Supporting Information to *Natural Gas to Liquid Transportation Fuels under Uncertainty Using Robust Optimization*

Logan R. Matthews[c,a,b], Yannis A. Guzman[c,a,b], Onur Onel[c,a,b], Alexander M. Niziolek[c,a,b], and Christodoulos A. Floudas[a,b]

[a]Artie McFerrin Department of Chemical Engineering, Texas A&M University, College Station, TX, USA

[b]Texas A&M Energy Institute, Texas A&M University, College Station, TX, USA

[c]Department of Chemical and Biological Engineering, Princeton University, Princeton, NJ, USA

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Appendix A Investment Cost Parameters

The units $u \in U_{INV}$ are listed in Table S1 along with their cost parameters that are used in the GTL superstructure model. 45 total units with investment cost parameters exist in the MINLP model, which leads to a total of 53 uncertain parameters when both price and investment cost uncertainty are considered simultaneously. The base costs listed in Table S1 are the parameters C_0 which are considered uncertain for the robust implementation, and are allowed to vary by up to 50% with a uniform distribution across all price possibilities.

Table S1: Investment cost parameters for units in the GTL superstructure refinery. All costs are in $2015 units.

Unit	Base Cost (MM$)	Base Flow	Units	Scale Basis	sf
	Synthesis Gas Generation				
Auto Thermal Reformer	21.33	12.20	kg/s	Feed	0.67
Steam Reformer	29.83	12.20	kg/s	Feed	0.67
	Syngas Cleaning				
Reverse Water-Gas Shift Reactor	3.64	150.00	kg/s	feed	0.67
Acid Gas and CO_2 Removal Unit	31.17	2.51	kmol/s	Feed	0.63
First CO_2 Compressor	7.26	10.00	MW	Electricity	0.67
Recycle CO_2 Compressor	7.26	10.00	MW	Electricity	0.67
CO_2 Sequestration Compressor	23.47	24.40	kg/s	Feed	0.60
	Hydrocarbon Production				
Methanol Synthesis Compressor	7.26	10.00	MW	Electricity	0.67
Methanol Synthesis Reactor	10.58	35.65	kg/s	Feed	0.60
Unreacted Methanol Feed Gas Compressor	7.26	10.00	MW	Electricity	0.67
Methanol Gas Expander	7.26	10.00	MW	Electricity	0.67
Fischer-Tropsch Compressor	7.26	10.00	MW	Electricity	0.67
Fischer-Tropsch Waxy Units	43.36	54.98	kg/s	feed	0.72
Fischer-Tropsch Non-waxy Units	43.36	54.98	kg/s	feed	0.72
	Hydrocarbon Upgrading				
Hydrocarbon Recovery Unit	0.79	1.82	kg/s	feed	0.70
Wax Hydrocracker	10.20	1.13	kg/s	feed	0.70
Distillate Hydrotreater	2.73	0.36	kg/s	feed	0.70
Kerosene Hydrotreater	2.73	0.36	kg/s	feed	0.70
Naphtha Hydrotreater	0.82	0.26	kg/s	feed	0.70
Naphtha Reformer with CCP Platforming	5.69	0.43	kg/s	feed	0.70
Naphtha Reformer with RZ Separation	6.20	0.43	kg/s	feed	0.70
C_4 Isomerizer	10.65	6.06	kg/s	feed	0.70
C_5-C_6 Isomerizer	1.05	0.15	kg/s	feed	0.70
C_3-C_4-C_5 Alkylation Unit	58.67	12.50	kg/s	feed	0.70
Saturated Gas Plant	8.78	4.34	kg/s	feed	0.70
ZSM-5 Hydrocarbon Conversion Unit	20.05	23.79	kg/s	feed	0.72
ZSM-5 Product Fractionation	12.80	4.23	kg/s	feed	0.67
Methanol to Gasoline Reactor	8.60	10.63	kg/s	feed	0.65
Methanol to Gasoline Product Upgrading	23.80	10.63	kg/s	feed	0.65
Olefins to Gasoline/Distillate Unit	25.38	10.63	kg/s	feed	0.65
	Water Treatment				
Biological Digestor	4.91	115.74	kg/s	Feed	0.71
Cooling Tower	60.56	1.75	kg/s	feed	0.65
Reverse Osmosis Unit	0.33	4.63	kg/s	feed	0.85
	Heat/Power Generation				
Gas Turbine Natural Gas Compressor	7.26	10.00	MW	Electricity	0.67
Gas Turbine Combustor	79.21	266.00	MW	Electricity	0.75
Light Gas Compressor	7.40	10.00	kg/s	feed	0.67
Steam Turbine	64.36	136.00	MW	Electricity	0.67
CO_2 Recovery Unit	97.41	448.70	kg/s	feed	0.63
	Hydrogen/Oxygen Production				
Water Gas Shift Unit	3.64	107.90	kg/s	feed	0.67
Pressure Swing Adsorption	7.72	0.29	kmol/s	Purge Gas	0.65
Air Separation Unit	241.60	145.00	kg/s	O_2	0.50
Electrolyzer	0.52	1.00	MW	Electricity	0.90
Air Compressor	5.86	10.00	MW	Electricity	0.67

Appendix B Size Parameters for the Case Studies

The initial size parameters calculated from *a priori* bounds for each of the case studies, with and without investment cost uncertainty, are included for completeness in Table S2.

Table S2: Initial values of Δ for each uncertainty set and probability of constraint violation using *a priori* bounds. The nominal and worst-case solutions can be found using the box uncertainty set with Ψ values of zero and one, respectively. Values for the box (B) and interval + polyhedral (IP) parameters were found using GMF6, while values for the interval + ellipsoidal (IE) set were found using GMF7'.

		$\|J\| = 8$			$\|J \cup U_{INV}\| = 53$	
ϵ^{pri}	Box Ψ	IE Ω	IP Γ	Box Ψ	IE Ω	IP Γ
0.00	1.0000	2.8284	8.0000	1.0000	7.2801	53.0000
0.05	0.9632	1.3589	3.8435	0.9632	1.4052	10.2299
0.10	0.9264	1.2026	3.4014	0.9264	1.2336	8.9806
0.15	0.8896	1.0975	3.1042	0.8896	1.1206	8.1579
0.20	0.8528	1.0147	2.8700	0.8528	1.0327	7.5181
0.25	0.8161	0.9445	2.6714	0.8161	0.9588	6.9804
0.30	0.7792	0.8823	2.4955	0.7792	0.8939	6.5075
0.35	0.7424	0.8255	2.3349	0.7424	0.8349	6.0784
0.40	0.7054	0.7726	2.1851	0.7054	0.7802	5.6801
0.45	0.6681	0.7223	2.0429	0.6681	0.7285	5.3037
0.50	0.6303	0.6739	1.9059	0.6303	0.6789	4.9424
0.55	0.5920	0.6266	1.7722	0.5920	0.6306	4.5909
0.60	0.5527	0.5798	1.6400	0.5527	0.5830	4.2443
0.65	0.5121	0.5330	1.5076	0.5121	0.5355	3.8982
0.70	0.4698	0.4854	1.3731	0.4698	0.4873	3.5476
0.75	0.4251	0.4364	1.2342	0.4251	0.4377	3.1865
0.80	0.3770	0.3846	1.0879	0.3770	0.3855	2.8067
0.85	0.3237	0.3285	0.9291	0.3237	0.3291	2.3956
0.90	0.2622	0.2647	0.7486	0.2622	0.2650	1.9291
0.95	0.1840	0.1848	0.5227	0.1840	0.1849	1.3461
1.00	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Appendix C Tabulated Iterative Results

The complete results over all iterations for the box uncertainty set are provided in Table S3. Results over all iterations for the interval + ellipsoidal and interval + polyhedral set may be found in the main text.

Table S3: Results from the iterative method for the box robust counterpart. The final *a posteriori* probabilities of constraint violation in the final iteration are within one percent error of the desired probabilities.

$\epsilon^{desired}$	Ψ	Profit ($/GJ)	ϵ^{post}_{GMF12}	Error (%)	PoR (%)	NPoR (%)
First Iteration						
0.00	1.0000	-5.51	0.0000	0.00	211.78	100.00
0.05	0.9632	-5.18	0.0001	99.80	205.14	96.87
0.10	0.9264	-4.78	0.0006	99.40	197.11	93.08
0.15	0.8896	-4.43	0.0020	98.67	190.02	89.73
0.20	0.8528	-4.02	0.0049	97.55	181.70	85.80
0.25	0.8161	-3.65	0.0097	96.12	174.14	82.23
0.30	0.7792	-3.28	0.0165	94.50	166.56	78.65
0.35	0.7424	-2.89	0.0252	92.80	158.72	74.95
0.40	0.7054	-2.48	0.0360	91.00	150.41	71.02
0.45	0.6681	-2.10	0.0490	89.11	142.60	67.33
0.50	0.6303	-1.71	0.0643	87.14	134.80	63.65
0.55	0.5920	-1.32	0.0821	85.07	126.83	59.89
0.60	0.5270	-0.93	0.1025	82.92	118.87	56.13
0.65	0.5121	-0.45	0.1261	80.60	109.20	51.56
0.70	0.4698	-0.06	0.1533	78.10	101.32	47.84
0.75	0.4251	0.43	0.1843	75.43	91.29	43.11
0.80	0.3770	0.93	0.2194	72.58	81.08	38.28
0.85	0.3237	1.48	0.2536	70.16	69.95	33.03
0.90	0.2622	2.17	0.3004	66.62	55.96	26.42
0.95	0.1840	2.99	0.3600	62.11	39.34	18.58
1.00	0.0000	4.93	0.5000	50.00	0.00	0.00
Second Iteration						
0.05	0.6656	-2.08	0.0499	0.20	142.13	67.11
0.10	0.5575	-0.95	0.0999	0.10	119.33	56.35
0.15	0.4749	-0.11	0.1499	0.07	102.14	48.23
0.20	0.4036	0.65	0.1999	0.05	86.82	41.00
0.25	0.3293	1.43	0.2494	0.24	71.04	33.55
0.30	Found from $\Psi = 0.2622$ in first iteration.					

Appendix D The Nominal Mathematical Model

This section shows the complete nominal mathematical model for process synthesis of a natural gas to liquid transportation fuel refinery. To incorporate price and investment cost uncertainty, the objective function is made robust as seen in Section 4 of the main text.

D.1 Nomenclature

The nomenclature required for understanding the nominal mathematical model for a natural gas to liquid transportation fuel refinery is shown in Table S4.

Table S4: Mathematical model nomenclature.

Symbol	Definition	Symbol	Definition
		Indices	
s	Species index	u	Process unit index
r	Reaction index	a	Atom index
p	Proximate analysis index	i	General counting index
		Sets	
$(u,u') \in UC$	All streams from unit u to unit u'	$(u,u',s) \in S^{UF}$	All species s within stream (u,u')
$s \in S_u^U$	All species s existing within unit u	$a \in A_u^U$	All atoms a existing within unit u
$u \in U_{Sp}^{Bal}$	All units u using a species balance	$u \in U_{At}^{Bal}$	All units u using an atom balance
$(u,r,s) \in R^U$	Set for the key species s of reaction r in unit u		
		Parameters	
$AR_{s,a}$	Atomic ratio of atom a in species s	$\nu_{r,s}$	Coefficient for species s in reaction r
fc_r^u	Conversion of key species of reaction r in unit u	$H_{u,u',s}^S$	Specific enthalpy of species s in stream (u,u')
cf_s^u	Specific carbon fraction conversion for unit u and species (or species subsets) s		
		Variables	
$N_{u,u',s}^S$	Molar flow of species s from unit u to unit u'	ξ_r^u	Extent of conversion of reaction r in unit u
$H_{u,u'}^T$	Total enthalpy of stream (u,u')	Q_u	Heat transfer to/from unit u
Q_u^L	Heat loss from unit u	W_u	Work need for/required by unit u
y_u	Logical existence of unit u	$N_{u,u'}^T$	Total molar flow from unit u to unit u'
$x_{u,u',s}^S$	Molar composition of species s from unit u to unit u'	$sp_{u,u'}$	Split fraction of stream going from unit u to unit u'
Q_u^L	Heat lost from unit u	$Cost_s^{NG}$	Total delivered cost of feedstock s
$Cost^{Seq}$	Total sequestration cost of CO_2	$Cost^{El}$	Total cost of electricity
$Cost^{El}$	Total cost (profit) of electricity	$Cost_u^U$	Total levelized cost of unit u
$Cost_{LPG}$	Total cost of selling LPG	$Cost_{GAS}$	Total cost of selling gasoline
$Cost_{DIE}$	Total cost of selling diesel	$Cost_{KER}$	Total cost of selling kerosene

D.2 Process Units

The set of all process units within the mixed-integer nonlinear optimization (MINLP) model is defined in Equation 1.

$$u \in U = \{\text{Complete set of process units listed in Table S5}\} \quad (1)$$

Each unit in the MINLP model is defined in Table S5. When multiple units of the same type appear due to different operating conditions, they are defined as u_n. Such units are modeled with binary variables. The subscripts u and u' may both be used to represent elements of the set U and will be used interchangeably in the indices for stream flows.

Table S5: Process units present in the GTL process synthesis model are listed below. Multiple forms of the same unit are described with the subscript n and denote units with a distinct set of operating conditions.

Unit Name	Unit Index	Unit Name	Unit Index
	Process Inlets		
Inlet Air	IN_{AIR}	Inlet Water	IN_{H2O}
Inlet Natural Gas	IN_{NG}	Inlet Butane	IN_{BUT}
	Process Outlets		
Outlet Gasoline	OUT_{GAS}	Outlet LPG	OUT_{LPG}
Outlet Kerosene	OUT_{KER}	Outlet Diesel	OUT_{DIE}
Outlet Sequestered CO_2	OUT_{CO_2}	Outlet Wastewater	OUT_{WW}
Outlet Vent	OUT_{V}		
	Natural Gas Conversion		
Auto Thermal Reactor	ATR	Steam Reformer	SMR
Natural Gas Compressor For Gas Turbine	CMP_GTF		
	Syngas Cleaning		
Dedicated Reverse Water Gas Shift Unit	RGS_n	RGS Effluent Cooler	X_{RGS}
Acid Gas Flash Vapor Cooler	X_{AGF}	Acid Gas Flash 2-Phase Cooler	X_{AGF_n}
Acid Gas Flash Unit	AGF	Acid Gas Thermal Analyzer	X_{AGR}
Acid Gas and CO_2 Removal Unit	AGR_{CREC}	First CO_2 Compressor	CO_2C
CO_2 Recycle Compressor	CO_2RC	CO_2 Sequestration Compressor	CO_2SC
	Hydrocarbon Production		
Iron MT fWGS nominal wax FT	MTFTWGS-N	Iron MT fWGS minimal wax FT	MTFTWGS-M
Fischer-Tropsch Compressor	FTC	Fischer-Tropsch Splitter	SP_{FT}
Low-Temperature Preheater	X_{LTFT}	Low-Temperature Splitter	SP_{LTFT}
Low-Temperature Iron-Based FT	LTFTRGS	Low-Temperature Cobalt-Based FT	LTFT
High-Temperature Preheater	X_{HTFT}	High-Temperature Splitter	SP_{HTFT}

Table S5: (continued)

Unit Name	Unit Index	Unit Name	Unit Index
High-Temperature Iron-Based FT	HTFTRGS	High-Temperature Cobalt-Based FT	HTFT
ZSM-5 hydrocarbon conversion unit	FT-ZSM5	ZSM-5 product fractionation	ZSM5F
Water-Soluble Oxygenates Separator	WSOS	Vapor-Phase Oxygenates Separator	VPOS
Primary Vapor-Liquid-Water Separator	VLWS	Methanol to gasoline ZSM-5 reactor	MTG
Methanol synthesis unit	MEOHS	Methanol flash unit	MEOH-F
Methanol Synthesis Compressor	MSC	Unreacted Methanol Feed Gas Compressor	MUC
Methanol degasser	MEDEG	Methanol Gas Expander	MGT
Methanol to olefins SAPO-34 reactor	MTO	MTO fractionation	MTO-F
	Hydrocarbon Recovery		
Hydrocarbon Recovery Column	HRC	Wax Hydrocracker	WHC
Distillate Hydrotreater	DHT	Kerosene Hydrotreater	KHT
Naphtha Hydrotreater	NHT	Naphtha Reformer	NRF
C_4 Isomerizer	C_4I	C_5-C_6 Isomerizer	C_{56}I
C_3-C_4-C_5 Alkylation Unit	C_{345}A	Saturated Gas Plant	SGP
Diesel Blender	DBL	Gasoline Blender	GBL
Olefins to gasoline/distillate	OGD	OGD fractionation	OGD-F
	Recycle Gas Treatment		
Light Gas Compressor	LGC	Light Gas Splitter	SP_{LG}
Fuel Combustor	FCM	Fuel Combuster Effluent Cooler	X_{FCM}
Fuel Combustor Flash Unit	FCF	First Gas Turbine Air Compressor	$GTAC_1$
Second Gas Turbine Air Compressor	$GTAC_2$	Gas Turbine Combustor	GTC
First Gas Turbine	GT_1	Second Gas Turbine	GT_2
Gas Turbine Effluent Cooler	X_{GT}	Gas Turbine Flash Unit	GTF
Gas Turbine Effluent Compressor	GTEC	CO_2 Recovery Unit	CO_2R
	Water Treatment		
Biological Digestor	BD	Reverse Osmosis	RO
Cooling Tower	CLTR	Process Cooling	COOL-P
Heat & Power System	HEP	Heat & Power Utilities	HEAT-P
Deaerator	DEA	Process Water Economizer	X_{WPR}
Process Water Boiler	X_{WBL}	Steam Turbine	ST

Table S5: (continued)

Unit Name	Unit Index	Unit Name	Unit Index
	Hydrogen/Oxygen Production		
PSA Effluent Splitter	SP_{PSA}	Pressure-swing Adsorption Unit	PSA
PSA Hydrogen Preheater	X_{H_2P}	PSA Hydrogen Splitter	SP_{H_2P}
Electrolyzer	EYZ	Electrolyzer Oxygen Preheater	X_{O_2E}
Electrolyzer Oxygen Splitter	SP_{O_2E}	Electrolyzer Hydrogen Preheater	X_{H_2E}
Electrolyzer Hydrogen Splitter	SP_{H_2E}	Air Compressor	AC
Air Separation Unit	ASU	Oxygen Compressor	OC
ASU Oxygen Preheater	X_{O_2A}	OC Oxygen Splitter	SP_{O_2C}
OC Oxygen Preheater	X_{O_2C}	Water Gas Shift Unit	WGS

Process Species

The complete set of species, defined formally in Equation 2 for the MINLP model, is listed in Table S6.

$$s \in S = \{\text{Complete set of species listed in Table S6}\} \tag{2}$$

Table S6: Species present in the MINLP model.

Species Name	Species Index	Species Name	Species Index	Species Name	Species Index
		Light Non-Hydrocarbon Gases			
Oxygen	O_2	Nitrogen	N_2	Argon	Ar
Nitric Oxide	NO	Nitrous Oxide	N_2O	Water	H_2O
Carbon Monoxide	CO	Hydrogen	H_2	Carbon Dioxide	CO_2

Table S6: Species present in the MINLP model.

Species Name	Species Index	Species Name	Species Index	Species Name	Species Index
			Hydrocarbons		
Methane	CH_4	Acetylene	C_2H_2	Ethylene	C_2H_4
Ethane	C_2H_6	Propylene	C_3H_6	Propane	C_3H_8
Isobutylene	iC_4H_8	1-Butene	nC_4H_8	Isobutane	iC_4H_{10}
n-Butane	nC_4H_{10}	1-Pentene	C_5H_{10}	2-Methylbutane	iC_5H_{12}
n-Pentane	nC_5H_{12}	1-Hexene	C_6H_{12}	2-Methylpentane	iC_6H_{14}
n-Hexane	nC_6H_{14}	1-Heptene	C_7H_{14}	n-Heptane	C_7H_{16}
1-Octene	C_8H_{16}	n-Octane	C_8H_{18}	1-Nonene	C_9H_{18}
n-Nonane	C_9H_{20}	1-Decene	$C_{10}H_{20}$	n-Decane	$C_{10}H_{22}$
1-Undecene	$C_{11}H_{22}$	n-Undecane	$C_{11}H_{24}$	1-Dodecene	$C_{12}H_{24}$
n-Dodecane	$C_{12}H_{26}$	1-Tridecene	$C_{13}H_{26}$	n-Tridecane	$C_{13}H_{28}$
1-Tetradecene	$C_{14}H_{28}$	n-Tetradecane	$C_{14}H_{30}$	1-Pentadecene	$C_{15}H_{30}$
n-Pentadecane	$C_{15}H_{32}$	1-Hexadecene	$C_{16}H_{32}$	n-Hexadecane	$C_{16}H_{34}$
1-Heptadecene	$C_{17}H_{34}$	n-Heptadecane	$C_{17}H_{36}$	1-Octadecene	$C_{18}H_{36}$
n-Octadecane	$C_{18}H_{38}$	1-Nonadecene	$C_{19}H_{38}$	n-Nonadecane	$C_{19}H_{40}$
1-Eicosene	$C_{20}H_{40}$	n-Eicosane	$C_{20}H_{42}$	C_{21} Pseudocomponent	$C_{21}OP$
C_{22} Pseudocomponent	$C_{22}OP$	C_{23} Pseudocomponent	$C_{23}OP$	C_{24} Pseudocomponent	$C_{24}OP$
C_{25} Pseudocomponent	$C_{25}OP$	C_{26} Pseudocomponent	$C_{26}OP$	C_{27} Pseudocomponent	$C_{27}OP$
C_{28} Pseudocomponent	$C_{28}OP$	C_{29} Pseudocomponent	$C_{29}OP$	C_{30+} Pseudocomponent	$C_{30}Wax$
VP Oxygenate	OXVAP	HP Oxygenate	OXHC	AP Oxygenate	OXH2O
Gasoline	GAS	Diesel	DIE	Kerosene	KER
Methanol	CH_3OH	LPG	LPG		

Indices/Sets

The following indices are utilized in the MINLP process synthesis model:

u : Process unit index

s : Species index

a : Atom index

p : Proximate analysis index

r : Reaction index

i : General counting index.

With the complete set of process units defined previously in set U of Equation 1, several subsets of units may be defined for specific areas of the GTL superstructure to ease the presentation of the mathematical model. Four examples of these subsets are defined below:

$$\begin{aligned} u_{RGS} &= \{u : u = \mathrm{RGS}_n\} \\ u_{ATR} &= \{u : u = \mathrm{ATR}_n\} \\ u \in U_{Fl} &= \{\text{Set of flash units}\} \\ u \in U_{Sp} &= \{\text{Set of splitter units}\}. \end{aligned}$$

Elements C, H, O, N, S, Cl, and Ar are included in the set of all atoms, A, included in the superstructure:

$$a \in A = \{\text{C, H, O, N, S, Cl, Ar}\}$$

All allowable unit connections, UC, are present in the following set:

$$UC = \{(u, u') : \exists \text{ a connection between unit } u \text{ and unit } u' \text{ in the superstructure}\}$$

Each connection between units has a subset of allowable species which may flow from unit u to unit u'. This set of species is defined by $s \in S^{UC}_{u,u'}$, and may be constructed from *a priori* knowledge of the unit operations in a GTL refinery. Combining all of the stream information into one set leads to $(u, u', s) \in S^{UF}$, defined below.

$$S^{UF} = \{(u, u', s) : \exists s \in S^{UC}_{u,u'}\}$$

Furthermore, the set of species that exist within a given unit (S^U) may defined based on the species entering and exiting the unit.

$$S^U = \{(s, u) : \exists (u, u', s) \in S^{UF} \text{ or } \exists (u', u, s) \in S^{UF}\}$$

Parameters

The atomic ratios ($AR_{s,a}$) of atom a in species s may be defined using the molecular formulas in Table S6 and the formulas given by Bechtel for pseudocomponents in their processes.

$$AR_{s,a} \quad : \quad \text{Atomic ratio of atom } a \text{ in species } s$$

Of course, the molecular weights of the species (MW_s) may be calculated utilizing the atomic ratios and the atomic weights of the atoms (AW_a).

$$AW_a \quad : \quad \text{Atomic weight of atom } a$$

$$MW_s = \sum_a AW_a \cdot AR_{s,a} \tag{3}$$

Variables

The following continuous variables exist in the MINLP GTL superstructure:

$N^S_{u,u',s}$	:	Molar flow of species s from unit u to unit u'
$N^T_{u,u'}$	:	Total molar flow from unit u to unit u'
ξ^u_r	:	Extent of reaction r in unit u
$x^S_{u,u',s}$	:	Molar composition of species s from unit u to unit u'
$sp_{u,u'}$	:	Split fraction of stream going from unit u to unit u'
$H^T_{u,u'}$	:	Total enthalpy flow from unit u to unit u'
Q^L_u	:	Heat lost from unit u
Q_u	:	Heat transferred to or absorbed from from unit u
$Cost^F_s$	:	Total delivered cost of feedstock s
$Cost^{Seq}$	:	Total sequestration cost of CO_2
$Cost^{El}$	:	Total cost (profit) of electricity
$Cost^U_u$	:	Total levelized cost of unit u
$Cost_p$	:	Total selling revenue of products

Binary variables (y_u) are also required in the GTL superstructure in order to model the logical existence of units. Units such as autothermal reformers, the methanol synthesis reactor, Fischer-Tropsch reactors, and many others are all modeled using binary variables.

y_u : Logical existence of process unit u (i.e., it takes the value of one if unit u is selected and zero otherwise)

General Constraints

The following constraints define the MINLP GTL superstructure at nominal conditions. Robust counterparts for the objective function are provided in Section 4 of the main text to allow for price and investment cost uncertainty to be considered in the optimization problem.

Material Balances

Species Balances

$$\sum_{(u',u)\in UC} N^S_{u',u,s} - \sum_{(u,r,s')\in R^U} \frac{\nu_{r,s}}{\nu_{r,s'}} \cdot \xi^u_r - \sum_{(u,u')\in UC} N^S_{u,u',s} \quad = 0 \quad \forall s \in S^U_u, u \in U^{Bal}_{Sp} \tag{4}$$

Extent of Reaction

$$\xi^u_r - fc^u_r \cdot \sum_{(u',u,s)\in S^{UF}} N^S_{u',u,s} \quad = 0 \quad \forall (u,r,s) \in R^U \tag{5}$$

Atom Balances

$$\sum_{(u',u,s)\in S^{UF}} AR_{s,a} \cdot N^S_{u',u,s} - \sum_{(u,u',s)\in S^{UF}} AR_{s,a} \cdot N^S_{u,u',s} \quad = 0 \quad \forall a \in A^U_u, u \in U^{Bal}_{At} \tag{6}$$

Total Mole Balance

$$N^T_{u',u} - \sum_{(u,u',s)\in S^{UF}} N^S_{u',u,s} \quad = 0 \quad \forall (u,u') \in UC \tag{7}$$

Mole Fractions Sum to 1

$$\sum_{(u,u',s)\in S^{UF}} x^S_{u,u',s} - 1 \quad = 0 \quad \forall (u,u') \in UC_{Comp} \tag{8}$$

Process Splitters

Set Unit Split Fractions

$$N^S_{u,u',s} - \sum_{(u',u'')\in UC} sp_{u',u''} \cdot N^S_{u',u'',s} \quad = 0 \quad \forall (u,u',s) \in S^{UF}, u \in U_{Sp} \tag{9}$$

Split Fractions Sum to 1

$$\sum_{(u,u')\in UC} sp_{u,u'} - 1 \quad = 0 \quad \forall(u) \in U_{Sp} \tag{10}$$

Flash Units

Upper Bound of Liquid Phase Split Fraction

$$x^S_{u,u_L,s} - min\{1, \frac{1}{K^{VLE}_{u,s}}\} \quad \leq 0 \quad \forall(u, u_L, s) \in S^{UF}, u \in U_{Fl} \tag{11}$$

Upper Bound of Vapor Phase Split Fraction

$$x^S_{u,u_V,s} - min\{1, K^{VLE}_{u,s}\} \quad \leq 0 \quad \forall(u, u_V, s) \in S^{UF}, u \in U_{Fl} \tag{12}$$

Set Liquid Phase Split Fraction

$$x^S_{u,u_L,s} \cdot N^T_{u,u_L} - N^S_{u,u_L,s} \quad = 0 \quad \forall u \in U_{Fl} \tag{13}$$

Set Vapor Phase Split Fraction

$$x^S_{u,u_V,s} \cdot N^T_{u,u_V} - N^S_{u,u_V,s} \quad = 0 \quad \forall u \in U_{Fl} \tag{14}$$

Set Phase Equilibrium

$$x^S_{u,u_V,s} - K^{VLE}_{u,s} \cdot x^S_{u,u_L,s} \quad = 0 \quad \forall u \in U_{Fl} \tag{15}$$

Energy Balances

Conservation of Energy

$$\sum_{(u,u')\in UC} H^T_{u,u'} - \sum_{(u',u)\in UC} H^T_{u',u} - Q_u - Q^L_u - Wu \quad = 0 \quad \forall u \in U/U_{Agg} \tag{16}$$

Total Heat Balance

$$H^T_{u,u'} - \sum_{(u,u',s)\in S^{UF}} H^S_{u,u',s} \quad = 0 \quad \forall (u,u') \in UC \tag{17}$$

Logical Unit Existence

Bound on Molar Flows

$$\sum_{(u',u)\in UC} N^T_{u',u} - UB^N_u \cdot y_u \quad \leq 0 \quad \forall u \in U^{Ex} \tag{18}$$

Upper Bound on Inlet Enthalpy Flow

$$H^T_{u',u} - UB^H_{u',u} \cdot y_u \quad \leq 0 \quad \forall (u',u) \in UC, u \in U^{Ex} \tag{19}$$

Lower Bound on Inlet Enthalpy Flow

$$LB^H_{u',u} \cdot y_u - H^T_{u',u} \quad \leq 0 \quad \forall (u',u) \in UC, u \in U^{Ex} \tag{20}$$

Upper Bound on Outlet Enthalpy Flow

$$H^T_{u,u'} - UB^H_{u',u} \cdot y_u \quad \leq 0 \quad \forall (u,u') \in UC, u \in U^{Ex} \tag{21}$$

Lower Bound on Outlet Enthalpy Flow

$$LB^H_{u,u'} \cdot y_u - H^T_{u,u'} \quad \leq 0 \quad \forall (u,u') \in UC, u \in U^{Ex} \tag{22}$$

Process Inlets

Known Stream Compositions

Set Stream Compositions for Inlet Streams

$$N^S_{u,u',s} - x^K_{u,s} \cdot N^T_{u,u'} \quad = 0 \quad \forall (u,u',s) \in S^{UF}, u = \{\mathrm{IN_{AIR}},\mathrm{IN_{BUT}},\mathrm{IN_{NG}}\} \tag{23}$$

Greenhouse Gas Emissions Reduction

Set Reduction from Petroleum Based Processes

$$GHG_{GTL} - GHG_{Red} \cdot (GHG_{Pet} + GHG_{Elec}) \quad = 0 \tag{24}$$

Sum Emissions from GTL Components

$$GHG_{GTL} - GHG^{Seq} - GHG^{Proc} - GHG^{Feed} - GHG^{Fuel} \quad = 0 \tag{25}$$

Set Emissions from Feedstock Acquisition

$$GHG^{Feed} - \sum_{u \in U_{In}} \sum_{(u,u',s) \in S^{UF}} GHG^{T}_{s} \cdot MW_{s} \cdot N^{S}_{u,u',s} \quad = 0 \tag{26}$$

Set Emissions from CO_2 Sequestration

$$GHG^{Seq} - GHG^{T}_{\mathrm{CO_2}} \cdot MW_{\mathrm{CO_2}} \cdot N^{S}_{\mathrm{CO_2SC,OUT_{CO_2},CO_2}} \quad = 0 \tag{27}$$

Set Emissions from CO_2 Venting

$$GHG^{Proc} - MW_{\mathrm{CO_2}} \cdot N^{S}_{\mathrm{CO_2R,OUT_V,CO_2}} \quad = 0 \tag{28}$$

Set Emissions from Fuel

$$\begin{aligned} & GHG^{Fuel} - \sum_{(u,u',s) \in S^{UF}} GHG^{F}_{s} \cdot MW_{\mathrm{s}} \cdot N^{S}_{u,u',s} = 0 \\ & u' = \{\mathrm{OUT_{GAS}, OUT_{LPG}, OUT_{KER}, OUT_{DIE}}\} \end{aligned} \tag{29}$$

Natural gas conversion

Auto-Thermal Reactor

Logical Use of One Temperature

$$\sum_{u \in U_{\mathrm{ATR}}} y_u - 1 \quad = 0 \tag{30}$$

Water-Gas-Shift Equilibrium

$$N^S_{u,u',\mathrm{CO_2}} \cdot N^S_{u,u',\mathrm{H_2}} - K^{RGS}_u \cdot N^S_{u,u',\mathrm{CO}} \cdot N^S_{u,u',\mathrm{H_2O}} \quad = 0 \quad \forall (u,u') \in UC, u \in U_{ATR} \tag{31}$$

CH_4 Steam Reforming Equilibrium

$$x^S_{u,u',\mathrm{CO}} \cdot {x^S_{u,u',\mathrm{H_2}}}^3 - K^{SR}_{u,\mathrm{CH_4}} \cdot x^S_{u,u',\mathrm{CH_4}} \cdot x^S_{u,u',\mathrm{H_2O}} \quad = 0 \quad \forall (u,u') \in UC, u \in U_{ATR} \tag{32}$$

Bypass of Inert Species

$$\sum_{(u',u,s) \in S^{UF}} N^S_{u',u,s} - \sum_{(u,u',s) \in S^{UF}} N^S_{u,u',s} \quad = 0 \quad \forall u \in U_{\mathrm{ATR}}, s \in S^{In}_{ATR} \tag{33}$$

Steam Reformer

Logical Use of One Temperature

$$\sum_{u \in U_{\mathrm{SMR}}} y_u - 1 \quad = 0 \tag{34}$$

Water-Gas-Shift Equilibrium

$$N^S_{u,u',\mathrm{CO_2}} \cdot N^S_{u,u',\mathrm{H_2}} - K^{RGS}_u \cdot N^S_{u,u',\mathrm{CO}} \cdot N^S_{u,u',\mathrm{H_2O}} \quad = 0 \quad \forall (u,u') \in UC, u \in U_{SMR} \tag{35}$$

CH_4 Steam Reforming Equilibrium

$$x^S_{u,u',\mathrm{CO}} \cdot {x^S_{u,u',\mathrm{H_2}}}^3 - K^{SR}_{u,\mathrm{CH_4}} \cdot x^S_{u,u',\mathrm{CH_4}} \cdot x^S_{u,u',\mathrm{H_2O}} \quad = 0 \quad \forall (u,u') \in UC, u \in U_{SMR} \tag{36}$$

Bypass of Inert Species

$$\sum_{(u',u,s)\in S^{UF}} N^S_{u',u,s} - \sum_{(u,u',s)\in S^{UF}} N^S_{u,u',s} \quad = 0 \quad \forall u \in U_{\text{SMR}}, s \in S^{In}_{SMR} \tag{37}$$

Acid Gas Recovery

Set CO_2 Molar Fraction in Clean Output

$$N^S_{\text{AGR},\text{SP}_{\text{AGR}},\text{CO}_2} - rf_{\text{AGR}} \cdot N^T_{\text{AGR},\text{SP}_{\text{CG}}} \quad = 0 \tag{38}$$

Set CO_2 Output Flow Rates

$$N^T_{\text{AGR},\text{CO}_2\text{C}} - sf_{\text{AGR}} \cdot (N^T_{\text{AGR},\text{CO}_2\text{C}} + N^T_{\text{AGR},\text{MX}_{\text{CO2RC}}}) \quad = 0 \tag{39}$$

Hydrocarbon Production

Fischer-Tropsch

Set Ratio of H_2 to CO in Cobalt-Based Inlet

$$\sum_{(u',u,\text{H}_2)\in S^{UF}} FTR_{u,\text{H}_2} - 2 \cdot \sum_{(u',u,\text{CO})\in S^{UF}} FTR_{u,\text{CO}} \quad = 0 \quad \forall u \in U_{CoFT} \tag{40}$$

Set Ratio of H_2 to CO and CO_2 in Iron-Based Inlet

$$\begin{aligned} &\sum_{(u',u,\text{H}_2)\in S^{UF}} FTR_{u,\text{H}_2} - \\ &2 \cdot \sum_{(u',u,\text{CO})\in S^{UF}} FTR_{u,\text{CO}} - 3 \cdot \sum_{(u',u,\text{CO}_2)\in S^{UF}} FTR_{u,\text{CO}_2} \end{aligned} \quad = 0 \quad \forall u \in U_{IrFT} \tag{41}$$

Adjust Weight Fraction of C_1 Species

$$W_1 = \frac{1}{2}(1 - \sum_{n=5}^{\infty} W_n) \tag{42}$$

Adjust Weight Fraction of C_2 Species

$$W_2 = \frac{1}{6}(1 - \sum_{n=5}^{\infty} W_n) \tag{43}$$

Adjust Weight Fraction of C_3 Species

$$W_3 = \frac{1}{6}(1 - \sum_{n=5}^{\infty} W_n) \tag{44}$$

Adjust Weight Fraction of C_4 Species

$$W_4 = \frac{1}{6}(1 - \sum_{n=5}^{\infty} W_n) \tag{45}$$

Set Weight Fraction of C_n Species from Anderson-Schultz-Flory Distribution

$$W_n = n(1-\alpha)^2\alpha^{n-1} \qquad \forall 5 \leq n \leq 29 \tag{46}$$

Set Weight Fraction of Wax

$$W_{Wax} = \sum_{n=30}^{\infty} n(1-\alpha)^2\alpha^{n-1} \tag{47}$$

Set Carbon Distribution from Weight Fractions

$$cr_n = \frac{n \cdot W_n}{\sum\limits_{n=1}^{29} n \cdot W_n + n_{Wax} \cdot W_{Wax}} \tag{48}$$

Alpha Values for Low Temperature FT Units

$$\text{Low Temperature} = 0.9341 \tag{49}$$

Alpha Values for High Temperature FT Units

$$\text{High Temperature} = 0.6215 \tag{50}$$

Select At Most One Low-Temperature Unit

$$y_{\text{LTFT}} + y_{\text{LTFTRGS}} + y_{\text{MTFTWGS-N}} - 1 \quad \leq 0 \tag{51}$$

Select At Most One High-Temperature Unit

$$y_{\text{HTFT}} + y_{\text{HTFTRGS}} + y_{\text{MTFTWGS-M}} - 1 \quad \leq 0 \tag{52}$$

Aqueous Phase Oxygenates Separator

Removal of Aqueous Phase Oxygenates

$$N^{S}_{\text{WSOS,VLWS},s} \quad = 0 \quad \forall s \in S_{APO} \tag{53}$$

Vapor Phase Oxygenates Separator

Removal of Vapor Phase Oxygenates

$$N^{S}_{\text{VPOS,HRC},s} \quad = 0 \quad \forall s \in S_{VPO} \tag{54}$$

Methanol Synthesis

Water-Gas-Shift Equilibrium

$$x^{S}_{u,u',\text{CO}_2} \cdot x^{S}_{u,u',\text{H}_2} - K^{RGS}_{u} \cdot x^{S}_{u,u',\text{CO}} \cdot x^{S}_{u,u',\text{H}_2\text{O}} \quad = 0 \quad \forall (u,u') \in UC, u \in U_{MEOH_S} \tag{55}$$

Methanol Synthesis Equilibrium

$$x^{S}_{u,u',\text{CH3OH}} - K^{MEOH_S}_{u} \cdot x^{S}_{u,u',\text{CO}} \cdot {x^{S}_{u,u',\text{H}_2}}^{2} \quad = 0 \quad \forall (u,u') \in UC, u \in U_{MEOH_S} \tag{56}$$

Hydrocarbon Upgrading

Hydrocarbon Upgrading Units

Set Carbon Distribution Fractions of Total Input

$$N^S_{u,u',s} \cdot AR_{s,\mathrm{C}} - cf_{u,u',s} \cdot \sum_{(u'',u,s') \in S^{UF}} N^S_{u'',u,s'} \cdot AR_{s',\mathrm{C}} \quad = 0 \quad \forall u \in U_{UG}, (u,u',s) \in s^{UF} \tag{57}$$

Set Carbon Distribution Fractions of Total Input for MTO

$$N^S_{MTO,u,s} \cdot AR_{s,\mathrm{C}} - cf_s^{MTO,u} \cdot \sum_{(u,MTO,CH_3OH) \in S^{UF}} N^S_{u,MTO,s} \cdot AR_{s,\mathrm{C}} \quad = 0 \tag{58}$$

Recycle Gas Treatment

Fuel Combustor

Set Inlet Combustor Oxygen Level

$$\sum_{(u,\mathrm{FCM}) \in UC} N^S_{u,\mathrm{FCM},\mathrm{O_2}} - er_{\mathrm{FCM}} \cdot \sum_{(\mathrm{SP_{LG}},\mathrm{FCM},s) \in S^{UF}} N^S_{\mathrm{SP_{LG}},\mathrm{FCM},s} \cdot sor_s \quad = 0 \tag{59}$$

Gas Turbine

Set Air Leakage From First Compressor

$$N^S_{\mathrm{GTAC_1},\mathrm{OUT_V},s} - lk_{\mathrm{GTAC_1}} \cdot N^S_{\mathrm{IN_{AIR}},\mathrm{GTAC_1},s} \quad = 0 \quad \forall (\mathrm{GTAC_1}, s) \in S^U \tag{60}$$

Set Air Bypass From First Compressor

$$N^S_{\mathrm{GTAC_1},\mathrm{GT_2},s} - by_{\mathrm{GTAC_1}} \cdot N^S_{\mathrm{IN_{AIR}},\mathrm{GTAC_1},s} \quad = 0 \quad \forall (\mathrm{GTAC_1}, s) \in S^U \tag{61}$$

Set Inlet Oxygen Flow Rate in Combustor

$$er_{\mathrm{GTC}} \cdot \sum_{(u,\mathrm{GTC},s) \in S^{UF}} sor_s \cdot N^S_{u,\mathrm{GTC},s} - \sum_{(u,\mathrm{GTC},s) \in S^{UF}} N^S_{u,\mathrm{GTC},\mathrm{O_2}} \quad = 0 \tag{62}$$

Set Heat Loss in Combustor

$$Q^L_{\text{GTC}} - hl_{\text{GTC}} \cdot (H^T_{\text{SP}_{\text{LG}},\text{GTC}} - H^T_{\text{X}_{\text{GTF}},\text{GTF}}) \quad = 0 \tag{63}$$

Wastewater Treatment

Biological Digestor

Set Biogas Ratio of CH_4 to CO_2

$$N^S_{\text{BD,CC,CH}_4} - cr_{\text{BD}} \cdot N^S_{\text{BD,CC,CO}_2} \quad = 0 \tag{64}$$

Reverse Osmosis

Set Removal Fraction of Solids

$$N^S_{\text{RO,SP}_{\text{RO}},s} - rf_{\text{RO}} \cdot N^S_{\text{MX}_{\text{RO}},\text{RO},s} \quad = 0 \quad \forall s \in S_{Sol} \tag{65}$$

Cooling Cycle

Cooling Tower Flow Rate from Energy Requirement

$$Q_C - hr_{\text{COOL-P}} \cdot N^S_{\text{CLTR,COOL-P,H}_2\text{O}} \quad = 0 \tag{66}$$

Cooling Tower Evaporation Loss

$$N^{Evap}_{\text{CLTR}} - 0.00085 \cdot \Delta T_{\text{CLTR}} \cdot N^S_{\text{CLTR,COOL-P,H}_2\text{O}} \quad = 0 \tag{67}$$

Cooling Tower Drift Loss

$$N^{Drift}_{\text{CLTR}} - 0.001 \cdot N^S_{\text{MX}_{\text{CLTR}},\text{CLTR,H}_2\text{O}} \quad = 0 \tag{68}$$

Sum Total Cooling Tower Losses

$$N_{\text{CLTR}}^{Evap} + N_{\text{CLTR}}^{Drift} - N_{\text{CLTR,OUT}_\text{V},\text{H}_2\text{O}}^{S} \quad = 0 \tag{69}$$

Set Known Cooling Tower Output Solid Concentrations

$$x_{\text{CLTR,SP}_\text{CLTR},s}^{Kn} \cdot N_{\text{CLTR,SP}_\text{CLTR}}^{T} - N_{\text{CLTR,SP}_\text{CLTR},s}^{S} \quad = 0 \quad \forall s \in S_{Sol} \tag{70}$$

Steam Cycle

Set Known Process Steam Boiler Output Solid Concentrations

$$x_{\text{X}_\text{PWB},\text{MX}_\text{BLR},s}^{Kn} \cdot N_{\text{X}_\text{PWB},\text{MX}_\text{BLR}}^{T} - N_{\text{X}_\text{PWB},\text{MX}_\text{BLR},s}^{S} \quad = 0 \quad \forall s \in S_{Sol} \tag{71}$$

Set Known Heat Engine Boiler Output Solid Concentrations

$$x_{\text{HEP,MX}_\text{BLR},s}^{Kn} \cdot N_{\text{HEP,MX}_\text{BLR}}^{T} - N_{\text{HEP,MX}_\text{BLR},s}^{S} \quad = 0 \quad \forall s \in S_{Sol} \tag{72}$$

Outlet Wastewater

Upper Bound on Output Wastewater Concentrations

$$N_{\text{MX}_\text{WW},\text{OUT}_\text{V},s}^{S} - x_{\text{MX}_\text{WW},\text{OUT}_\text{V},s}^{Max} \cdot N_{\text{MX}_\text{WW},\text{OUT}_\text{V}}^{T} \quad \leq 0 \quad \forall s \in S_{WW} \tag{73}$$

Hydrogen/Oxygen Production

Pressure-Swing Adsorption

Set Recovery Fraction of H_2 from Inlet

$$N_{\text{PSA,SP}_{\text{H}_2\text{P}},\text{H}_2}^{S} - Rev_{\text{PSA}}^{\text{H}_2} \cdot \sum_{(u,\text{PSA}) \in UC} N_{u,\text{PSA},\text{H}_2}^{S} \quad = 0 \tag{74}$$

Set Inlet Mole Fraction of H_2

$$\sum_{(u,\text{PSA})\in UC} N^S_{u,\text{PSA},\text{H}_2} - In^{\text{H}_2}_{\text{PSA}} \cdot \sum_{(u,\text{PSA})\in UC} N^T_{u,\text{PSA}} \quad = 0 \tag{75}$$

Air Separation Unit

Recovery Fraction of O_2

$$N^S_{\text{ASU},\text{OUT}_\text{V},s} - (1 - sf_{\text{ASU}}) \cdot N^S_{\text{AC},\text{ASU},s} \quad = 0 \quad \forall s \in S^U_{ASU} \tag{76}$$

Process Hot/Cold/Power Utility Requirements

Set Electricity Needed for Process Units

$$Q^{El}_P - \sum_{u\in U_{Util}} S_u \cdot El^{Base}_u \quad = 0 \tag{77}$$

Set Cooling Water Needed for Process Units

$$Q^{CW}_P - \sum_{u\in U_{Util}} S_u \cdot CW^{Base}_u \quad = 0 \tag{78}$$

Set Heating Fuel Needed for Process Units

$$Q_{\text{FCM}} - \sum_{u\in U_{Util}} S_u \cdot F^{Base}_u \quad = 0 \tag{79}$$

Set Utilities Needed for Process Units

$$Q^{HU}_{u,ut} - S_u \cdot U^{Base}_{u,ut} \quad = 0 \quad \forall ut, u \in U_{Util} \tag{80}$$

Process Costs

Feedstock Costs

Levelized Cost of Natural Gas Feedstock

$$Cost_{NG} = \sum_{(\mathrm{IN_{NG}},u)\in UC} \frac{(\sum\limits_{s\in S_{NG}} MW_s \cdot N^S_{\mathrm{IN_{NG}},u,s}) \cdot C^F_{NG}}{Prod \cdot LHV_{Prod}} \tag{81}$$

Levelized Cost of Freshwater Feedstock

$$Cost_{\mathrm{H_2O}} = \frac{MW_{\mathrm{H_2O}} \cdot N^S_{\mathrm{IN_{H_2O}},\mathrm{SP_{WRI}},\mathrm{H_2O}} \cdot C^F_{\mathrm{H_2O}}}{Prod \cdot LHV_{Prod}} \tag{82}$$

Levelized Cost of Butane Feedstock

$$Cost_{BUT} = \sum_{(\mathrm{IN_{BUT}},u)\in UC} \frac{(\sum\limits_{s\in S_{BUT}} MW_s \cdot N^S_{\mathrm{IN_{BUT}},u,s}) \cdot C^F_{BUT}}{Prod \cdot LHV_{Prod}} \tag{83}$$

Product Revenues

Levelized Cost of Gasoline

$$Cost_{GAS} = \sum_{(u,\mathrm{OUT_{GAS}})\in UC} \frac{(\sum\limits_{s\in S_{GAS}} MW_s \cdot N^S_{\mathrm{u,OUT_{GAS}},s}) \cdot C^P_{GAS}}{Prod \cdot LHV_{Prod}} \tag{84}$$

Levelized Cost of Diesel

$$Cost_{DIE} = \sum_{(u,\mathrm{OUT_{DIE}})\in UC} \frac{(\sum\limits_{s\in S_{DIE}} MW_s \cdot N^S_{\mathrm{u,OUT_{DIE}},s}) \cdot C^P_{DIE}}{Prod \cdot LHV_{Prod}} \tag{85}$$

Levelized Cost of Kerosene

$$Cost_{KER} = \sum_{(u,\mathrm{OUT_{KER}})\in UC} \frac{(\sum\limits_{s\in S_{KER}} MW_s \cdot N^S_{\mathrm{u,OUT_{KER}},s}) \cdot C^P_{KER}}{Prod \cdot LHV_{Prod}} \tag{86}$$

Levelized Cost of LPG

$$Cost_{LPG} = \sum_{(u,\mathrm{OUT_{PRO}})\in UC} \frac{(\sum_{s\in S_{PRO}} MW_s \cdot N^S_{\mathrm{u,OUT_{PRO}},s}) \cdot C^P_{LPG}}{Prod \cdot LHV_{Prod}} \tag{87}$$

Electricity Costs

Levelized Cost of Electricity

$$Cost^{El} = \frac{F^{El}_{In} \cdot C^{El}_{In} - F^{El}_{Out} \cdot C^{El}_{Out}}{Prod \cdot LHV_{Prod}} \tag{88}$$

CO_2 Sequestration Costs

Levelized Cost of CO_2 Sequestration

$$Cost^{Seq} = \frac{MW_{\mathrm{CO_2}} \cdot N^S_{\mathrm{CO_2SC,OUT_{CO_2},CO_2}} \cdot C^{Seq}}{Prod \cdot LHV_{Prod}} \tag{89}$$

Levelized Investment Costs

Total Overnight Cost of Process Units

$$TOC_u = (1 + IC_u) \cdot (1 + BOP_u) \cdot C_{o,u} \cdot \frac{S_u}{S_{o,u}}^{sf_u} \tag{90}$$

Variable Capital Costs of Process Units

$$CC_u = LCCR \cdot IDCF \cdot TOC_u \tag{91}$$

Levelized Cost of Process Units

$$Cost^U_u = \frac{CC_u \cdot (1 + OM)}{CAP \cdot Prod \cdot LHV_{Prod}} \tag{92}$$

Objective Function

Levelized Profit of Fuels & Chemicals Production

$$\text{MIN} \quad \sum_{f \in Feed} Cost_f + Cost^{El} + Cost^{Seq} + \sum_{u \in U_{Inv}} Cost_u^U - \sum_{p \in Products} Cost_p \tag{93}$$

Simultaneous Heat and Power Integration

Pinch Points

Set Pinch Points Based on Inlet Temperatures

$$\left\{ \begin{array}{l} T_{pi} = T_{u,u'}^{HP-in} \quad \forall (u,u') \in HP; \quad T_{pi} = T_u \quad \forall u \in HPt^{HB}; \\ T_{pi} = T_{ut} \quad \forall (ut,pi) \in HPt - PI^{Ut}; \quad T_{pi} = T_{b,c,t}^{PC-in} \quad \forall (b,c,t) \in HEP; \quad T_{pi} = T_c \\ T_{pi} = T_{u,u'}^{CP-in} + \Delta T \quad \forall (u,u') \in CP; \quad T_{pi} = T_{b,c}^{EC-in} + \Delta T \quad \forall (b,c) \in CP^{EC}; \\ T_{pi} = T_{b,t}^{SH-in} + \Delta T \quad \forall (b,t) \in CP^{SH}; \quad T_{pi} = T_{ut} + \Delta T \quad \forall (ut,pi) \in CPt - PI^{Ut}; \\ T_{pi} = T_b + \Delta T \end{array} \right\} \tag{94}$$

Temperature Differences

Process Unit Hot Stream Inlets

$$\Delta T_{u,u',pi}^{HP-in} = \max\{0, T_{u,u'}^{HP-in} - T_{pi}\} \tag{95}$$

Process Unit Hot Stream Outlets

$$\Delta T_{u,u',pi}^{HP-out} = \max\{0, T_{u,u'}^{HP-out} - T_{pi}\} \tag{96}$$

Process Unit Cold Stream Inlets

$$\Delta T_{u,u',pi}^{CP-in} = \max\{0, T_{u,u'}^{CP-in} - (T_{pi} - \Delta T)\} \tag{97}$$

Process Unit Cold Stream Outlets

$$\Delta T^{CP-out}_{u,u',pi} \quad = \quad \max\{0, T^{CP-out}_{u,u'} - (T_{pi} - \Delta T)\} \tag{98}$$

Heat Engine Precooler Inlets

$$\Delta T^{PC-in}_{b,c,t,pi} \quad = \quad \max\{0, T^{PC-in}_{b,c,t} - T_{pi}\} \tag{99}$$

Heat Engine Precooler Outlets

$$\Delta T^{PC-out}_{b,c,t,pi} \quad = \quad \max\{0, T^{PC-out}_{b,c,t} - T_{pi}\} \tag{100}$$

Heat Engine Economizer Inlets

$$\Delta T^{EC-in}_{b,c,pi} \quad = \quad \max\{0, T^{EC-in}_{b,c} - (T_{pi} - \Delta T)\} \tag{101}$$

Heat Engine Economizer Outlets

$$\Delta T^{EC-out}_{b,c,pi} \quad = \quad \max\{0, T^{EC-out}_{b,c} - (T_{pi} - \Delta T)\} \tag{102}$$

Heat Engine Superheater Inlets

$$\Delta T^{SH-in}_{b,t,pi} \quad = \quad \max\{0, T^{SH-in}_{b,t} - (T_{pi} - \Delta T)\} \tag{103}$$

Heat Engine Superheater Outlets

$$\Delta T^{SH-out}_{b,t,pi} \quad = \quad \max\{0, T^{SH-out}_{b,t} - (T_{pi} - \Delta T)\} \tag{104}$$

Heat Engine Logical Existence

Bound on Heat Engine Flow Rate

$$F^{Up}_{b,c,t} \cdot y^{En}_{b,c,t} \quad \geq F^{En}_{b,c,t} \quad \forall (b,c,t) \in HEP \tag{105}$$

Bound on Total Amount of Heat Engines

$$\sum_{(b,c,t)\in HEP} y^{En}_{b,c,t} \quad \leq EnMax \tag{106}$$

Heat Balances

Heat Engine Electricity Balance

$$\sum_{(b,c,t)\in HEP} (w^{Tur}_{b,c,t} - w^{Pum}_{b,c,t}) \cdot F^{En}_{b,c,t} \quad = F_{El} \tag{107}$$

Upper Heat Balance for Pinch Points

$$\begin{aligned} Q^H_{pi} = \quad & \sum_{(u,u')\in HP} \sum_s N^s_{u,u',s} \cdot Cp^P_{u,u',s} \cdot (\Delta T^{HP-in}_{u,u',pi} - \Delta T^{HP-out}_{u,u',pi}) \\ & + \sum_{(b,c,t)\in HEP} F^{En}_{b,c,t} \cdot Cp^{HE-P} \cdot (\Delta T^{PC-in}_{b,c,t,pi} - \Delta T^{PC-out}_{b,c,t,pi}) \\ & + \sum_{(ut,pi)\in HPt-PI^{Ut}} \sum_{(u,ut)\in HPt} Q^{HU}_{u,ut} + \\ & + \sum_{(u,pi)\in HPt-PI^{HB}} Q_u + \sum_b \sum_{(c,pi)\in HPt-PI^C} \sum_t F^{En}_{b,c,t} \cdot dH^C_c \end{aligned} \tag{108}$$

Lower Heat Balance for Pinch Points

$$\begin{aligned} Q^C_{pi} = \quad & \sum_{(u,u')\in CP} \sum_s N^s_{u,u',s} \cdot Cp^P_{u,u',s} \cdot (\Delta T^{CP-out}_{u,u',pi} - \Delta T^{CP-in}_{u,u',pi}) \\ & + \sum_{(b,c,t)\in HEP} F^{En}_{b,c,t} \cdot Cp^{HE-E} \cdot (\Delta T^{EC-out}_{b,c,pi} - \Delta T^{EC-in}_{b,c,pi}) \\ & + \sum_{(b,c,t)\in HEP} F^{En}_{b,c,t} \cdot Cp^{HE-S} \cdot (\Delta T^{SH-out}_{b,t,pi} - \Delta T^{SH-in}_{b,t,pi}) \\ & + \sum_{(ut,pi)\in CPt-PI^{Ut}} \sum_{(u,ut)\in CPt} Q^{HU}_{u,ut} + \sum_{(b,pi)\in CPt-PI^B} \sum_c \sum_t F^{En}_{b,c,t} \cdot dH^B_b \end{aligned} \tag{109}$$

Pinch Point Heating Deficit

$$z_{pi} = Q^C_{pi} - Q^H_{pi} \tag{110}$$

Negativity of Pinch Deficits

$$z_{pi} \leq 0 \tag{111}$$

Total Heating Deficit

$$\Omega - Q_c = 0 \tag{112}$$

Total Heat Balance

$$\begin{aligned}
\Omega = \quad & \sum_{(u,u')\in HP} \sum_{s} N^{s}_{u,u',s} \cdot Cp^{P}_{u,u',s} \cdot (T^{HP-in}_{u,u'} - T^{HP-out}_{u,u'}) \\
& + \sum_{(b,c,t)\in HEP} F^{En}_{b,c,t} \cdot Cp^{HE-P} \cdot (T^{PC-in}_{b,c,t} - T^{PC-out}_{b,c,t}) \\
& + \sum_{(u,ut)\in HPt} Q^{HU}_{u,ut} + \sum_{u\in HPt^{HB}} Q_u + \sum_{(b,c,t)\in HEP} F^{En}_{b,c,t} \cdot dH^{C}_{c} \\
& - \sum_{(u,u')\in CP} \sum_{s} N^{s}_{u,u',s} \cdot Cp^{P}_{u,u',s} \cdot (T^{CP-out}_{u,u'} - T^{CP-in}_{u,u'}) \\
& - \sum_{(b,c,t)\in HEP} F^{En}_{b,c,t} \cdot Cp^{HE-E} \cdot (T^{EC-out}_{b,c} - T^{EC-in}_{b,c}) \\
& - \sum_{(b,c,t)\in HEP} F^{En}_{b,c,t} \cdot Cp^{HE-S} \cdot (T^{SH-out}_{b,t} - T^{SH-in}_{b,t}) \\
& - \sum_{(u,ut)\in CPt} Q^{HU}_{u,ut} - \sum_{(b,c,t)\in HEP} F^{En}_{b,c,t} \cdot dH^{B}_{b}
\end{aligned} \tag{113}$$