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Economic and Environmental Optimization and Analysis of Biomass to Fuels: Present and Future

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S1. Mathematical Formulation

S1.1 Notation

Indexes are given as lower-case italicized roman characters, sets and subsets as capital bold roman characters, parameters as italicized Greek characters, and variables as capital italicized roman characters.

Sets

$b \in \boldsymbol{B}$	Biomass feedstocks
$c \in \mathbf{C}$	Carbon capture options
$e \in \mathbf{E}$	Energy purchase
$f \in \mathbf{F}$	Fuel types
$s \in \mathbf{S}$	Scaling exponents
$t \in \mathbf{T}$	Technology
$y \in \mathbf{Y}$	Years

Subsets

B_t^T	Feedstock b used in technology t
$\mathbf{C}_{t,e,f}^{\mathrm{S}}$	Carbon capture options for the combination of technology t, energy purchase e, and fuel f
$\mathbf{F}^{\mathrm{L}}$	Liquid fuels
$\mathbf{Y}^{C}$	Construction years
$\mathbf{Y}^{\mathrm{S}}$	Startup years
$\mathbf{Y}^{\mathrm{O}}$	Operating years
$\mathbf{Y}^{\mathrm{OF}}$	First operating year
$\mathbf{Y}^{\mathrm{OL}}$	Last operating year

Parameters

$\gamma_{t,e,f,c,s}^{GEN}$	General plant capital cost corresponding to scaling exponent s for technology t, energy purchase e, fuel f, and carbon capture $c \in \mathbf{C}_{t,e,f}^{\mathrm{S}}$ at reference capacity ($)
$\gamma_{t,e,f,c,s}^{ST}$	Steam plant capital cost corresponding to scaling exponent s for technology t, energy purchase e, fuel f, and carbon capture $c \in \mathbf{C}_{t,e,f}^{\mathrm{S}}$ at reference capacity ($)
δ^{DIS}	Discount rate

δ_y^{GEN} Depreciation rate for general plant in year $y \in \mathbf{Y}^{\mathrm{O}}$
δ_y^{ST} Depreciation rate for steam plant in year $y \in \mathbf{Y}^{\mathrm{O}}$
ϵ_y^{C} Percent of construction costs incurred in year $y \in \mathbf{Y}^{C}$
$\epsilon_{t,f}^{CG}$ Cost growth parameter of technology t and fuel $f \in \mathbf{F}^{\mathrm{L}}$
$\epsilon_{t,f,y}^{PER}$ Plant performance of technology t and fuel $f \in \mathbf{F}^{\mathrm{L}}$ in year $y \in \mathbf{Y}^{\mathrm{O}}$
ϵ_y^{SF} Percent of fixed costs incurred during startup in year $y \in \mathbf{Y}^{\mathrm{S}}$
ϵ_y^{SP} Percent of production during startup in year $y \in \mathbf{Y}^{\mathrm{S}}$
ϵ_y^{ST} Percent of year $y \in \mathbf{Y}^{\mathrm{O}}$ spent in startup
ϵ_y^{SV} Percent of variable costs incurred during startup in year $y \in \mathbf{Y}^{\mathrm{S}}$
ζ^{REF} Reference capacity (Mg feedstock/day)
ζ Capacity (Mg feedstock/day)
$\eta_{t,e,c}^{E}$ Amount of electricity in excess for technology t, energy purchase e, liquid fuel production, and carbon capture $c \in \mathbf{C}_{t,e,f}^{\mathrm{S}}$ (MWh/Mg feedstock)
$\eta_{t,e,f,c}^{F}$ Fuel production for technology t, energy purchase e, fuel f, and carbon capture $c \in \mathbf{C}_{t,e,f}^{\mathrm{S}}$ (GGE/Mg feedstock)
κ_b^{FD} Cost of feedstock b (\$/Mg)
$\kappa_{t,e,f,c}^{FX}$ Fixed cost for technology t, energy purchase e, fuel f, and carbon capture $c \in \mathbf{C}_{t,e,f}^{\mathrm{S}}$ (\$/yr)
$\kappa_{t,e,f,c}^{M}$ Material cost for technology t, energy purchase e, fuel f, and carbon capture $c \in \mathbf{C}_{t,e,f}^{\mathrm{S}}$ (\$/Mg feedstock)
$\kappa_{t,e,f,c}^{O}$ Operating cost for technology t, energy purchase e, fuel f, and carbon capture $c \in \mathbf{C}_{t,e,f}^{\mathrm{S}}$ (\$/Mg feedstock)
μ^{L} Upper bound of yearly losses (\$/yr)
μ^{T} Upper bound for taxes paid (\$/yr)
ν^{O} Overhead rate
ν^{WC} Working capital percent
π^{E} Purchase/sell price of electricity (\$/MWh)
π^{SEQ} Sequestration credit (\$/Mg CO_2)
π^{TR} Transportation and injection cost of CO_2 (\$/Mg CO_2)
σ_s Value of scaling exponent
τ Tax rate
χ_f^{E} Efficiency of fuel f in an engine
$\psi_{t,e,f,c}^{CCS}$ CO_2 sequestered for technology t, energy purchase e, fuel f, and carbon capture $c \in \mathbf{C}_{t,e,f}^{\mathrm{S}}$ (Mg CO_2e/Mg feedstock)
$\psi_{t,e,f,c}^{CHE}$ CO_2e emissions from biorefinery chemical consumption for technology t, energy purchase e, fuel f, and carbon capture $c \in \mathbf{C}_{t,e,f}^{\mathrm{S}}$ (Mg CO_2e/Mg feedstock)
ψ_e^{EP} Incurred CO_2e emissions from energy purchased (Mg CO_2e/MWh)
ψ_f^{F} Mitigated CO_2e emissions from fuel sold (Mg CO_2e/GGE)
ψ_b^{H} CO_2 emissions from harvesting biomass b (Mg CO_2e/Mg feedstock)
ψ_b^{SOC} CO_2 sequestered in soil organic carbon by biomass b (Mg CO_2e/Mg feedstock)
ψ_b^{TR} CO_2 emissions from transport of biomass b (Mg CO_2e/Mg feedstock)
ω^{OP} Operating days per year

Variables

Real variables

INC_y^{AN}	Annual income in year y (\$/yr)
INC_y^{TX}	Taxable income in year y (\$/yr)
$MFSP$	Minimum fuel selling price (\$/GGE)
$MFSP^F$	Minimum fuel selling price normalized to forward motion (\$/GJ forward motion)
REV_y	Revenue in year y (\$/yr)
Non-negative continuous variables	
ACI_y	Annual cash inflow (\$/yr)
C_y^{OP}	Operating cost in year y (\$/yr)
C_y^{FX}	Fixed cost in year y (\$/yr)
C_y^{TR}	Cost of transporting CO_2 in year y (\$/yr)
C_y^{SEQ}	Credit from sequestration of CO_2 in year y (\$/yr)
FCI	Fixed capital investment (\$)
FCI^{GEN}	Fixed capital investment for general plant (\$)
FCI^{ST}	Fixed capital investment for steam plant (\$)
GHG^D	Direct GHG sequestration (Mg CO_2/Mg feedstock)
GHG^{NET}	GHG sequestration balance with direct sequestration and mitigated emissions (Mg CO_2/Mg feedstock)
L_y	Losses in year y (\$/yr)
L_y^D	Dummy variable for losses in year y (\$/yr)
T_y	Taxes paid in year y (\$/yr)
T_y^D	Dummy variable for taxes in year y (\$/yr)
TCI	Total capital investment (\$)
Binary variables	
$Z_{t,e,f,c}^S$	=1 if strategy (technology t, energy purchase e, fuel f, and carbon capture c) is selected
Y_y^L	=1 if there are net losses in year y
Y_y^T	=1 if there are taxes paid in year y

S1.2 Mathematical Model

The mathematical model is presented below. For comparisons between liquid fuels, we minimize $MFSP$, and for comparisons of all fuel types, we minimize the breakeven price normalized to forward motion, $MFSP^F$.

$$FCI^{GEN} = (1+\nu^O) \sum_{t,e,f,s,c \in \boldsymbol{C}_{t,e,f}^S} Z_{t,e,f,c}^S \, \gamma_{t,e,f,c,s}^{GEN} \left(\frac{\zeta}{\zeta^{REF}}\right)^{\sigma_s} \tag{S1.1}$$

$$FCI^{ST} = (1+\nu^O) \sum_{t,e,f,s,c \in \boldsymbol{C}_{t,e,f}^S} Z_{t,e,f,c}^S \, \gamma_{t,e,f,c,s}^{ST} \left(\frac{\zeta}{\zeta^{REF}}\right)^{\sigma_s} \tag{S1.2}$$

$$\sum_{t,e,f,c \in \boldsymbol{C}_{t,e,f}^S} Z_{t,e,f,c}^S = 1 \tag{S1.3}$$

$$FCI = FCI^{GEN} + FCI^{ST} \tag{S1.4}$$

$$TCI = FCI(1+\nu^{WC}) \tag{S1.5}$$

$$INC_y^{AN} = \left(\epsilon_y^{ST}\epsilon_y^{SP} + 1 - \epsilon_y^{ST}\right) \sum_{t,e,f,c \in \boldsymbol{C}_{t,e,f}^S} Z_{t,e,f,c}^S \omega^{OP} \zeta \left(\eta_{t,e,f,c}^F MFSP + \eta_{t,e,c}^E \pi^E\right) \quad y \in \mathbf{Y}^{\mathrm{O}} \tag{S1.6}$$

$$C_y^{OP} = \left(\epsilon_y^{ST}\epsilon_y^{SV} + 1 - \epsilon_y^{ST}\right) \sum_{t,e,f,c \in \boldsymbol{C}_{t,e,f}^S, b \in B_t^T} Z_{t,e,f,c}^S \omega^{OP} \zeta \left(\kappa_{t,e,f,c}^M + \kappa_{t,e,f,c}^O + \kappa_b^{FD}\right) \quad y \in \mathbf{Y}^{\mathrm{O}} \tag{S1.7}$$

$$C_y^{TR} = \left(\epsilon_y^{ST}\epsilon_y^{SP} + 1 - \epsilon_y^{ST}\right) \sum_{t,e,f,c \in \boldsymbol{C}_{t,e,f}^S} Z_{t,e,f,c}^S \omega^{OP} \zeta \psi_{t,e,f,c}^{CCS} \pi^{TR} \quad y \in \mathbf{Y}^{\mathrm{O}} \tag{S1.8}$$

$$C_y^{FX} = \left(\epsilon_y^{ST}\epsilon_y^{SF} + 1 - \epsilon_y^{ST}\right) \sum_{t,e,f,c \in \boldsymbol{C}_{t,e,f}^S} Z_{t,e,f,c}^S \kappa_{t,e,f,c}^{FX} \quad y \in \mathbf{Y}^{\mathrm{O}} \tag{S1.9}$$

$$C_y^{SEQ} = \left(\epsilon_y^{ST}\epsilon_y^{SP} + 1 - \epsilon_y^{ST}\right) \sum_{t,e,f,c \in \boldsymbol{C}_{t,e,f}^S} Z_{t,e,f,c}^S \omega^{OP} \zeta \psi_{t,e,f,c}^{CCS} \pi^{SEQ} \quad y \in \mathbf{Y}^{\mathrm{O}} \tag{S1.10}$$

$$REV_y = INC_y^{AN} + C_y^{SEQ} - \left(C_y^{OP} + C_y^{TR} + C_y^{FX} + \delta_y^{GEN} FCI^{GEN} + \delta_y^{ST} FCI^{ST}\right) \quad y \in \mathbf{Y}^{\mathrm{O}} \tag{S1.11}$$

$$L_y^D - L_y = INC_{y-1}^{TX} + C_y^{SEQ} \quad y \in \mathbf{Y}^{\mathrm{O}} \setminus \mathbf{Y}^{\mathrm{OF}} \tag{S1.12}$$

$$L_y \leq Y_y^L \mu^L \quad y \in \mathbf{Y}^{\mathrm{O}} \setminus \mathbf{Y}^{\mathrm{OF}} \tag{S1.13}$$

$$L_y^D \leq (1 - Y_y^L)\mu^L \quad y \in \mathbf{Y}^{\mathrm{O}} \setminus \mathbf{Y}^{\mathrm{OF}} \tag{S1.14}$$

$$INC_y^{TX} = \begin{cases} REV_y & y \in \mathbf{Y}^{\mathrm{OF}} \\ REV_y - L_y & y \in \mathbf{Y}^{\mathrm{O}} \setminus \mathbf{Y}^{\mathrm{OF}} \end{cases} \tag{S1.15}$$

$$T_y - T_y^D = \tau \, INC_y^{TX} \quad y \in \mathbf{Y}^{\mathrm{O}} \tag{S1.16}$$

$$T_y \leq Y_y^T \mu^T \quad y \in \mathbf{Y}^{\mathrm{O}} \tag{S1.17}$$

$$T_y^D \leq \left(1 - Y_y^T\right)\mu^T \quad y \in \mathbf{Y}^{\mathrm{O}} \tag{S1.18}$$

$$ACI_y = INC_y^{AN} + C_y^{SEQ} - (C_y^{OP} + C_y^{TR} + C_y^{FX} + T_y) \tag{S1.19}$$

$$\sum_{y \in \mathbf{Y}^{\mathrm{C}}} \epsilon_y^C (1 + \delta^{DIS})^{-y} FCI + \epsilon^{WC} FCI \left(1 - \sum_{y \in \mathbf{Y}^{\mathrm{OL}}} (1 + \delta^{DIS})^{-y}\right) = \sum_{y \in \mathbf{Y}^{\mathrm{O}}} ACI_y (1 + \delta^{DIS})^{-y} \tag{S1.20}$$

$$MFSP^F \sum_{t,e,f,c \in \boldsymbol{C}_{t,e,f}^S} Z_{t,e,f,c}^S \chi_f = MFSP \left(8.32 \frac{GGE}{GJ}\right) \tag{S1.21}$$

$$GHG^D = \sum_{t,e,f,c \in \boldsymbol{C}_{t,e,f}^S, b \in B_t^T} Z_{t,e,f,c}^S \left(\psi_b^{SOC} - \psi_b^H - \psi_b^{TR} + \psi_{t,e,f,c}^{CCS}\right) \tag{S1.22}$$

$$GHG^{NET} = GHG^D - \sum_{t,e,f \in \mathbf{F}^{\mathrm{L}}, c \in \boldsymbol{C}_{t,e,f}^S} Z_{t,e,f,c}^S \eta_{t,e,c}^E \psi_e^{EP} + \sum_{t,e,f,c \in \boldsymbol{C}_{t,e,f}^S} Z_{t,e,f,c}^S \left(\eta_{t,e,f,c}^F \psi_f^F - \psi_{t,e,f,c}^{CHE}\right) \tag{S1.23}$$

S2. Feedstock and transportation data

Table S2.1. Biomass growth data.

Parameter	Units	Value	
		Switchgrass	Poplar
Yield	Mg/h/yr	7.3[1]	9.2[1]
Percent of Land Available	%	1.4[2]	1.4[1]
Farm Price	$/Mg	44.9[3]	58.7[4]
Fuel Emissions	g $CO_2e/m^2/yr$	4.6[1]	0.6[1]
Fertilizer Emissions	g $CO_2e/m^2/yr$	33.8[1]	-[1]
N_2O Emissions	g $CO_2e/m^2/yr$	56.9[1]	27.1[1]
CH_4 Oxidation	g $CO_2e/m^2/yr$	-0.9[1]	-1.2[1]
SOC Sequestration	g $CO_2e/m^2/yr$	-115[1]	-115

For transportation, we use the model developed by Ng *et al.*[5]

Table S2.2. Biomass transportation data.[5]

Parameter	Units	Value	
		Switchgrass	Poplar
Biomass Handling Cost	$/Mg	19.3	*
Depot Cost	$/Mg	19.7	18.2
Truck Fixed Cost	$/Mg	7.5	4.7
Truck-Depot-Truck Fixed Cost	$/Mg	11.1	10.9
Truck-Depot-Rail Fixed Cost	$/Mg	26.7	27
Truck Variable Cost	$/Mg/km	0.218	0.142
Truck-Depot-Truck Variable Cost	$/Mg/km	0.07	0.098
Truck-Depot-Rail Variable Cost	$/Mg/km	0.012	0.022
Biomass Handling Energy	MJ/Mg	681	681
Depot Energy	MJ/Mg	882	882
Truck Variable Energy	MJ/Mg/km	5.27	3.43
Truck-Depot-Truck Variable Energy	MJ/Mg/km	1.13	1.11
Truck-Depot-Rail Variable Energy	MJ/Mg/km	0.177	0.18

*included in farm price of poplar

S3. Economic assumptions

Additional costs beyond installed capital costs are assumed as described in Table S3.1.

Table S3.1. Additional indirect costs.

Item	Parameter in model	Amount
Warehouse, site development, additional piping	ν^{O}	10% of total direct costs
Prorateable costs		10% of total direct costs
Field expenses		10% of total direct costs
Home office and construction		20% of total direct costs
Project contingency		10% of total direct costs
Working capital	ν^{WC}	15% of fixed capital investment

Fixed capital investment is calculated as the sum of installed costs and indirect costs. Total capital investment is calculated as the sum of fixed capital investment and working capital. The project is assumed to be 100% equity financed. Discounted cash flow analysis parameters and scaling exponents are given in Tables S3.2 and S3.3, respectively.

Table S3.2. Discounted cash flow analysis parameters.[6]

Item	Set/Parameter in model	Value
Plant life	$\lvert \mathbf{Y}^{O} \rvert$	30 years
Discount rate	δ^{DIS}	10%
Income tax rate	τ	35%
General plant depreciation	δ_y^{GEN}	200% declining balance
General plant recovery period		7 years
Steam plant depreciation	δ_y^{ST}	150% declining balance
Steam plant recovery period		20 years
Construction period	$\lvert \mathbf{Y}^{C} \rvert$	3 years
First year's expenditures	$\epsilon_{y_{-2}}^{C}$	8%
Second year's expenditures	$\epsilon_{y_{-1}}^{C}$	60%
Third year's expenditures	$\epsilon_{y_0}^{C}$	32%
Startup time	$\epsilon_{y_1}^{ST}$	0.5 years
Revenues during startup	$\epsilon_{y_1}^{SP}$	50%
Variable costs incurred during startup	$\epsilon_{y_1}^{SV}$	75%
Fixed costs incurred during startup	$\epsilon_{y_1}^{SF}$	100%

Table S3.3. Scaling exponents

$s \in \mathbf{S}$	s_1	s_2	s_3	s_4	s_5	s_6	s_7	s_8	s_9
σ_s	1	0.9	0.8	0.75	0.72	0.7	0.65	0.6	0.5

We assume an electricity purchase/sell price (π^{E}) of \$60/MWh. The cost of transporting and injecting CO_2 into saline aquifers (π^{TR}) is \$12/Mg CO_2.

S4. Pioneer Plant Analysis

For calculating the additional costs and reduced performance of a pioneer plant, we use the methodology developed by the RAND Corporation.[7] In this method, the total capital investment and plant performance of the pioneer plant are calculated according to Eqs. (S4.1 and (S4.2, respectively.

$$TCI_{pioneer} = \frac{TCI_{n^{th}}}{CG} \tag{S4.1}$$

$$Cost_{pioneer,y} = \max(PER + 20(\mathrm{y} - 1), 100)\ Cost_{n^{th},y} \tag{S4.2}$$

CG is the cost growth and PER is the fraction of peak performance in the first year of operation. CG and PER are determined by Eqs. (S4.3 and (S4.4, respectively.

$$CG = 1.12196 - 0.00297 \times PNEW - 0.02125 \times IMP - 0.01137 \times COMP + 0.00111 \times INCL - 0.06351 \times PDEF \tag{S4.3}$$

$$PER = 85.77 - 9.69 \times NSTEP + 0.33 \times BALQ - 4.12 \times WST - 17.91 \times SLDS \tag{S4.4}$$

The descriptions of the parameters in Eqs. (S4.3 and (S4.4 are given in Table S4.1.

Table S4.1. Pioneer plant analysis parameters.

Parameter	Full Name: Description	Range	Value		
			Fermentation	Pyrolysis	Gasification
PNEW	Percent new: percentage of equipment cost data for new equipment	0-100	30	40	30
IMP	Impurities: a factor of impurities present in the process	0-5	3	4	4
COMP	Complexities: number of consecutively linked plant areas	≥1	6	5	9
INCL	Inclusiveness: percent of land purchase/lease, initial plant inventory/parts/ catalysts, and pre-operating personnel costs included in the analysis	0-100	0	0	33
PDEF	Project definition: a factor of level of detail in the analysis	2-8	4	8	7
NSTEP	New steps: number of new process areas	≥0	3	3	2
BALQ	Balance equations: percentage of mass and energy balance equations based on commercial plant data	0-100	60	0	0
WST	Waste: a factor of waste disposal	0-5	2	4	4
SLDS	Solids: a factor based on the presence of solids	0 or 1	1	1	1
$\epsilon_{t,f}^{CG}$			0.65	0.35	0.44
ϵ_{t,f,y_1}^{PER}			60%	22%	32%
References			8,9	10,11	12,13

For the pioneer plant analysis, model equations S1.1-2 and S1.6-10 are replaced with equations S4.5-11, and only liquid fuels ($f \in \mathbf{F}^{\mathrm{L}}$) are considered.

$$FCI^{GEN} = (1+\epsilon^{O}) \sum_{t,e,f,s,c \in \boldsymbol{C}^{S}_{t,e,f}} \frac{Z^{S}_{t,e,f,c}\gamma^{GEN}_{t,e,f,c,s}}{\epsilon^{CG}_{t,f}} \left(\frac{\zeta}{\zeta^{REF}}\right)^{\sigma_s} \quad y \in \mathbf{Y}^{\mathrm{O}} \tag{S4.5}$$

$$FCI^{ST} = (1+\epsilon^{O}) \sum_{t,e,f,s,c \in \boldsymbol{C}^{S}_{t,e,f}} \frac{Z^{S}_{t,e,f,c}\gamma^{ST}_{t,e,f,c,s}}{\epsilon^{CG}_{t,f}} \left(\frac{\zeta}{\zeta^{REF}}\right)^{\sigma_s} \quad y \in \mathbf{Y}^{\mathrm{O}} \tag{S4.6}$$

$$INC^{AN}_{y} = \left(\epsilon^{ST}_{y}\epsilon^{SP}_{y} + 1 - \epsilon^{ST}_{y}\right) \sum_{t,e,f,c \in \boldsymbol{C}^{S}_{t,e,f}} \frac{Z^{S}_{t,e,f,c}\omega^{OP}\zeta\left(\eta^{F}_{t,e,f,c}MFSP + \eta^{E}_{t,e,c}\pi^{E}\right)}{\epsilon^{PER}_{t,f,y}} \quad y \in \mathbf{Y}^{\mathrm{O}} \tag{S4.7}$$

$$C^{OP}_{y} = \left(\epsilon^{ST}_{y}\epsilon^{SV}_{y} + 1 - \epsilon^{ST}_{y}\right) \sum_{t,e,f,c \in \boldsymbol{C}^{S}_{t,e,f}, b \in B^{T}_{t}} \frac{Z^{S}_{t,e,f,c}\omega^{OP}\zeta\left(\kappa^{M}_{t,e,f,c} + \kappa^{O}_{t,e,f,c} + \kappa^{FD}_{b}\right)}{\epsilon^{PER}_{t,f,y}} \quad y \in \mathbf{Y}^{\mathrm{O}} \tag{S4.8}$$

$$C^{TR}_{y} = \left(\epsilon^{ST}_{y}\epsilon^{SP}_{y} + 1 - \epsilon^{ST}_{y}\right) \sum_{t,e,f,c \in \boldsymbol{C}^{S}_{t,e,f}} \frac{Z^{S}_{t,e,f,c}\omega^{OP}\zeta\psi^{CCS}_{t,e,f,c}\pi^{TR}}{\epsilon^{PER}_{t,f,y}} \quad y \in \mathbf{Y}^{\mathrm{O}} \tag{S4.9}$$

$$C^{FX}_{y} = \left(\epsilon^{ST}_{y}\epsilon^{SF}_{y} + 1 - \epsilon^{ST}_{y}\right) \sum_{t,e,f,c \in \boldsymbol{C}^{S}_{t,e,f}} \frac{Z^{S}_{t,e,f,c}\kappa^{FX}_{t,e,f,c}}{\epsilon^{PER}_{t,f,y}} \quad y \in \mathbf{Y}^{\mathrm{O}} \tag{S4.10}$$

$$C^{SEQ}_{y} = \left(\epsilon^{ST}_{y}\epsilon^{SP}_{y} + 1 - \epsilon^{ST}_{y}\right) \sum_{t,e,f,c \in \boldsymbol{C}^{S}_{t,e,f}} \frac{Z^{S}_{t,e,f,c}\omega^{OP}\zeta\psi^{CCS}_{t,e,f,c}\pi^{SEQ}}{\epsilon^{PER}_{t,f,y}} \quad y \in \mathbf{Y}^{\mathrm{O}} \tag{S4.11}$$

S5. Strategy parameters and illustration

A conceptual illustration of how we define a strategy is shown in Figure S5.1. A strategy is defined by the technology $t \in \mathbf{T}$, energy $e \in \mathbf{E}$ purchased, fuel $f \in \mathbf{F}$ produced, and carbon capture $c \in \mathbf{C}$.

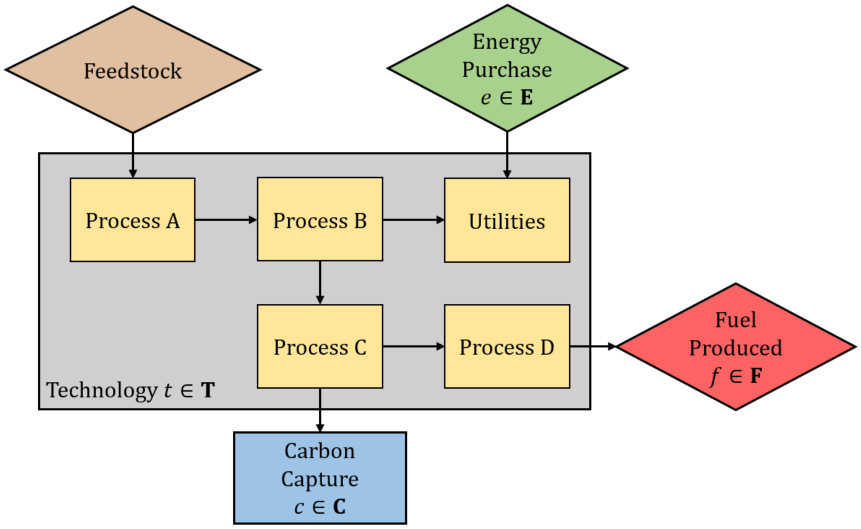

Figure S5.1. Illustration of an example strategy,

Parameters for each strategy, and the references from which data is taken, are provided in Tables S5.1-3.

Table S5.1. Process costs and parameters for fermentation to ethanol.

Technology $t \in \mathbf{T}$			*Fer*	*Fer*	*Fer*	*Fer*	*Fer*
Energy Purchased $e \in \mathbf{E}$			–	–	–	–	*Elec*
Fuel $f \in \mathbf{F}$			*Liq*	*Liq*	*Liq*	*Liq*	*Liq*
Carbon Capture $c \in \mathbf{C}$			–	*Fer*	*FerBio*	*FerBioFlu*	*FerBioFlu*
$\gamma^{GEN}_{t,e,f,c,s}$	s_1	MM$	65.3	65.3	65.3	65.3	65.3
	s_3	MM$	13.6	28.8	47.0	63.1	117.6
	s_6	MM$	91.3	91.3	91.3	91.3	91.3
	s_8	MM$	30.1	30.1	30.1	30.1	30.1
	s_9	MM$	0.7	0.7	0.7	0.7	0.7
$\gamma^{ST}_{t,e,f,c,s}$	s_4	MM$	19.1	19.1	18.4	15.8	9.9
	s_6	MM$	57.6	57.6	57.6	57.6	57.6
	s_7	MM$	1.0	1.0	1.0	1.0	1.0
	s_8	MM$	0.2	0.2	0.2	0.2	0.2
$\kappa^{FX}_{t,e,f,c}$	MM$/yr		12.6	12.6	12.6	12.6	12.6
$\kappa^{M}_{t,e,f,c}$	$/Mg feedstock		34.9	36.7	37.3	38.0	39.4
$\kappa^{O}_{t,e,f,c}$	$/Mg feedstock		2.0	2.0	2.0	2.0	2.0
$\eta^{E}_{t,e,c}$	MWh/Mg feedstock		0.188	0.152	0.107	-	-0.226
$\eta^{F}_{t,e,f,c}$	GGE/Mg feedstock		62.3	62.3	62.3	62.3	62.3
$\psi^{CCS}_{t,e,f,c}$	Mg CO_2/Mg feedstock		-	0.47	0.65	0.80	1.12
$\psi^{CHE}_{t,e,f,c}$	Mg CO_2e/Mg feedstock		0.142	0.142	0.142	0.142	0.142
References			6	6,14	6,14	6,14	6,14

**Bio*: Biogas, *Elec*: Electricity, *Fer*: Fermentation, *Flu*: Flue gas, *Liq*: Liquid fuel

Table S5.2. Process costs and parameters for gasoline/diesel production.

Technology $t \in \mathbf{T}$		*Pyr*	*Pyr*	*Pyr*	*Pyr*	*Pyr*	*Gas*	*Gas*	*Gas*	*Gas*	*Gas*
Energy Purchased $e \in \mathbf{E}$		*H2*	*H2*	*H2Elec*	–	–	–	*Elec*	*Elec*	–	–
Fuel $f \in \mathbf{F}$		*Liq*	*Liq*	*Liq*	*Liq*	*Liq*	*Liq*	*Liq*	*Liq*	*Liq*	*Liq*
Carbon Capture $c \in \mathbf{C}$		–	*Flu*	*Flu*	–	*Flu*	–	*Syn*	*SynFlu*	*Syn*	*SynFlu*
$\gamma^{GEN}_{t,e,f,c,\cdot}$	s_1 MM$	65.8	65.8	65.8	77.9	77.9	2.5	2.5	2.5	2.5	1.8
	s_2 MM$	0.2	0.2	0.2	8.7	8.7	0.2	0.2	0.2	0.2	0.2
	s_3 MM$	4.4	59.5	70.1	5.0	5.0	3.5	12.4	60.9	14.2	66.5
	s_4 MM$	26.6	21.9	20.4	26.6	26.6	-	-	-	-	-
	s_6 MM$	130.6	130.6	130.6	140.3	140.3	103.5	103.5	101.9	103.5	101.9
	s_7 MM$	0.2	0.2	0.2	0.2	0.2	-	-	-	-	-
	s_8 MM$	-	-	-	-	-	68.9	68.9	68.9	68.9	68.9
	s_9 MM$	66.7	66.7	66.7	67.3	67.3	2.1	2.1	2.1	2.1	2.1
$\gamma^{ST}_{t,e,f,c,\cdot}$	s_1 MM$	-	-	-	-	-	3.3	3.3	3.3	3.2	2.4
	s_3 MM$	-	-	-	-	-	1.4	1.4	1.4	1.8	5.0
	s_4 MM$	-	-	-	-	-	36.1	36.1	20.3	37.9	53.8
	s_6 MM$	-	-	-	-	-	1.2	1.2	1.2	1.2	0.9
	s_7 MM$	-	-	-	-	-	0.4	0.4	0.4	0.4	0.2
	s_9 MM$	-	-	-	-	-	1.3	1.3	1.3	1.3	1.1
$\kappa^{FX}_{t,e,f,c}$	MM$/yr	25.8	25.8	25.8	28.4	28.4	20.3	20.3	20.3	20.3	20.3
$\kappa^{M}_{t,e,f,c}$	$/Mg feedstock	23.3	23.3	23.3	12.1	4.7	17.3	17.3	17.3	17.2	12.8
$\kappa^{O}_{t,e,f,c}$	$/Mg feedstock	2.3	5.2	5.9	2.4	23.3	1.5	3.1	4.2	3.4	13.0
$\eta^{E}_{t,e,c}$	MWh/Mg feedstock	0.411	-	-0.096	0.193	-	-	-0.010	-0.392	-	-
$\eta^{F}_{t,e,f,c}$	GGE/Mg feedstock	67.7	67.7	67.7	67.7	26.3	56.4	56.4	56.4	55.8	40.6
$\psi^{CCS}_{t,e,f,c}$	Mg CO_2/Mg feedstock	-	0.79	0.98	-	1.22	-	0.42	1.16	0.42	1.26
$\psi^{CHE}_{t,e,f,c}$	Mg CO_2e/Mg feedstock	0.132	0.132	0.132	0.011	0.011	0.009	0.009	0.009	0.009	0.009
References		10,11	10,11,15	10,11,15	10,11	10,11,15	12,13	12,13,15	12,13,15	12,13,15	12,13,15

**Elec*: Electricity, *Flu*: Flue gas, *Gas:* Gasification, *Liq*: Liquid fuel, *Pyr*: Pyrolysis, *Syn:* Syngas

Table S5.3. Process costs and parameters for nonliquid fuel production.

Technology $t \in \mathbf{T}$			*Gas*	*Gas*	*Gas*	*Gas*	*Gas*	*Gas*	*Comb*	*Comb*
Energy Purchased $e \in \mathbf{E}$			–	–	–	–	–	–	–	–
Fuel $f \in \mathbf{F}$			*H2*	*H2*	*H2*	*Elec*	*Elec*	*Elec*	*Elec*	*Elec*
Carbon Capture $c \in \mathbf{C}$			–	*Syn*	*SynFlu*	–	*Syn*	*SynFlu*	–	*Flu*
$\gamma^{GEN}_{t,e,f,c,s}$	s_1	MM$	11.7	11.7	11.7	11.7	11.7	11.7	11.7	11.7
	s_2	MM$	18.0	18.0	18.0	18.0	18.0	18.0	18.0	18.0
	s_3	MM$	10.4	33.5	74.7	10.4	33.5	91.0	-	133.3
	s_6	MM$	138.1	137.5	131.2	116.5	116.5	116.5	-	-
	s_8	MM$	4.6	4.6	4.6	4.6	4.6	4.6	-	-
	s_9	MM$	6.6	6.9	9.1	12.5	12.5	12.5	13.5	13.5
$\gamma^{ST}_{t,e,f,c,s}$	s_3	MM$	2.0	2.4	3.1	11.8	11.8	9.7	7.4	5.3
	s_4	MM$	32.6	38.7	48.7	172.7	172.7	143.9	111.6	81.2
	s_6	MM$	22.4	24.7	33.8	70.5	70.5	64.3	26.4	19.6
$\kappa^{FX}_{t,e,f,c}$		MM$/yr	17.0	17.0	17.0	17.0	17.0	17.0	17.0	17.0
$\kappa^{M}_{t,e,f,c}$		$/Mg feedstock	9.9	9.5	6.2	1.0	1.0	1.0	0.0	0.0
$\kappa^{O}_{t,e,f,c}$		$/Mg feedstock	24.0	26.7	29.3	24.0	26.7	29.4	24.0	29.1
$\eta^{F}_{t,e,f,c}$		GGE/Mg feedstock	88.9	85.8	60.5	65.8	63.8	44.1	40.3	21.5
$\psi^{CCS}_{t,e,f,c}$		Mg CO_2/Mg feedstock	-	0.85	1.56	-	0.85	1.60	-	1.38
$\psi^{CHE}_{t,e,f,c}$		Mg CO_2e/Mg feedstock	0.009	0.009	0.009	0.009	0.009	0.009	0.009	0.009
References			16,17	14,16,17	14,16,17	16	14,16	14,16	16	14,16

S6. Energy Production Forecasts

The assumed electricity and hydrogen production mix, and the average emissions per kWh, for every five years from 2020-2050 are given in Table S6.1 and Table S6.2.

Table S6.1. Electricity and hydrogen production mix and emissions for the reference scenario.[18]

Production Source	Units	2020	2025	2030	2035	2040	2045	2050
Annual Electricity Production								
Onshore Wind	TWh	411	413	510	613	942	1177	1300
Offshore Wind	TWh	0.1	3.7	11.1	23.4	28.7	38.7	173
Rooftop PV	TWh	50.1	79.5	102	130	174	221	268
Utility PV	TWh	49.1	54.5	72.9	131	182	199	257
Hydro	TWh	300	312	295	296	304	294	295
Geothermal	TWh	14.6	14.5	14.6	14.6	14.2	14.2	13.9
Nuclear	TWh	802	775	733	620	558	456	394
Natural Gas	TWh	1547	1791	2184	2446	2263	2339	2245
Natural Gas + CCS	TWh	0	0	0.3	0.4	0.4	0.4	0.4
Biomass	TWh	16.8	20.1	14	8.9	3.8	4.4	5.6
Biomass + CCS	TWh	0	0	0.1	0.1	0.1	0.1	0.1
Coal	TWh	965	844	534	394	366	342	310
Average Emissions	gCO_2e/kWh	0.600	0.538	0.486	0.465	0.416	0.402	0.366
Annual Hydrogen Production								
Biomass	TWh	0	0	0	0	0	0	0
Fossil	TWh	248.9	259.7	265.3	265.3	265.0	261.4	260.6
Electrolysis	TWh	0.2	0.2	0.3	0.4	0.6	1.0	1.6
Average Emissions	gCO_2e/kWh	0.290	0.290	0.290	0.290	0.290	0.290	0.290

Table S6.2. Electricity and hydrogen production mix and emissions for the high electrification scenario.[19]

Production Source	Units	2020	2025	2030	2035	2040	2045	2050
Annual Electricity Production								
Onshore Wind	TWh	412	764	1446	2119	3029	3710	4485
Offshore Wind	TWh	0.093	3.9	20.3	80.7	182	455	934
Rooftop PV	TWh	50.1	79.4	102	127	168	212	252
Utility PV	TWh	88.9	295	656	1169	1694	2268	2833
Hydro	TWh	300	312	295	295	302	292	292
Geothermal	TWh	14.5	14.5	14.3	14.2	13.8	13.7	13.1
Nuclear	TWh	802	775	733	620	558	467	503
Natural Gas	TWh	1490	1742	1453	1117	853	443	202
Natural Gas + CCS	TWh	0	0	1.42	114	152	181	231
Biomass	TWh	18.2	19.7	39.5	26.3	18.7	13.4	0.436
Biomass + CCS	TWh	0	0	21.7	21.9	53.7	76.5	79.7
Coal	TWh	982	284	0.599	0.598	0.526	0.429	0.152
Average Emissions	gCO_2e/kWh	0.600	0.368	0.226	0.161	0.117	0.074	0.057
Annual Hydrogen Production								
Biomass	TWh	0	0	0	821	1529	3114	4763
Fossil	TWh	896	953	1111	785	915	931	560
Electrolysis	TWh	0.9	0.7	0.8	1.5	17.5	406	2706
Average Emissions	gCO_2e/kWh	0.290	0.289	0.289	0.289	0.287	0.230	0.108

S7. Biorefinery Carbon Balances

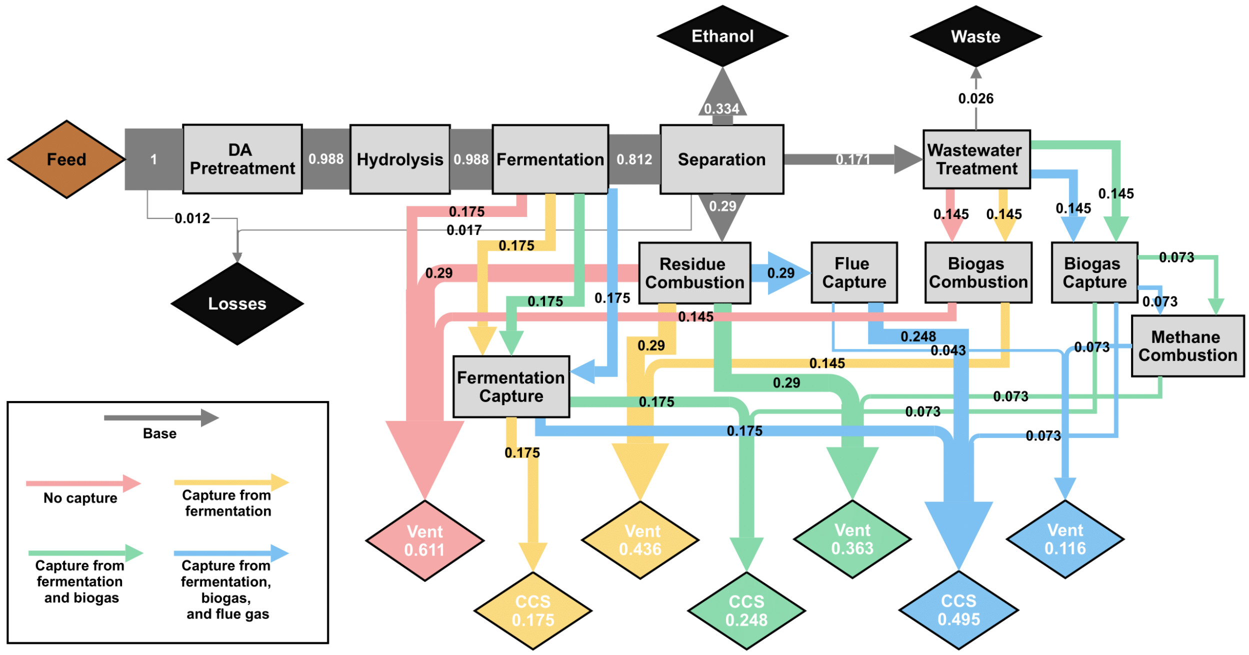

Figure S7.1. Carbon molar flows normalized to 1 mole of carbon in the feedstock for a biorefinery producing ethanol via fermentation.

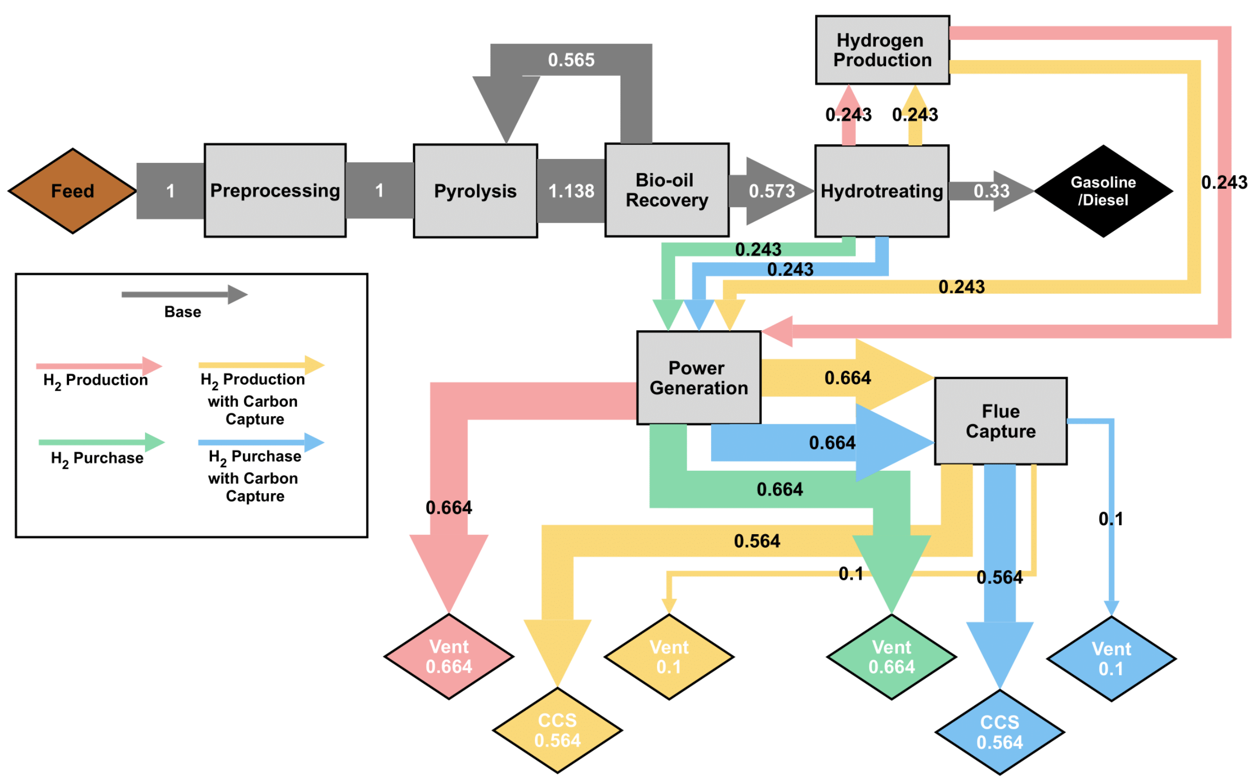

Figure S7.2. Carbon molar flows normalized to 1 mole of carbon in the feedstock for a biorefinery producing gasoline/diesel via pyrolysis.

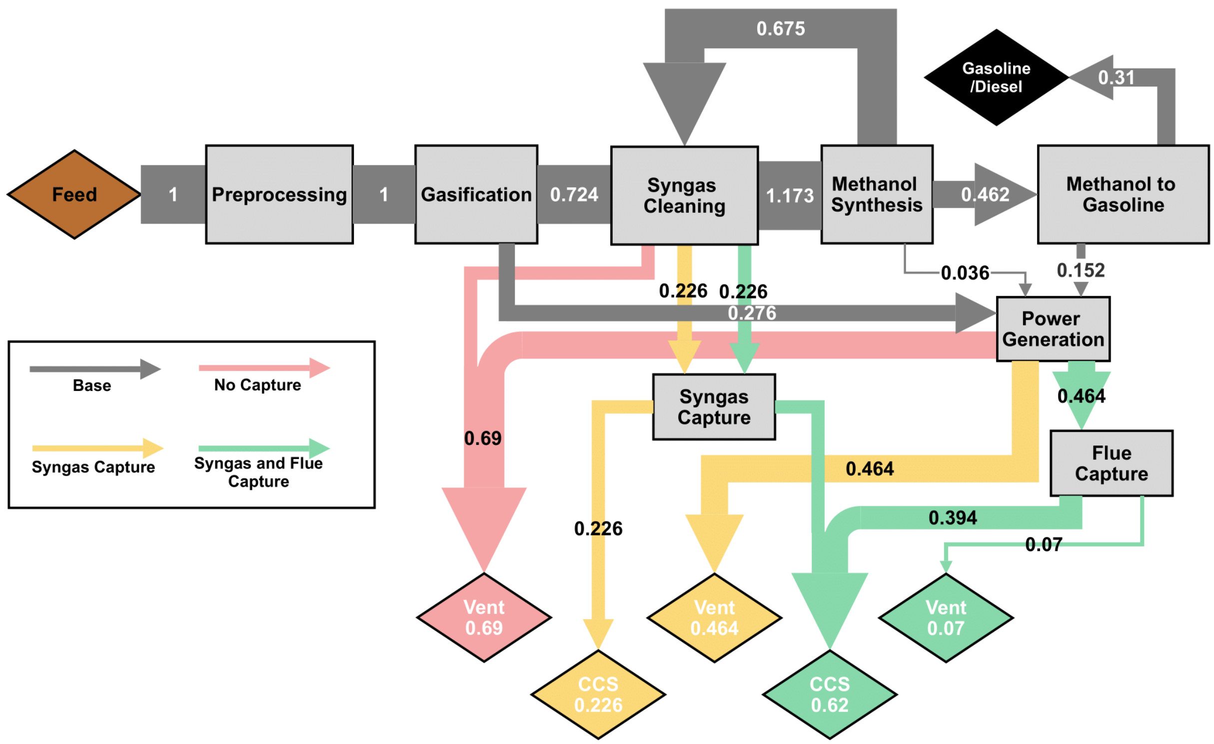

Figure S7.3. Carbon molar flows normalized to 1 mole of carbon in the feedstock for a biorefinery producing gasoline via gasification.

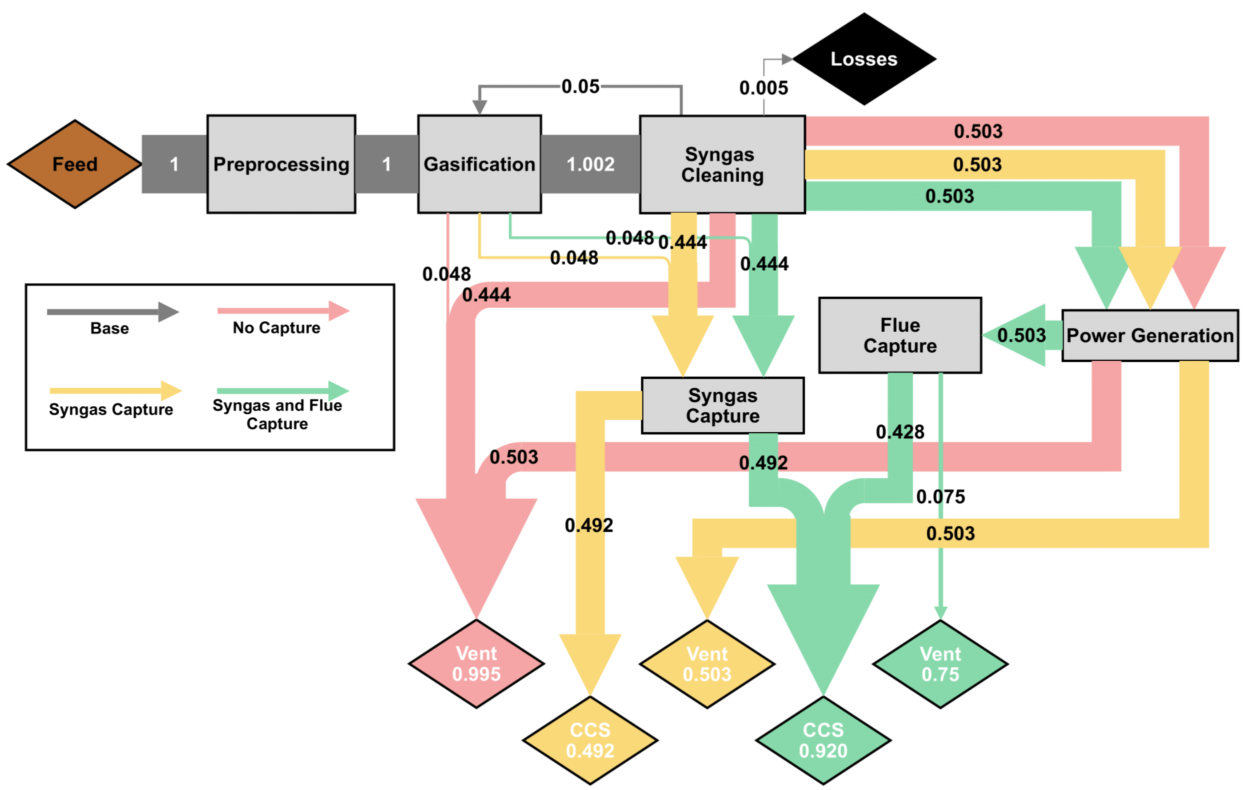

Figure S7.4. Carbon molar flows normalized to 1 mole of carbon in the feedstock for a biorefinery producing electricity via gasification and combustion.

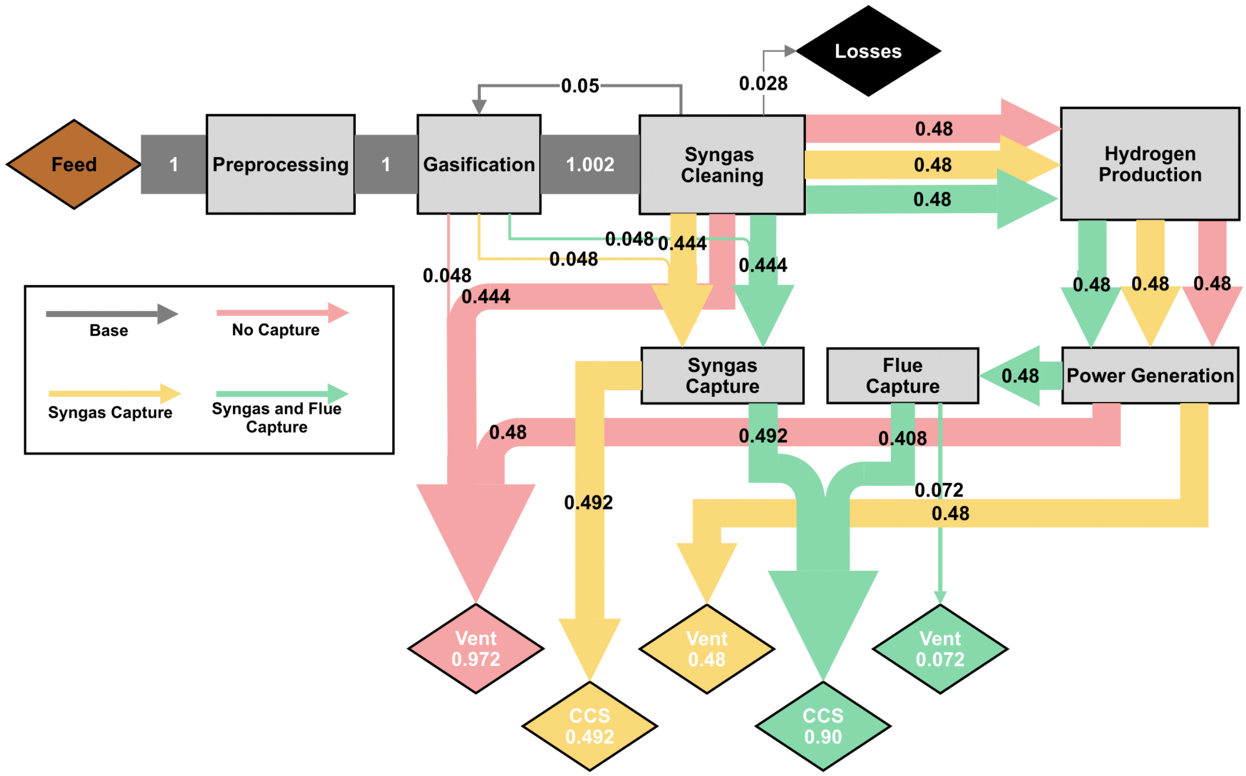

Figure S7.5. Carbon molar flows normalized to 1 mole of carbon in the feedstock for a biorefinery producing hydrogen via gasification and water-gas shift.

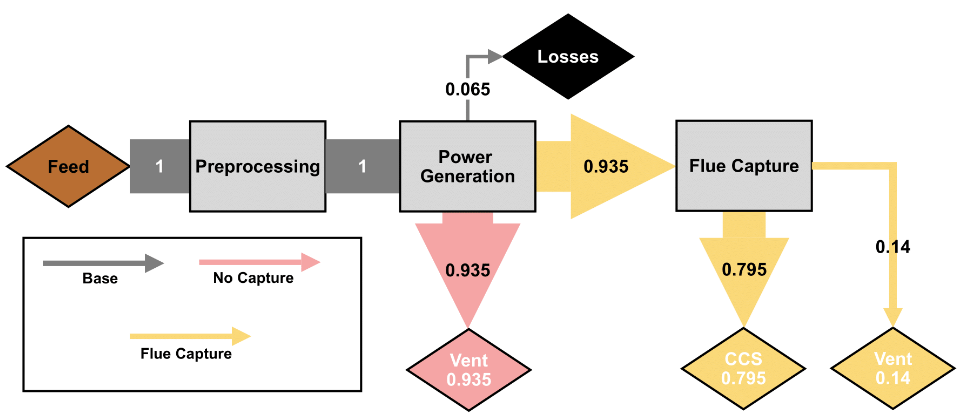

Figure S7.6. Carbon molar flows normalized to 1 mole of carbon in the feedstock for a biorefinery producing electricity via direct combustion.

S8. Carbon Capture Technology

We consider the general effect of separation energy requirement and capital cost, both normalized to the CO_2 flow, on the cost of flue gas capture, as shown in Figure S8.1. Capital costs per CO_2 flow is used to encompass both the relative capital costs of different capture technologies, and the economies of scale of a single capture technology. Similarly, the separation energy encompasses both the relative energy requirements of different capture technologies, and the change in energy requirement based on different CO_2 concentrations in the flue gas. Capture technologies, such as monoethanolamine (MEA) absorption, can include both heat and electricity requirements, so the electricity requirement is converted to the heat required to generate that amount of electricity in a turbogenerator with an efficiency of 75%. We estimate the sequestration credit needed to incentivize capture from flue gas with MEA as \$48-58/Mg CO_2, depending on the capacity of the biorefinery and on the CO_2 concentration in flue gas. Membrane separation is not as established of a technology as MEA absorption, so we do not report the capital cost.[20]

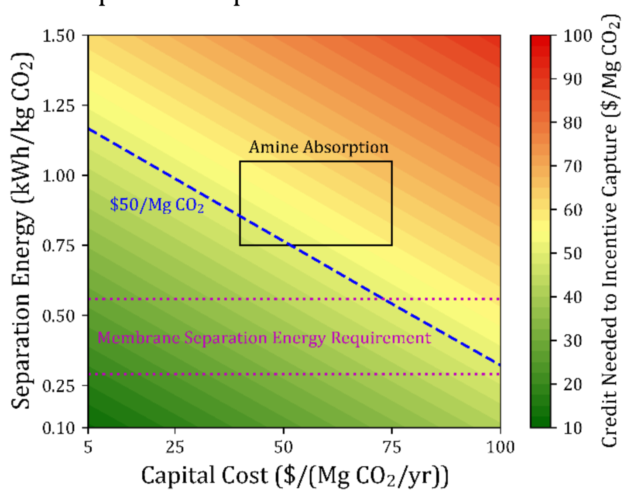

Figure S8.1. Sequestration credit needed to incentivize carbon capture from flue gas as a function of separation energy and capital cost. Amine absorption capital costs and energy requirements and membrane energy requirement are taken from literature data.[14,21]

S9. Impact of Biomass Availability

Biomass availability, both in terms of yield in a single field and in terms of what percent of land is available for crop growth, can vary significantly across the landscape.[22] Therefore, we investigate the effect of biomass availability and biorefinery capacity on fuel cost for Pyr.H2.Liq.– (see Figure S9.1).

As expected, as biomass availability increases, the breakeven cost of fuel decreases because the feedstock is transported over shorter distances, decreasing the average delivered feedstock cost. For a given biomass availability, as the capacity increases, feedstock costs increase while fixed and capital costs per unit of fuel decrease due to economies of scale. At low capacities, increasing capacity has a significant effect on decreasing costs, but the rate of cost savings decreases as the capacity continues to increase. The rate of increase of the feedstock cost depends on transportation method that is economically optimal at a given biomass availability and biorefinery capacity. Direct truck transport has the highest variable transportation cost, followed by depot and truck, then depot and rail.

In the case of low biomass availability, the feedstock cost increases rapidly at low capacities when truck transport is used. However, this rapid increase coincides with the rapid decrease in fixed costs, so increasing capacity is still favorable. As the capacity increases and the rate of increase in feedstock cost slows as depots are used for transportation and the rate of fixed costs savings slow, the breakeven cost continues to slowly decline. At biomass availabilities above 24 Mg/km^2, the interplay between these two economic forces is different. At low capacities, increasing capacity results in the same fixed cost savings as at lower biomass availabilities, but the average feedstock cost increases more slowly because of the higher biomass availability, making the breakeven cost drop dramatically. At capacities above 17,000 Mg/day, the fixed and capital cost savings from increasing capacity have reduced significantly. However, the feedstock cost still increases relatively quickly as capacity increases. In fact, these feedstock costs increase faster than the fixed and capital costs decrease as capacity increases, causing a minimum in breakeven price. At biomass availabilities above 24 Mg/km^2, this minimum in breakeven price occurs at capacities where direct truck transport of biomass is preferred, and the cost-optimal capacity increases as the biomass availability increases.

Figure S9.1B shows the optimal capacity as a function of sequestration credit and biomass availability. At low sequestration credits where Pyr.H2.Liq.– is preferred, the optimal capacity depends on biomass availability as shown in Figure S9.1A, but is independent of the sequestration credit applied. At higher credits that incentivize flue gas capture, the optimal capacity does change with sequestration credit even with the same strategy. We use an after-tax refundable tax credit in our model, so at sufficiently high sequestration credits, negative pre-tax income with the sequestration credit can result in no payment of income tax. Increasing the sequestration credit beyond this does not have the added benefit of reducing taxable income, so slightly smaller biorefineries with lower transportation costs that take full advantage of the sequestration credit offsetting the slightly higher fixed and capital costs is optimal. However, the biorefinery cannot become indefinitely small without the increased fixed and capital costs outweighing the decreases transportation costs, so beyond a sequestration credit of \$60-70 Mg/CO_2, depending on the biomass availability, the optimal capacity is once again independent of sequestration credit until a new strategy is chosen. This results in a narrow band where the optimal capacity results in exactly no income tax paid. This changing capacity within the same strategy would be different for different tax rates, and may not appear at all for different types of carbon incentives.

With biomass productions of 30-34 Mg/km^2, Pyr.H2Elec.Liq.Flu uses a biorefinery with the maximum capacity considered of 30,000 Mg/day, while Pyr.H2.Liq.– uses a biorefinery with a smaller capacity. With a lower capacity, Pyr.H2.Liq.– can adjust its capacity to minimize its cost of fuel production, while Pyr.H2Elec.Liq.Flu is limited by the maximum capacity, so a slightly higher sequestration credit is required to incentivize Pyr.H2Elec.Liq.Flu. Once the biomass production increases more, the cost-optimal capacity of Pyr.H2Elec.Liq.Flu decreases to below the maximum and can then adjust its capacity just like Pyr.H2.Liq.–.

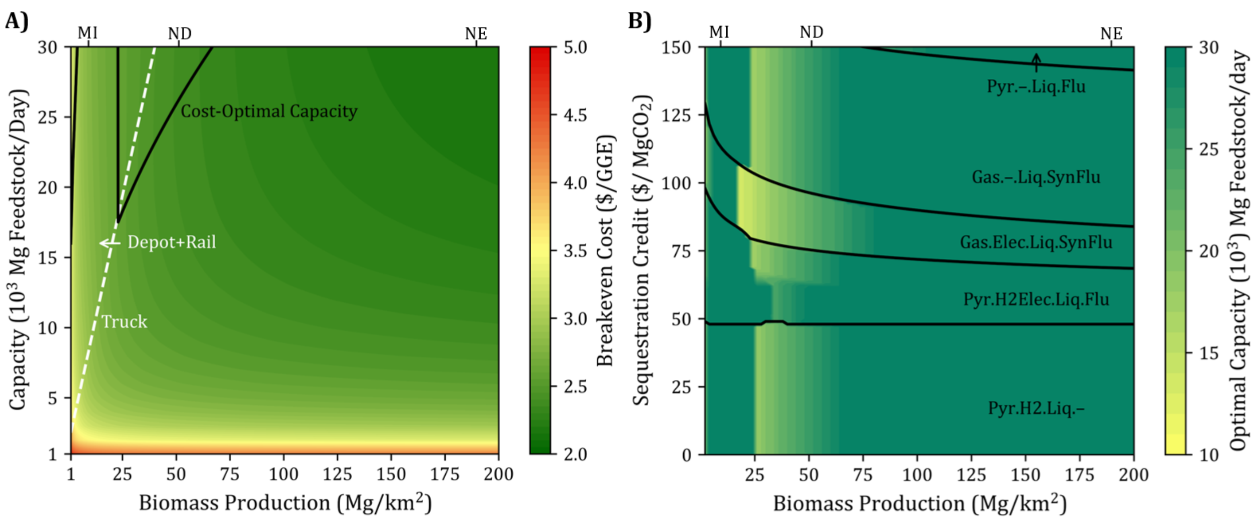

Figure S9.1. A) Effect of biomass availability and capacity on breakeven cost for Pyr.H2.Liq.– with no sequestration credit. Dashed white lines indicate capacities at which a new transportation is used for each biomass availability. Black line indicates cost-optimal capacities for a given biomass availability. B) Effect of biomass production and sequestration credit on cost-optimal biorefinery strategy and capacity. Black lines indicate transition to a new biorefinery strategy. For both plots, tick marks and abbreviations above the plot show the average biomass availability of marginal lands for representative US Midwest states (Michigan: 10 Mg/ha, North Dakota: 5.6 Mg/ha, Nebraska: 6.0 Mg/ha), normalized to total land area in the state.[2] (MI: Michigan, ND: North Dakota, NE: Nebraska).

S10. Future GHG Mitigation of Liquid Fuel Production

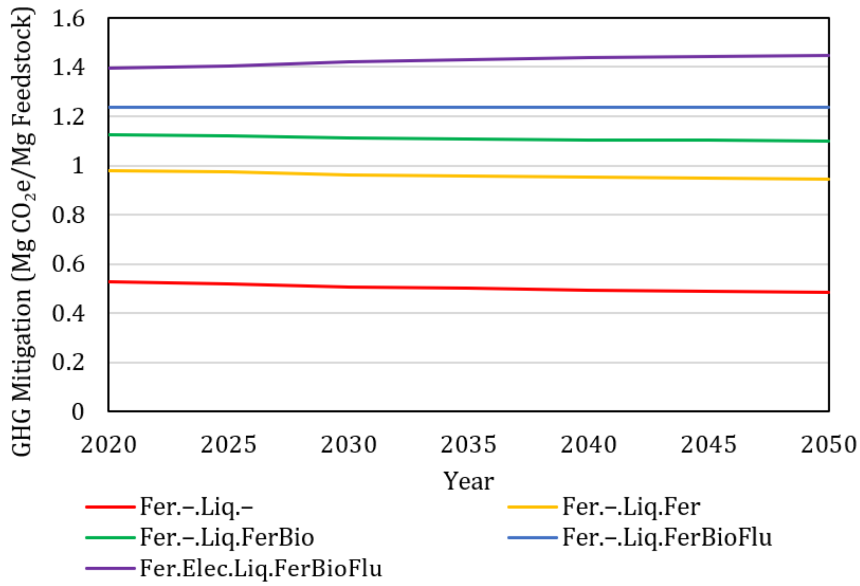

Figure S10.1. Expected GHG mitigation over time of biorefinery strategies using fermentation to produce liquid fuels.

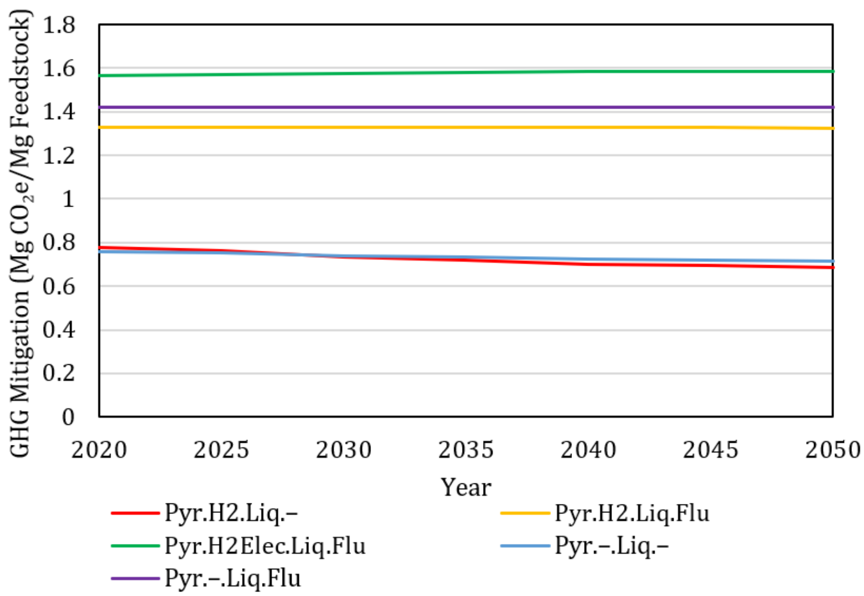

Figure S10.2. Expected GHG mitigation over time of biorefinery strategies using pyrolysis to produce liquid fuels.

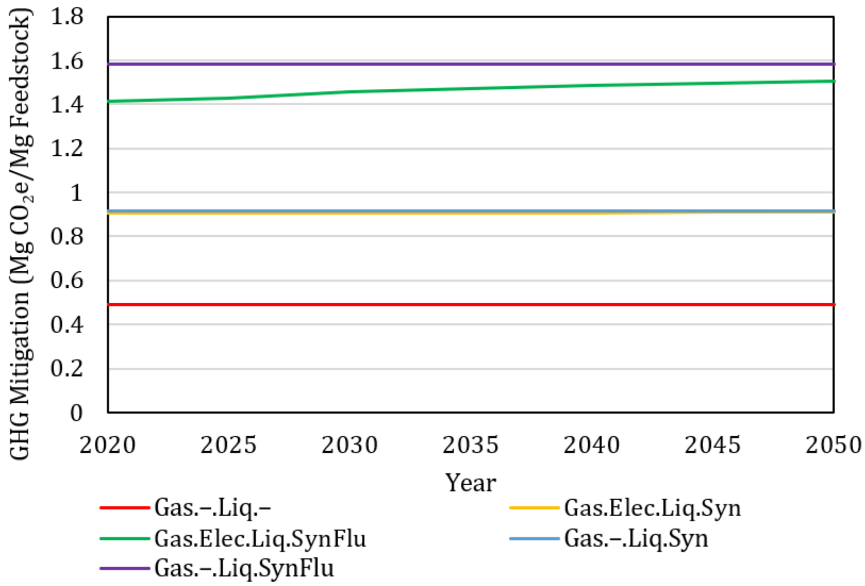

Figure S10.3. Expected GHG mitigation over time of biorefinery strategies using gasification to produce liquid fuels.

S11. Energetic Self-Sufficiency Mitigation

For strategy Gas.–.Liq.SynFlu, the total GHG mitigation is 1.710 Mg CO_2e/Mg feedstock. If 0.392 MWh/Mg feedstock of renewable electricity were purchased, the corresponding strategy would be Gas.Elec.SynFlu. but with no emission penalty for electricity purchase, which would have a total GHG mitigation of 1.774.

However, that 0.392 MWh/Mg feedstock of renewable electricity is consumed at the biorefinery for strategy Gas.Elec.Liq.SynFlu, but not for strategy Gas.–.Liq.SynFlu. Therefore, we need to consider the mitigation that could be achieved by directly using that electricity for transportation, displacing additional fossil gasoline. With assumed efficiencies of 0.8 for an electric motor, and 0.3 for an internal combustion engine, 0.392 MWh of electricity would displace $0.392\left(\frac{0.8}{0.3}\right)$ =1.045 MWh of gasoline. With assumed emissions for gasoline of 10.8 kg CO_2e/gallon of gasoline, the emissions displaced are:

$$1.045 \text{ MWh gasoline}\left(\frac{1 \text{ gallon gasoline}}{0.0337 \text{ MWh}}\right)\left(\frac{0.0108 \text{ Mg CO}_2\text{e}}{\text{gallon gasoline}}\right) = 0.335 \text{ Mg CO}_2\text{e}$$

So, including the benefit of the 0.392 MWh of renewable electricity displacing fossil gasoline, it is more environmentally beneficial to maintain an energetically self-sufficient biorefinery, and use renewable electricity directly for transportation. The GHG mitigation breakdown for these two strategies is shown in Table S11.1.

Table S11.1. GHG mitigation breakdown.

	GHG Source	GHG Mitigation ($Mg\ CO_2e$/Mg feedstock)	
		Gas.Elec.Liq.SynFlu	Gas.–.Liq.SynFlu
Biorefinery	Harvesting	-0.029	-0.029
	Transport	-0.080	-0.080
	SOC Sequestration	0.125	0.125
	CCS	1.157	1.263
	Chemicals	-0.008	-0.008
	Electricity Credit	0	0
	Gasoline Credit	0.609	0.439
	Total at Biorefinery	1.774	1.710
Renewable Electricity	Displaced Fossil Gasoline	0	0.335
Biorefinery and Renewable Electricity	Total GHG Mitigation	1.774	2.045

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