. Development of fossil fuel prices in different models using the SRES scenario (IPCC SRES, 2000; Lejour, 2003; Personal communication IIASA)

	Gas			Coal			Oil		
	2000	2020	2050	2000	2020	2050	2000	2020	2050
A1-ASF	1	1	1.06	1	1.07	1.27	1	1.2	1.61
A1-Minicam	1	1.17	1.58	1	1.14	1.36	1	1.22	1.48
GE-CPB	1	1.08	1.28	-	-	-	1	1.07	1.32
A1B-Message	1	1.72	2.14	1	1.32	1.05	1	1.79	1.53
A1G-Message	1	1.15	2.55	1	1.1	1.5	1	1.48	2.33
A1T-Message	1	1.12	1.65	1	1.03	1.29	1	1.41	1.7
A1C-Message	1	1.16	2.16	1	1.46	1.88	1	1.47	1.93
B1-ASF	1	0.98	0.96	1	1.07	1.13	1	1.16	1.43
B1-Minicam	1	1.07	1.34	1	1.14	1.21	1	1.13	0.97
SE-CPB	1	1.04	1	-	-	-	1	1.05	0.93
B1G-Message	1	1.33	1.61	1	1.59	1.15	1	1.83	2.14
B1-Message	1	1.22	1.3	1	1.49	0.97	1	1.66	1.21
B1T-Message	1	1.26	0.94	1	1.31	0.94	1	1.62	1.15
A2-ASF	1	1	1	1	1	1.13	1	1.07	1.41
A2-Minicam	1	1.2	2.14	1	1.16	1.36	1	1.26	1.64
TM-CPB	1	1.19	1.24	-	-	-	1	1.14	1.32
A2-Message	1	1.38	2.4	1	1.01	1.54	1	1.88	3.31
B2-ASF	1	1	0.98	1	1	1.07	1	1.07	1.39
B2-Minicam	1	1.13	1.41	1	1.14	1.21	1	1.11	1.09
RC-CPB	1	1	0.9	-	-	-	1	1.05	1.11
B2-Message	1	1.19	1.8	1	1.76	1.38	1	1.51	2.64

The CPB model used the SRES scenarios as basis for comparable scenarios used for modeling the European economy. The other models are included in the special report of the IPCC on emission scenarios.

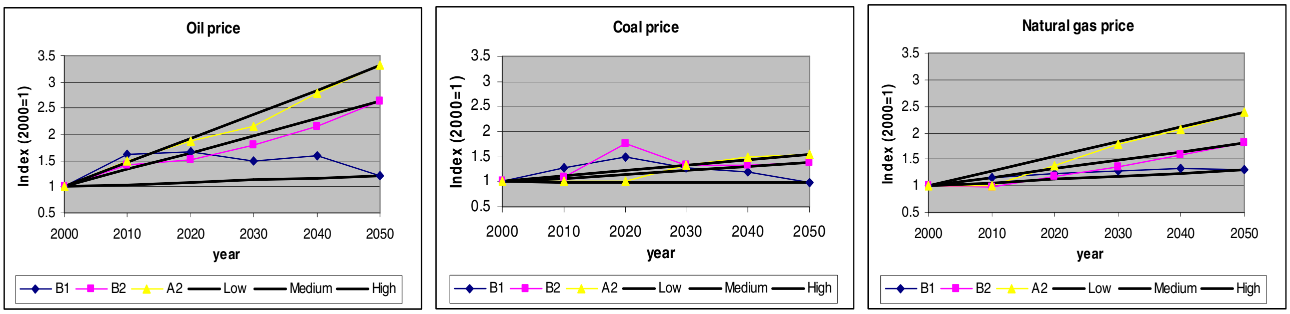

Figure S2. Fossil fuel prices in the three different scenarios[1)]

[1)] In this study, we used the fossil fuel prices from the Message model for our market projections for the coming 5 decades. Fuel prices in our LOW scenario are represented by the B1 scenario, in our MEDIUM scenario by the B2 scenario and in our HIGH scenario by the A2 scenario. In order to make our scenarios consistent - i.e., to ensure that in each year the fossil fuel price is highest in the HIGH scenario - we linearised the fossil fuel price trends (see Figure 4-4). It should hence be noted that fossil fuel prices in our scenarios are no projections of future crude oil price, but represent different images of the future under certain circumstances. Using a value of 25 US$/barrel as a price base, crude oil prices in our scenarios range from 30 to 66 and 83 US$/barrel in 2050 in the three scenarios.

Estimation of total production of organic chemicals in EU-25. Based on the insight gained from detailed material flow analyses of the petrochemical sector in the Netherlands and in Germany (Neelis et al., 2005a; Neelis et al., 2005b; Weiss et al. 2007) it has been estimated that the total production of all organic chemicals (without double counting related to intermediates) can be estimated by multiplying the total production of polymers by a factor of 1.35. For Germany and the Netherlands, the resulting values represent 92-99% of the chemical feedstock use reported in international energy balances (IEA 2003)

Table S3: Production volume of *selected chemicals* in Europe used as base chemical market demand in 2000

Petrochemical	**Volume** (kton)	**Year and region**	**Reference**
PE (HDPE, LDPE, LLDE)	11,300	2000, Western Europe[a]	CEFIC 2005
Ethylene	19,403	2000, Western Europe	CEFIC 2005
PTT	524	2000[b]	APME 2003
Nylon 6	1,255	2000, Western Europe[c]	APME 2003
PET	3,500	2000, EU-25[d]	APME 2003
PS	3,365	2000, EU-25[d]	APME 2003
Ethyl acetate	310	1999, Western Europe[e]	Weissermel and Arpe 2003
Maleic Anhydride	380	1999, Western Europe[f]	Weissermel and Arpe 2003
Adipic acid	1,000	1999, Western Europe[g]	Weissermel and Arpe 2003
Acetic acid	1,400	1999, Western Europe[h]	Weissermel and Arpe 2003
n-Butanol	930	1999, Western Europe[i]	Weissermel and Arpe 2003

[a] About 11700 kton ethylene are needed for the production of 11300 kton polyethylene. This demand of ethylene can only be replaced once within the market potentials.
[b] Consumption figure of other polymers in Western Europe.
[c] 44% of polyamide consumption as consumption (PA 6/66/other) for Western Europe was in the ratio of 44/46/10 in 1988. (Ullmann 1997)
[d] Consumption data. Data for PS includes expanded polystyrol.
[e] Production outside Western Europe, USA and Japan was about 510 kton in 1999.
[f] Production outside Western Europe, USA and Japan was about 530 kton in 1999.
[g] Production outside Western Europe, USA and Japan was about 390 kton in 1999.
[h] Production outside Western Europe, USA and Japan was about 3610 kton in 1999.
[i] Production volume includes all types of Butanol. Production outside Western Europe, USA and Japan was about 246 kton in 1999.

Table S4. Processes for the production of reference petrochemicals. Base data on the petrochemical processes are from SRI 2000.

Petrochemical	Process
Acetic acid	From MEOH by low pressure carbonylation, supported Rh Catalyst
Adipic acid	From cyclohexane
n-Butanol	From propylene, cobalt phosphine catalyst
Ethyl acetate	Ethyl acetate via pervaporation-assisted esterification of acetic acid
Ethylene	From wide-range naphtha steamcracking
HDPE	By liquid phase slurry process
PET	From DMT and EG
PS	General purpose PS, continous bulk polymerization
PTT	Via polycondensation of 1,3-propanediol (from Ethylene oxide) and purified terephthalic acid
Nylon 6	From Caprolactam
Maleic Anhydride	From n-butane, moving bed reactor

The process data used refer to a capacity of 100 Gg/yr for the bio-based chemicals and a typical world scale process for petrochemicals has been assumed.

Table S5. Processes for the production of bio-based chemicals selected from processes studied in Patel et al. (2005)

Bio-based chemical	**State –of –the Art Technology**	**Future technology**
Acetic acid	Acetic acid via anaerobic fermentation on dextrose substrate; workup via extraction using TOPO; Generic Approach (today); *BioAcet-Anaer-GA-Tex1*	Acetic acid via anaerobic fermentation on dextrose substrate; workup via evaporation+distillation; Generic Approach (future); *BioAcet-Anaer-GA-Fevd*
Adipic acid	Adipic acid via aerobic fermentation on glucose substrate; workup via evaporation, crystallisation; Generic Approach (today); *BioAdip-Aer-GA-Tc*	Adipic acid via aerobic fermentation on glucose substrate; workup via electrodialysis; Generic Approach (future); *BioAdip-Aer-GA-Fed*
n-Butanol	ABE via anaerobic fermentation on dextrose substrate; workup via distillation; Generic Approach (today); *ABE-Anaer-GA-Td*	ABE via anaerobic fermentation on dextrose substrate; workup via pervaporation; Generic Approach (future); *ABE-Anaer-GA-Fpv*
Ethyl lactate	Ethyl lactate via pervaporation-assisted esterification of lactic acid on dextrose substrate. One step process; low pH fermentation of lactic acid; lactic acid is not isolated. (Shell confidential data); *EL-Sh-pv*	No specific process data, price, energy and GHG emission depreciation as for PLA assumed
Ethylene	Dehydration of Bio-ethanol (Shell confidential data); Bio-ethanol via anaerobic continuous fermentation on dextrose substrate; workup via distillation; Generic Approach (present); *BioEtOH-Anaer-GA-Tdcont*	Dehydration of Ethanol (Shell confidential data); Bio-ethanol via anaerobic fermentation on dextrose substrate; workup via pervaporation; Generic Approach (future); *BioEtOH-Anaer-GA-Fpv*
PHA	Mid chain length poly(hydroxyalkanoate) in latex form via fermentation on dextrose; Generic Approach (present); *PHA–GA-Toa*	Mid chain length poly(hydroxyalkanoate) in latex form via fermentation on dextrose; Generic Approach (present); *PHA–GA-Toa (future worse than today case)*
PLA	Poly(lactic acid) via polycondensation of lactic acid (NatureWorks). lactic acid via fermentation by xxx on dextrose; workup via unspecified process involving neutralisation & acidification. NatureWorks process; supplementary data from SRI process designs; *PLA-LA-NW-Tu*	Poly(lactic acid) via polycondensation of lactic acid (NatureWorks). Lactic acid via fermentation on dextrose; workup via electrodialysis. Generic approach, future case; *PLA-LA-NW-Fu*
PTT	Poly(trimethylene terephthalate) via polycondensation of bio-1,3-propanediol and purified terephthalic acid, Bio-1,3-PDO via aerobic cont. bioprocess on dextrose substrate, workup by evaporation and distillation; Generic Approach today; *BioPTT-Aer-GA-Tevcont*.	Poly(trimethylene terephthalate) via polycondensation of bio-1,3-propanediol and purified terephthalic acid, Bio-1,3-PDO via aerobic cont. bioprocess on dextrose substrate, workup by pervaporation of PDO, Generic Approach future; *BioPDO-Aer-GA-FpvPDO*
Succinic acid	Bio-succinic acid via fermentation by Actinobacillus succinogenes 130Z on dextrose substrate; workup via electrodialysis; Generic Approach, today. *BioSA-GA-Ted*	Bio-succinic acid via fermentation by Actinobacillus succinogenes 130Z on dextrose substrate; workup via crystallisation and redox; Generic Approach, future; *BioSA-GA-Fcrx*

Table S6. Land use of biobased chemical production for current and future technology based on (Patel et al., 2007)

Specific land use ha/t	Current technology starch	Future technology starch	Current technology lignoc	Future technology lignoc
PHA	0.41	0.31	0.17	0.13
PTT	0.12	0.09	0.05	0.04
PLA	0.18	0.18	0.06	0.07
Ethyl lactate	0.22	0.22	0.08	0.09
Ethylene	0.47	0.45	0.19	0.18
Succinic Acid	0.25	0.15	0.17	0.08
Adipic acid	0.74	0.27	0.30	0.11
Acetic acid	0.26	0.14	0.10	0.06
n-Butanol	0.30	0.26	0.12	0.10

Results

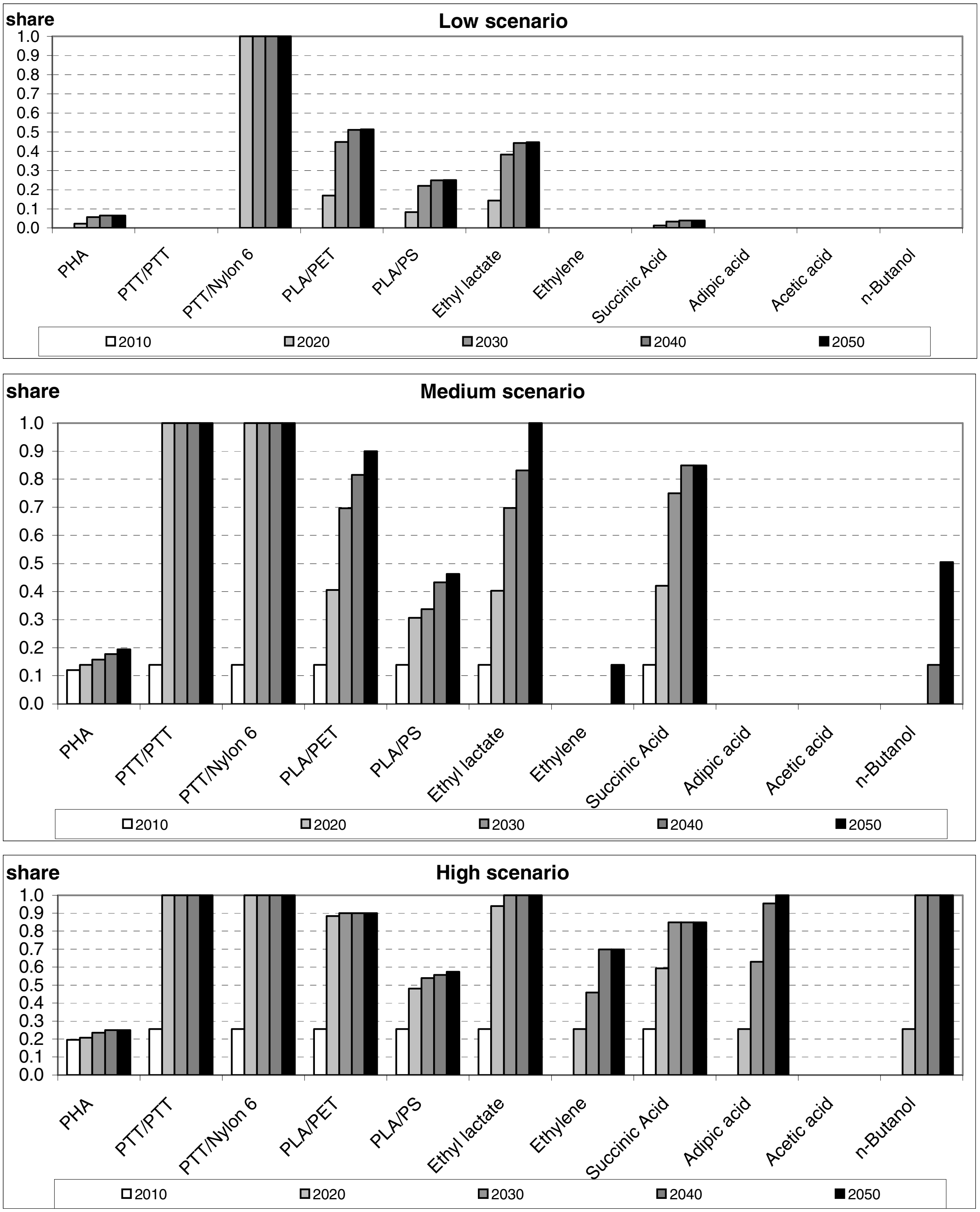

Figure S2. Share of bio-based chemical production relative to the selected reference petrochemical product in Europe for the three scenarios for the years 2010 to 2050

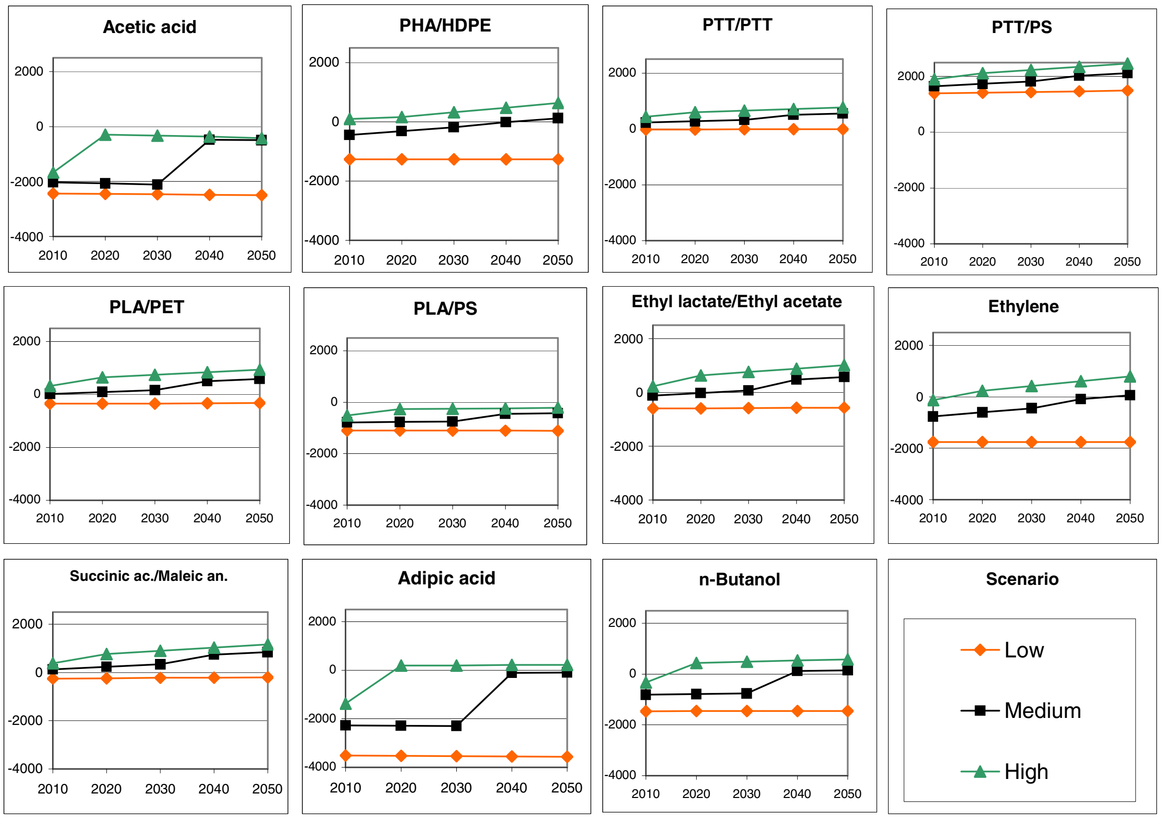

Figure S3. Differences between the product values of the reference petrochemical and the bio-based chemical in /t (positive values show an advantage of the bio-based chemical)

Discussion

Estimated savings compared to the total organic chemical industry. When relating the estimated savings to the *total organic chemical industry* we assume that there are no significant savings due to White Biotechnology other than those studied in this article. This concerns both other White Biotechnology products and other, more efficient process routes leading to the same products. Our arguments are that i) the most promising White Biotechnology chemicals have been taken into account, ii) the assumptions made in the economic calculation for the bio-based chemicals represent upper limits (Hermann and Patel, 2006) and iii) no technological progress has been assumed for the production of petrochemicals. Moreover, a sugar price of 70 /t (as assumed in the scenario HIGH) is likely to be too low for the long run (see below). We hence implicitly assume that these factors, which tend to lead to an overestimation of the saving potentials, compensate possible savings due to White Biotechnology products and processes, which have not been taken into account in this study.

Development of sugar prices. In several world regions, *fermentable sugar* is nowadays available at lower prices than in Europe. The difference is largest between Europe and sugar cane producing countries such as Brazil with a sugar price of 70 /tonne in 2000, which we have assumed in the scenario HIGH. As a consequence of industrialization of the developing world and improved social standards, the wages and hence also sugar prices will converge to some extent across the globe. In 2050 there will most likely still be a gap in production cost for sugar across the world due to incomplete socio-economic convergence and for climatic and fertility reasons but the size of this gap is likely to be substantially smaller than today. Moreover, due to the increasing production and use of bioenergy (liquid biofuels and solid biofuels) the biomass prices are likely to become increasingly correlated to fossil fuel prices. This effect has already been visible in the recent past when the expansion of bioethanol in combination with high oil prices was accompanied by a rise in sugar prices. To establish a quantitative relation between biomass prices and fossil fuel prices, a very comprehensive model would be required including the global and regional supply of agricultural and forest products and their use. Such a model is far beyond the scope of this project. The calculated market potentials presented in this article for low sugar prices hence may be overestimated, i.e. the real market potentials of the bio-based bulk chemicals may be lower than calculated in our projections. While these arguments speak for higher biomass prices relative to fossil fuels, one could also argue that oil prices may rise excessively due to surging demand especially from developing countries. The increase in oil price would then clearly outpace the rise in sugar prices. Under these conditions the market potentials for bio-based chemicals presented in this chapter could be clearly underestimated.

GHG emission reduction. In the SRES marker scenarios of the IPCC, about 7 to 18 Gt CO_2 are emitted from fossil fuels and industrial sources in the whole OECD in 2050. In 2000, about 31% of

OECD CO_2 emissions are emitted in OECD Europe. (IEA 2002). Multiplication of this percentage with the emissions in the OECD according to the IPCC scenarios results in an estimate of about 2 to 6 Gt CO_2 for OECD Europe in 2050. In comparison, GHG emission reductions of between 0.01 and 0.48 Gt CO_2 by White Biotechnology chemicals according to our calculations (the range covers all three scenarios for starch and for lignocellulosics) are limited.

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