Supporting Information

Spatially explicit multi-objective optimisation for the strategic design of first and second generation biorefineries including carbon and water footprints

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The supporting information comprises the economic formulation used in the model following Giarola *et al.* (2011) (for more details see the original reference). The values of some critical parameters used in the model is also reported in Tables S1-S3.

The modelling framework is summarised as follows.

- Annual cash flow

$$CF_t = PBT_t + D_t - TAX_t\,, \quad \forall\, t \tag{A.1}$$

- Gross profits

$$PBT_t = Inc_t - VarC_t - FixC_t - D_t\,, \quad \forall\, t \tag{A.2}$$

$$Inc_t = \sum_g \sum_k \sum_j P^T_{j,k,g,t} \cdot MP_j\,, \quad \forall\, t \tag{A.3}$$

- Fixed costs

$$D_t = \sum_p \sum_k \sum_g \lambda_{p,k,g,t} CI_{k,p} \cdot dk_t\,, \quad \forall\, t \tag{A.4}$$

$$FixC_t = \phi \cdot Inc_t\,, \quad \forall\, t \tag{A.5}$$

- Variable costs

$$VarC_t = BPC_t + TCb_t + TCf_t + EPC_t, \quad \forall\, t \tag{A.6}$$

$$BPC_t = \sum_g \sum_i Pb_{i,g,t} \cdot UPC_{i,g}\,, \quad \forall\, t \tag{A.7}$$

$$TCb_t = \sum_{i,m} UTC_m \cdot \left(\sum_{\mathrm{g,g'}} \mathrm{Qb}_{\mathrm{i,g,m,g',t}} \cdot LD_{g,g'} \cdot \tau_{g,m,g'} \right) + \sum_{i,g} \mathrm{UTC}^* \cdot \mathrm{Pb}_{\mathrm{i,g,t}} \cdot \mathrm{LD}_{\mathrm{g,g'}}\,, \quad \forall\, t \tag{A.8}$$

$$TCf_t = \sum_{i,m} UTC_m \cdot \left(\sum_{g,g'} Qf_{g,m,g',t} \cdot LD_{g,g'} \cdot \tau_{g,m,g'} \right), \quad \forall\, t \tag{A.9}$$

$$EPC_t = \sum_k coef_{'slope',k} \cdot \sum_g P^T_{'ethanol',k,g,t} + coef_{'\mathrm{int}\,ercept',k} \cdot \sum_g Y_{g,k,t}\,, \qquad \forall t \tag{A.10}$$

- Taxation

$$TAX_t \geq Tr \cdot PBT_t, \quad \forall\, t \tag{A.11}$$

$$TAX_t \geq 0 , \quad \forall \, t \tag{A.12}$$

- Capacity planning constraints

$$PCap^{\min} \cdot Y_{k,g,t} \leq P^{T}_{'ethanol',k,g,t} \leq \sum_{p} \lambda_{\mathrm{p,k,g,t}} \cdot 3 \cdot ER_p , \quad \forall \, k, g, t \tag{A.13}$$

$$Db_{i,g,t} = \sum_{k} \frac{Pf_{i,k,g,t}}{\gamma_i} \cdot \left(1 + burn_{i,k}\right), \qquad \forall i, g, t \tag{A.14}$$

- Sustainability constraints

$$Pb_{i,g,t} \leq BA_{g,i} , \quad \forall \, i, g, t \tag{A.15}$$

$$BA_{g,i} = GS_g \cdot BY_{i,g} \cdot AD_g \cdot BCD_g^{\max}, \quad \forall \, \mathrm{g}, i \tag{A.16}$$

$$TPot_{i,t} \cdot quota_i \geq \sum_{g} Pb_{i,g,t} \cdot IBF_g , \quad \forall \, \mathrm{i, t} \tag{A.17}$$

$$TPot_{i,t} = \sum_{g} BA_{i,g} \cdot IBF_g , \quad \forall \, i, t \tag{A.18}$$

- Production constraints

$$Pf_{i,k,g,t} = P^{T}_{'ethanol',k,g,t} \cdot \beta_{\mathrm{i,k}} , \quad \forall \, i, k, g, t \tag{A.19}$$

$$P^{T}_{'ethanol',k,g,t} = \sum_{i} Pf_{i,k,g,t} , \quad \forall \, k, g, t \tag{A.20}$$

$$P^{T}_{'DDGS',k,g,t} = Pf_{'corn',k,g,t} \cdot \delta , \quad \forall \, k, g, t \tag{A.21}$$

$$P^{T}_{'power',k,g,t} = P^{T}_{'ethanol',k,g,t} \cdot \frac{\omega_k}{\rho} , \quad \forall \, k, g, t \tag{A.22}$$

- Capital costs linearisation constraints

$$TCI_t = \sum_{p} \sum_{k} \sum_{g} \lambda^{plan}_{p,k,g,t} \cdot CI_{k,p} , \quad \forall \, t \tag{A.23}$$

$$D_t = \sum_{p} \sum_{k} \sum_{g} \lambda_{p,k,g,t} \cdot CI_{k,p} \cdot dk_t , \quad \forall \, t \tag{A.24}$$

$$\lambda_{p,k,g,t} = \lambda_{p,k,g,t-1} + \lambda^{plan}_{p,k,g,t} , \quad \forall \, k, g, t, p \tag{A.25}$$

$$\lambda_{p,k,g,t} - y_{p-1,k,g,t} - y_{p,k,g,t} \leq 0, \quad \forall\, k,g,t,p \in sub(p) \tag{A.26}$$

$$\lambda^{plan}_{p,k,g,t} - y_{p-1,k,g,t} - y_{p,k,g,t} \leq 0, \quad \forall\, k,g,t,p \in sub(p) \tag{A.27}$$

$$y_{p,k,g,t} = 0, \quad \forall\, k,g,t, \quad p = 6 \tag{A.28}$$

$$\sum_{p=1}^{P-1} y_{p,k,g,t} = Y_{k,g,t}, \quad \forall\, k,g,t \tag{A.29}$$

$$\sum_{p} \lambda_{p,k,g,t} = Y_{k,g,t}, \quad \forall\, k,g,t \tag{A.30}$$

$$\sum_{p} \lambda^{plan}_{p,k,g,t} = Y^{plan}_{k,g,t}, \quad \forall\, k,g,t \tag{A.31}$$

- Planning constraints

$$Y_{k,g,t} = Y_{k,g,t-1} + Y^{plan}_{k,g,t} \qquad \forall k,g,t \tag{A.32}$$

$$Y^{plan}_{k,g,'1'} = Y^{start}_{k,g} \qquad \forall k,g \tag{A.33}$$

$$\sum_{k} Y_{k,g,t} = 1 \qquad \forall g,t \tag{A.34}$$

Table S1. *values for water consumption (direct contribution) related to corn cultivation,* $f^{WF}_{'corn','bp'}$.[m^3/t$_{corn}$]

g	$f^{WF}_{'corn','bp'}$	g	$f^{WF}_{'corn','bp'}$	g	$f^{WF}_{'corn','bp'}$
1	79.96	21	68.91	41	155.73
2	79.96	22	63.47	42	150.18
3	79.96	23	39.46	43	158.71
4	49.93	24	118.61	44	142.96
5	35.93	25	127.78	45	157.54
6	35.93	26	140.51	46	179.12
7	64.63	27	135.18	47	179.25
8	81.65	28	115.50	48	171.93
9	71.94	29	117.43	49	181.07
10	42.12	30	106.79	50	187.29
11	52.62	31	106.59	51	180.57
12	57.40	32	105.97	52	174.38
13	51.49	33	132.07	53	0.00
14	49.93	34	78.40	54	213.97
15	87.87	35	124.70	55	177.18
16	71.18	36	130.78	56	184.96
17	42.16	37	191.57	57	192.73
18	100.59	38	171.05	58	173.99
19	86.61	39	173.18	59	173.99
20	83.49	40	170.07	60	116.25

Table S2. *water consumption related to biomass and ethanol transportation*

Transport mode	*Water consumption ($L_{H2O}/(t_{trans}*km)$*
small truck	3.10E-02
truck	6.42E-03
train	1.10E-03
barge	4.52E-04
ship	3.32E-04
trans ship	3.14E-04

Table S3. *Parameters* ω_k *and* ec_k^{WF} *representing the biomass-to-power conversion yields and the credits for avoided impact on water resources achieved by each technology* k.

technology k	ω_k [kWh/$L_{ethanol}$]	ec_k^{WF} [$m^3_{H_2O}$/$t_{ethanol}$]
1	0	170.5
2	0.743	13.7
3	0.496	179.7
4	0.602	11.1
5	0.482	103.0
6	0.515	74.5
7	0.533	59.5
8	0.482	8.9
9	0.515	9.5
10	0.533	9.9

List of symbols

Acronyms

CHP	Combined Heat and Power
DDGS	Distiller's Dried Grains with Solubles
WF	Water Footprint

Sets

$c \in C$	set of production costs regression coefficients $C = \{slope, intercept\}$
$g \in G$	*grid squares,* $G=\{1,\dots,60\}$
$g' \in G$	*set of square regions different than g*
$i \in I$	set of biomass typology, $I = \{corn, stover\}$
$j \in J$	set of product, $J = \{ethanol, DDGS, power\}$
$k \in K$	set of conversion technologies, $K = \{1,\dots,10\}$
$m \in M$	set of means of transport, $M = \{truck, rail, barge, ship, tship\}$
$l \in L$	environmental objective functions, $L = \{CF, WF\}$
$p \in P$	set of plant scale index, $P = \{1,\dots,6\}$
$s \in S$	set of life cycle stages, $S = \{bp, bpt, bt, fp, ft\}$
$t \in T$	set of time intervals (years), $T = \{1,\dots,20\}$
$tech(k) \subset K$	subset of conversion technologies producing DDGS to be sold, $tech(k) = \{1,3,5,6,7\}$
$fratio(k) \subset K$	subset of conversion technologies using both biomass typology for ethanol production, $fratio(k) = \{5,6,7,8,9,10\}$

sub(p) $\subset$ *P* — *subset of discretisation intervals, sub(p)={1,..,5}*

Scalars

δ	DDGS conversion factor [$t_{DDGS}/t_{ethanol}$]
ρ	ethanol density [kg/L]
Tr	taxation rate
ϕ	fixed costs over incomes
$PCap^{min}$	minimum ethanol production capacity [t/y]

Parameters

$\beta_{i,k}$	fraction of ethanol rate from biomass type *i* for each technology *k*
AD_g	arable land density [$km^2_{arable}/km^2_{grid\ surface}$]
$BA_{g,i}$	biomass *i* available for ethanol production in grid *g* [t/y]
BCD_g^{max}	maximum cultivation density in region *g* [$km^2_{cultivation}/km^2_{arable}$]
$burn_{i,k}$	fraction of biomass *i* fed to the CHP station in technology *k*
$BY_{i,g}$	cultivation yields for each biomass *i* in grid *g* [t/ha]
$coef_{c,k}$	coefficients (slope [€/$t_{ethanol}$], intercept [€]) for linear regression of production costs for technology *k*
$CI_{k,p}$	capital investment at each linearisation interval *p* for the conversion technology *k* [M€]
dk_t	depreciation charge at time *t*
ec_k^l	credits for avoided emissions of conversion technology *k* on climate change [kg CO_2-eq/t] (l = CF) or on water resources [$m^3_{H_2O}$/t] (l = WF)]

$f^{l}_{i,s,g}$ impact factors for biomass *i* and cell *g* on climate change [kg CO_2-eq/t] (l = CF) or on water resources [$m^3_{H_2O}$/t] (l = WF)] for biomass production ($s = bp$)

ER_p ethanol production rate for each plant size *p* [t_{EtOH}/year]

GS_g grid surface of cell *g* [km^2]

IBF_g internal biomass production feasibility, binary parameter

γ_i conversion of biomass *i* to ethanol [$t_{ethanol}/t_{biomass}$]

$LD_{g,g'}$ local delivery distance between grids *g* and *g'* [km]

MP_j market price of product *j* [€/t] or [€/MWh]

$quota_i$ maximum quota of collectable biomass *i* for ethanol production

$\tau_{g,m,g'}$ tortuosity factor of transport mode *m* between *g* and *g'* [-]

$UPC_{i,g}$ unit purchase cost for biomass *i* in grid *g* [€/t]

UTC_m unit transport cost via mean *m* [€/t]

UTC^* unit transport cost for local transport of biomass [€/t]

ω_k electricity sold potential of technology *k* ($kWh/L_{ethanol}$)

Continuous variables

BPC_t biomass purchase cost at time *t* [€/y]

CF_t cash flow at time *t* [€/y]

D_t depreciation charge at time *t* [€/y]

$Db_{i,g,t}$ biomass *i* demand in region *g* at time *t* [t/y]

EPC_t ethanol production cost at time *t* [€/y]

$FixC_t$ fixed costs at time *t* [€/y]

Inc_t gross earnings at time *t* [€/y]

$\lambda_{p,k,g,t}$ linearisation variables for TCI for technology *k* at interval *p* in region *g* at time *t*

$\lambda^{plan}_{p,k,g,t}$ linearisation variables for TCI for technology *k* at interval *p* in region *g* at time *t*

$Pb_{i,g,t}$ production rate of biomass *i* in cell *g* at time *t* [t/y]

PBT_t profit before taxes at time *t* [€/y]

$Pf_{i,k,g,t}$ ethanol production rate from biomass *i* through facility *k* at time *t* in grid *g* [t/y]

$P^T_{j,k,g,t}$ total production rate for product *j* through technology *k* at time *t* in grid *g* [t/y]

$Qb_{i,g,m,g',t}$ flow rate of biomass *i* between *g* and *g'* with transport mode *m* in time period *t* [t/y]

$Qf_{g,m,g',t}$ ethanol flow rate between *g* and *g'* with transport mode *m* in time period *t* [t/y]

TAX_t tax amount at time *t* [€/y]

TCb_t biomass transport cost at time *t* [€/y]

TCf_t ethanol transport cost at time *t* [€/y]

TCI_t total capital investment at time *t*[€]

$TPot_{i,t}$ total potential production of biomass *i* at time *t* [t/y]

$VarC_t$ variable costs at time *t* [€/y]

Binary variables

$Y_{k,g,t}$ 1 if a production facility *k* is already established in region *g* at time *t*, 0 otherwise

$Y^{plan}_{k,g,t}$ 1 if the establishment of a new conversion facilities *k* is to be planned in region *g* during time period *t,* 0 otherwise

$Y^{start}_{k,g}$ 1 if establishment of a new conversion facilities *k* is to be planned in region *g* at the beginning, 0 otherwise

$y_{p,k,g,t}$ supporting variable for linearisation of plant scale