U.S. DEPARTMENT OF ENERGY | National Energy Technology Laboratory

OFFICE OF FOSSIL ENERGY

Coal and Biomass to Liquids (CBTL) Greenhouse Gas Optimization Tool Documentation

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Disclaimer

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DOE Contract Number DE-FE0004001

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Acronyms and Abbreviations

AR4	Fourth Assessment Report (IPCC)
AR5	Fifth Assessment Report (IPCC)
Btu	British thermal unit
CH_4	Methane
CO_2	Carbon dioxide
CO_2e	Carbon dioxide equivalent
ECF	Energy conversion facility
EFG	Entrained flow gasifier
EU	End use
GHG	Greenhouse gas
GWP	Global warming potential
HRSG	Heat recovery steam generator
I-6	Illinois No. 6
IPCC	Intergovernmental Panel on Climate Change
kg	Kilogram
km	Kilometer
lb	Pound
LCA	Life cycle analysis
mi	Mile
MSW	Municipal solid waste
MWe	Megawatt electric
MWh	Megawatt-hour
N_2O	Nitrous Oxide
NETL	National Energy Technology Laboratory
NGCC	Natural gas combined cycle
PRB	Powder River Basin
PT	Product Transport
RMA	Raw material acquisition
RMT	Raw material transport
SF_6	Sulfur hexafluoride
scf	Standard cubic foot
SCPC	Supercritical pulverized coal
TRIG	Transport reactor integrated gasifier
U.S.	United States

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1 Introduction

The Connecticut Center for Advanced Technology (CCAT) has received funding from the Defense Logistics Agency (DLA) to demonstrate how liquid fuel can be produced from coal and meet the Energy Independence and Security Act (EISA) of 2007 greenhouse gas (GHG) requirement for Department of Defense (DOD) fuel purchases of synthetic fuel. Section 526 of EISA requires that any fuel purchases have a life-cycle CO_2 emission less or equal to than conventional petroleum fuel. Specifically, Section 526 of EISA provides that:

> *No Federal agency shall enter into a contract for procurement of an alternative or synthetic fuel, including a fuel produced from nonconventional petroleum sources, for any mobility-related use, other than for research or testing, unless the contract specifies that the life cycle greenhouse gas emissions associated with the production and combustion of the fuel supplied under the contract must, on an ongoing basis, be less than or equal to such emissions from the equivalent conventional fuel produced from conventional petroleum sources (Energy Independence and Security Act of 2007).*

As discussed previously, Section 526 of EISA requires that potential alternative fuel sources demonstrate GHG emissions that are equal to or lower than conventional fuel, on a *life cycle* basis, prior to contractual procurement by a federal agency. Life cycle emissions are evaluated via Life Cycle Analysis (LCA), a method used to estimate and compare the environmental flows associated with the production of a product or service.

NETL previously studied pathway for producing jet fuel via Fischer-Tropsch process from feeds of Montana Rosebud coal and Southern Pine biomass, utilizing Transport Reactor Integrated Gasification (TRIG) and Entrained Flow Gasification (EFG) technologies for CCAT (NETL, 2014a, 2015a, 2015b). In addition to technical and economic analyses, those studies also included an LCA of all of the scenarios to determine compliance with EISA Section 526. The scenarios evaluated in those previous studies were based on a fixed feed composition of Montana Rosebud coal and Southern Pine biomass. The goal of this analysis, referred to as the CBTL GHG Optimization Tool from hereon, is to provide CCAT with additional modeling flexibility, specifically:

(1) The addition of different types of coal and biomass, as well as customized fractions of those feedstocks. The CBTL GHG Optimization Tool gives users the ability to choose from three coal types (Illinois No. 6 bituminous coal, Montana Rosebud sub-bituminous coal, or North Dakota Lignite) and three biomass types (Southern pine, switchgrass, or municipal solid waste).

(2) The ability to vent a user-specified percentage of the captured CO_2 upstream of final compression.

(3) The ability to adjust the overall efficiency of the facility operation.

To provide that capability, NETL has included cases that were previously modeled and published. In addition to the studies already performed for CCAT, the CBTL GHG Optimization Tool relies on two studies: *Production of Zero Sulfur Diesel Fuel from Domestic Coal: Configurational Options to Reduce Environmental Impact* and *Cost and Performance Baseline for Fossil Energy Plants Volume 4: Coal-to-Liquids via Fischer-Tropsch Synthesis* (NETL, 2011, 2014b). These studies will be referred to as Zero S Diesel and CTL Baseline for the remainder of this document. The coal and biomass feed combinations are limited to those that were previously modeled. Additional information is presented in **Section 3** of this document.

The inputs and outputs of this model will be consistent with those in the existing *CCAT CBTL Jet Fuel* model. In addition to the new feedstock options, the model will also allow the user to adjust the fraction of the captured CO_2 that is vented and adjust the overall efficiency of the plant. The CBTL GHG Optimization Tool will resemble the modeling structure developed in background tabs of the existing *CCAT CBTL Jet Fuel Excel* model. Life cycle GHG results are provided at the same level of detail depicted in the 'Environmental Results' tab of the *CCAT CBTL Jet Fuel Excel* model. That is information on the process-level emissions (for example, coal mining, biomass production, etc.) for each GHG (CO_2, CH_4, N_2O, and SF_6). The results will also be aggregated to the life cycle stage level (raw material acquisition, raw material transport, energy conversion facility, product transport, and end use. The functional unit of this analysis is the combustion of 1 MJ LHV of blended jet fuel at 50/50 by volume. All results are expressed on the basis of this functional unit. The results will be deterministic point-estimates only. There will not be any stochastic modeling capabilities integrated into the tool.

Additionally, this tool will have also have optimization functionality, whereby the user can enter a life cycle GHG target (e.g. EISA Section 526), and the model was adjust the values for the selected parameter to match the configuration to the target. The remainder of this document provides instructions for using the model and background information on the development of it.

2 Model Use Instructions

The following sections describe the steps that are necessary to correctly configure the required Excel settings and operate the CBTL GHG Optimization Tool. The model is deterministic and thus does not require the Microsoft Excel Add-In to run successfully.

2.1 Excel Settings

2.1.1 Macro Enabling

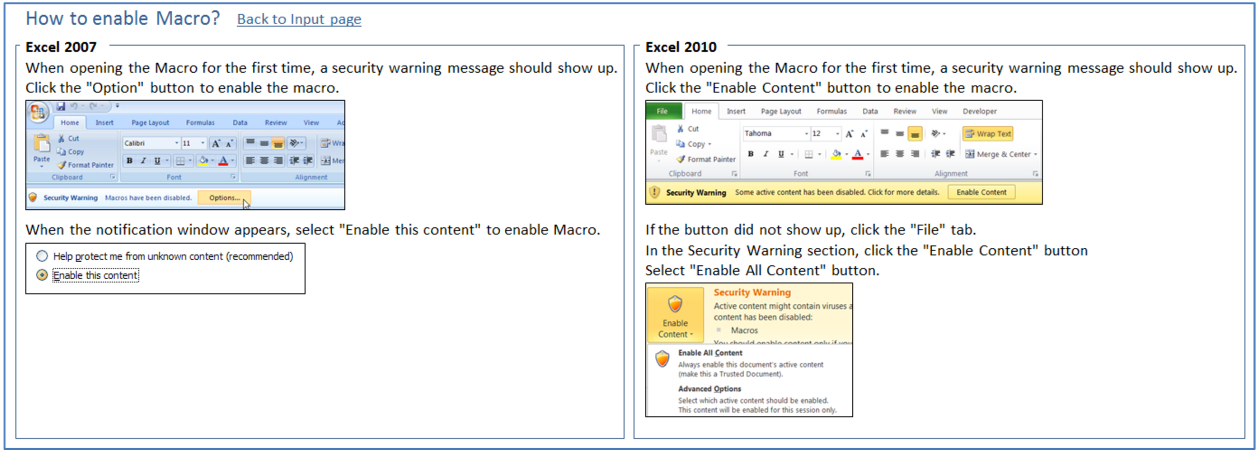
To use the model, Excel Macros must be enabled.

2.1.1.1 Excel 2007

- When opening Excel, a security warning message should appear just below the tool bars. The general instruction can be activated through clicking the "How to enable" link in the Input sheet, as shown in

- **Figure** 2-1.
- If no button appears in the security message, click on the Office button in the top left corner of the screen (**Figure 2-2**). Select the Excel Options button at the bottom of the menu (**Figure 2-3**). Within the Excel Options dialog, select the Trust Center on the left menu and then the Trust Center Settings button at the bottom right of the window (
- **Figure** 2-4). To enable the Macros, select the Macro Settings from the left menu and then the bottom option marked “Enable all macros” (**Figure 2-5**).

Figure 2-1: General Macro-Enabling Instructions



How to enable Macro? Back to Input page

Excel 2007

When opening the Macro for the first time, a security warning message should show up. Click the "Option" button to enable the macro.

When the notification window appears, select "Enable this content" to enable Macro.

○ Help protect me from unknown content (recommended)

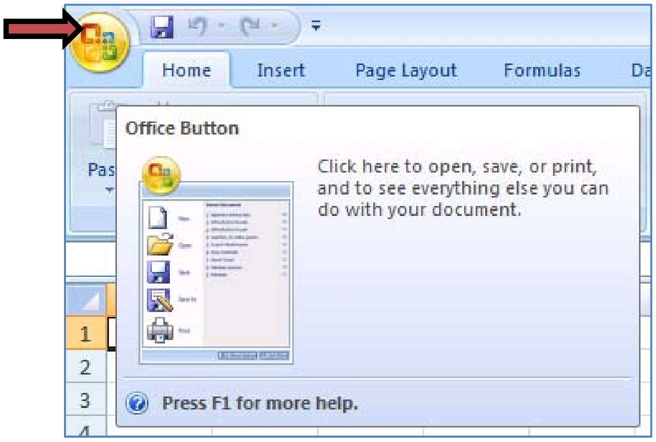
● Enable this content

Excel 2010

When opening the Macro for the first time, a security warning message should show up. Click the "Enable Content" button to enable the macro.

If the button did not show up, click the "File" tab.
In the Security Warning section, click the "Enable Content" button
Select "Enable All Content" button.

Figure 2-2: Office Button Location



Office Button

Click here to open, save, or print, and to see everything else you can do with your document.

Press F1 for more help.

Figure 2-3: Excel Options Location

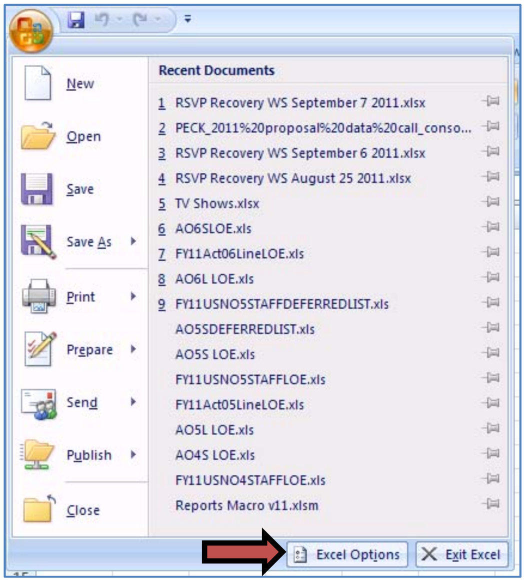
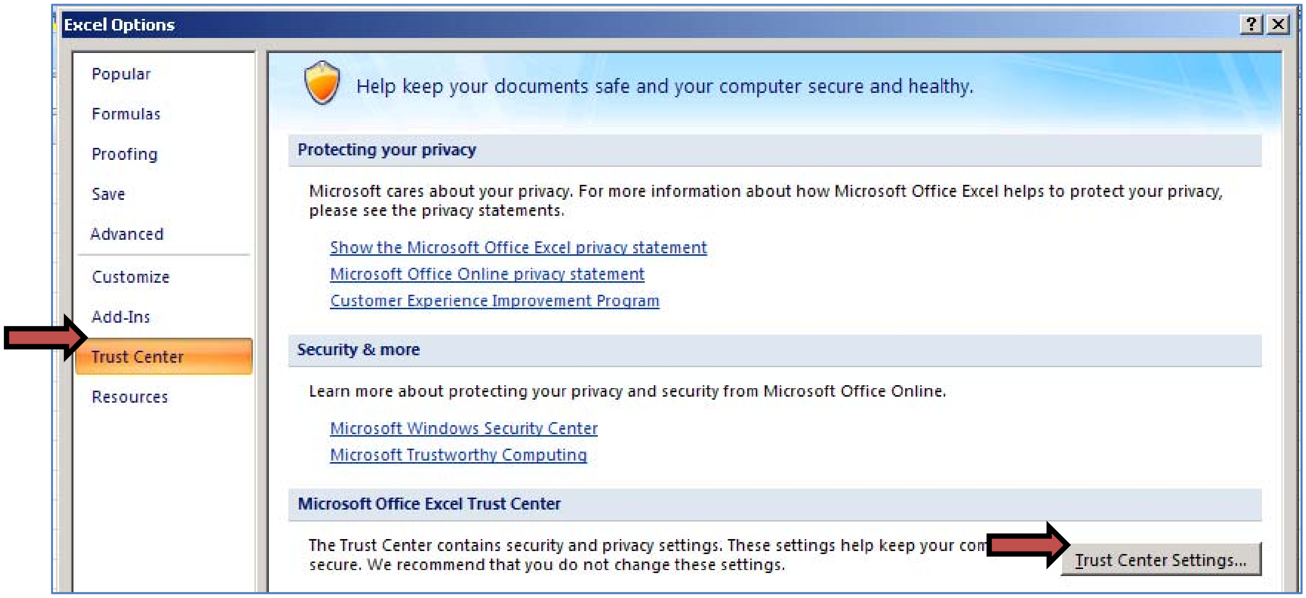


Figure 2-4: Opening the Trust Center



Help keep your documents safe and your computer secure and healthy.

Protecting your privacy

Microsoft cares about your privacy. For more information about how Microsoft Office Excel helps to protect your privacy, please see the privacy statements.

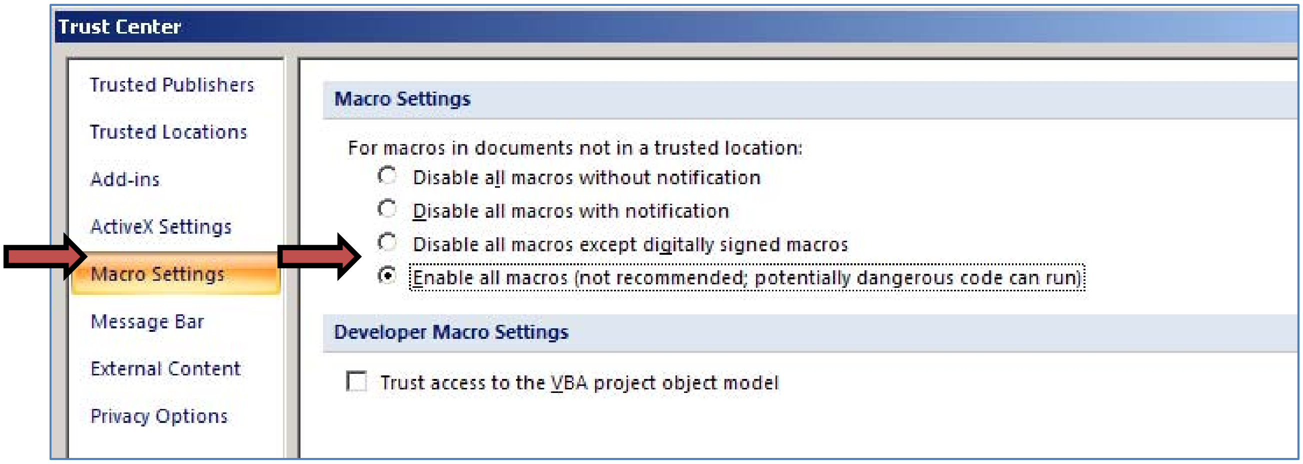
Security & more

Learn more about protecting your privacy and security from Microsoft Office Online.

Microsoft Office Excel Trust Center

The Trust Center contains security and privacy settings. These settings help keep your com secure. We recommend that you do not change these settings.

Figure 2-5: Enabling of Macros



Macro Settings

For macros in documents not in a trusted location:

○ Disable all macros without notification
○ Disable all macros with notification
○ Disable all macros except digitally signed macros
● Enable all macros (not recommended; potentially dangerous code can run)

Developer Macro Settings

☐ Trust access to the VBA project object model

2.1.1.2 Excel 2010

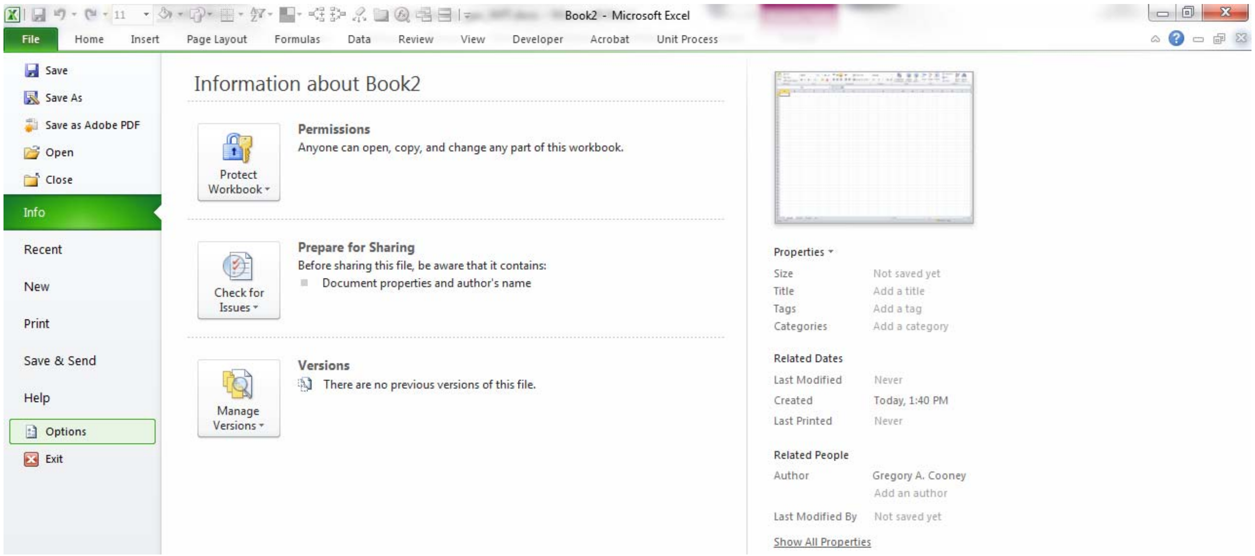
- When opening Excel, a security warning message should appear just below the tool bars. The general instruction can be activated through clicking the “How to enable” link in the Input sheet, as shown in

- **Figure** 2-1.
- If there is no security warning message or the wrong option is selected, switch to the File tab. In the Security Warning section, clicking on the Enable Content button will open a drop-down menu. Select the option "Enable content for this session only."

2.1.2 Microsoft Excel Solver Add-In

This model relies on the use of the Solver Add-In to Microsoft Excel. As such, the add-in must be enabled before the model can be used. To check that the Solver Add-In is functional, navigated to the file tab in Excel and click "Options" as shown in **Figure 2-5**. In the "Excel Options" window, select "Add-Ins" on the left hand panel as shown in **Figure 2-6**. At the bottom of the window, next to "Manage" ensure that "Excel Add-ins" is selected in the dropdown list and then select "Go." In the Add-Ins dialog box, shown in **Figure 2-7**, ensure that the checkbox for "Solver Add-In" is selected and then click "OK."

Figure 2-6: Excel Options



Information about Book2

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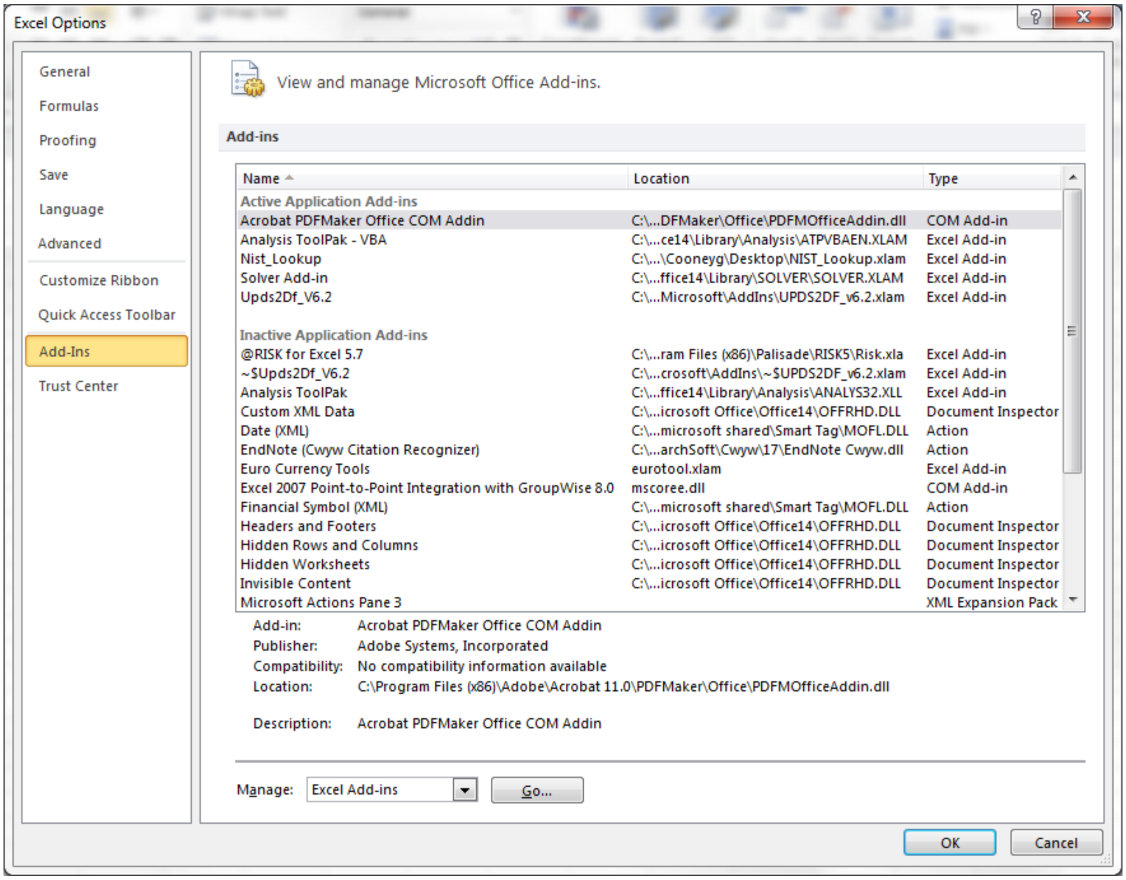
Categories: Add a category

Related Dates
Last Modified: Never
Created: Today, 1:40 PM
Last Printed: Never

Related People
Author: Gregory A. Cooney
Add an author
Last Modified By: Not saved yet

Figure 2-7: Excel Options – Add-Ins



View and manage Microsoft Office Add-ins.

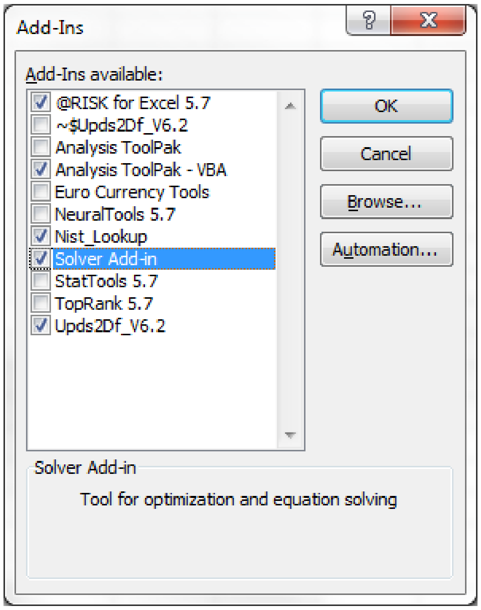
Add-ins

Name	Location	Type
Active Application Add-ins		
Acrobat PDFMaker Office COM Addin	C:\...DFMaker\Office\PDFMOfficeAddin.dll	COM Add-in
Analysis ToolPak - VBA	C:\...ce14\Library\Analysis\ATPVBAEN.XLAM	Excel Add-in
Nist_Lookup	C:\...\Cooneyg\Desktop\NIST_Lookup.xlam	Excel Add-in
Solver Add-in	C:\...ffice14\Library\SOLVER\SOLVER.XLAM	Excel Add-in
Upds2Df_V6.2	C:\...Microsoft\AddIns\UPDS2DF_v6.2.xlam	Excel Add-in
Inactive Application Add-ins		
@RISK for Excel 5.7	C:\...ram Files (x86)\Palisade\RISK5\Risk.xla	Excel Add-in
~$Upds2Df_V6.2	C:\...crosoft\AddIns\~$UPDS2DF_v6.2.xlam	Excel Add-in
Analysis ToolPak	C:\...ffice14\Library\Analysis\ANALYS32.XLL	Excel Add-in
Custom XML Data	C:\...icrosoft Office\Office14\OFFRHD.DLL	Document Inspector
Date (XML)	C:\...microsoft shared\Smart Tag\MOFL.DLL	Action
EndNote (Cwyw Citation Recognizer)	C:\...archSoft\Cwyw\17\EndNote Cwyw.dll	Action
Euro Currency Tools	eurotool.xlam	Excel Add-in
Excel 2007 Point-to-Point Integration with GroupWise 8.0	mscoree.dll	COM Add-in
Financial Symbol (XML)	C:\...microsoft shared\Smart Tag\MOFL.DLL	Action
Headers and Footers	C:\...icrosoft Office\Office14\OFFRHD.DLL	Document Inspector
Hidden Rows and Columns	C:\...icrosoft Office\Office14\OFFRHD.DLL	Document Inspector
Hidden Worksheets	C:\...icrosoft Office\Office14\OFFRHD.DLL	Document Inspector
Invisible Content	C:\...icrosoft Office\Office14\OFFRHD.DLL	Document Inspector
Microsoft Actions Pane 3		XML Expansion Pack

Add-in:	Acrobat PDFMaker Office COM Addin
Publisher:	Adobe Systems, Incorporated
Compatibility:	No compatibility information available
Location:	C:\Program Files (x86)\Adobe\Acrobat 11.0\PDFMaker\Office\PDFMOfficeAddin.dll
Description:	Acrobat PDFMaker Office COM Addin

Manage: Excel Add-ins

Figure 2-8: Add-Ins Selection Dialog Box



Add-Ins available:

☑ @RISK for Excel 5.7
☐ ~$Upds2Df_V6.2
☐ Analysis ToolPak
☑ Analysis ToolPak - VBA
☐ Euro Currency Tools
☐ NeuralTools 5.7
☑ Nist_Lookup
☑ Solver Add-in
☐ StatTools 5.7
☐ TopRank 5.7
☑ Upds2Df_V6.2

Solver Add-in

Tool for optimization and equation solving

2.2 Model Dashboard

The main interface for utilizing the CBTL GHG Optimization Tool is the ‘Dashboard’ tab. All of the inputs, model selections, and outputs of the model are displayed on the ‘Dashboard’ tab in the Excel workbook. The remainder of this section will step through the process of setting up and configuring the model. The ribbon interface for the CBTL GHG Optimization Tool is depicted in **Figure 2-9**. When first starting the model, the user should select the ‘Scenario Editor’ button in the ribbon to establish the configuration. Upon selecting the ‘Scenario Editor’ button, the user will see the interface shown in **Figure 2-10**. From that interface, the user can select the coal, biomass, and gasifier types, as well as a recycle or once-through configuration. The options that are available to the users are based on cases that NETL has previously modeled. The selection matrix is shown in

Table 3-1. After making selections for all of the dropdown boxes in **Figure 2-10**, the user can close the dialog box. The choices that the user has made for the facility configuration are shown in cells D2:D5 on the ‘Dashboard’ tab as shown in **Figure 2-11**.

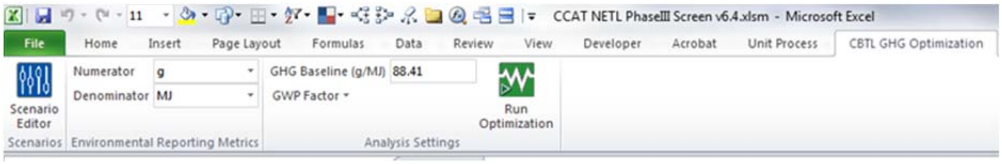
The next step to configuring the model is to set values for the biomass percentage, plant efficiency, and fraction of captured CO_2 vented. These choices can be specified in cells D8:D10 on the ‘Dashboard’ tab as shown in **Figure 2-11**. The minimum and maximum values in columns E and F are utilized in the Optimization, which will be discussed later. In addition to the Model Inputs, users have additional options to customize the parameters that drive the impacts of individual processes on the total life cycle GHG emissions. These can be configured in cells D13:D28, as shown in **Figure 2-12** and are consistent with the parameters available to users in the existing *CCAT CBTL Jet Fuel* Model (NETL, 2014a).

The outputs from the model are consistent with the *CCAT CBTL Jet Fuel* Model and are shown in both tabular (**Figure 2-13**) and graphical format (**Figure 2-14**).

After the model has been configured, the design parameters (biomass percentage, plant efficiency, and fraction of vented CO_2) and life cycle parameters can be altered at any time and the user will see the updated results instantaneously. If the user wants to change the coal, biomass, or gasifier types or the recycle/once-through configuration, they must do so by using the ‘Scenario Editor’ button in the ribbon.

The optimization utilized in the tool adopts the Excel’s built-in solver add-in. Users need to activate the add-in in order to use this function. The target is the total GHG emission (cell D60 on the ‘Dashboard’ tab). The solver will change variable values with their constraints to reach the GHG Baseline value. The default of the GHG Baseline value is set to 88.41 g/MJ (NETL, 2008). Users can change the target value for the optimization in the ribbon GHG Baseline box. The variables included in the optimization are D11:D13 (three design parameters), D16:D32 (LC stage parameters). Users should also change the Min and Max values for each parameter to give the solution space a proper boundary.

Figure 2-9: CBTL GHG Optimization Tool Ribbon Interface

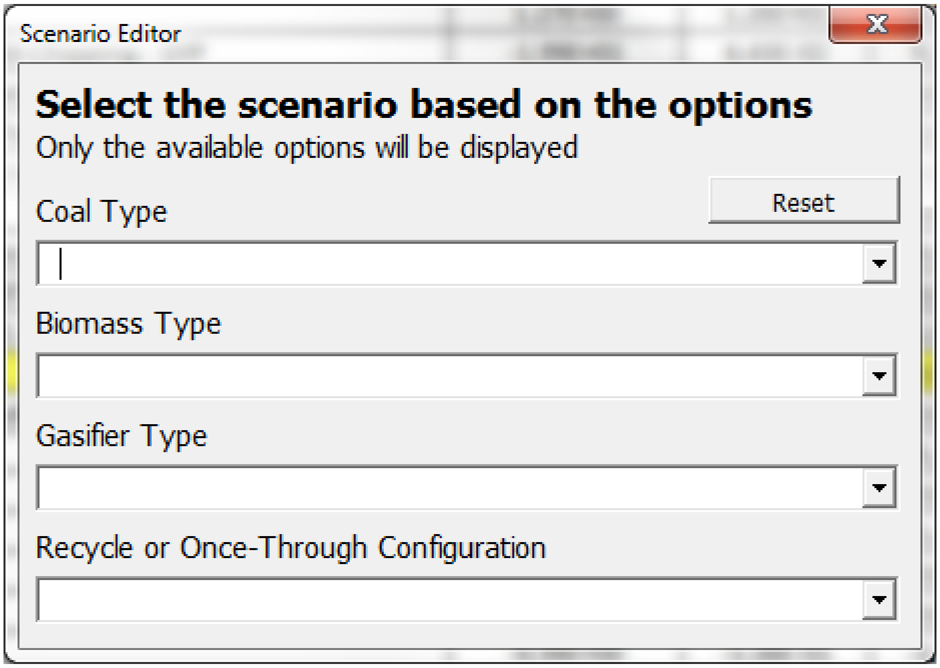


Numerator g

Denominator MJ

GHG Baseline (g/MJ) 88.41

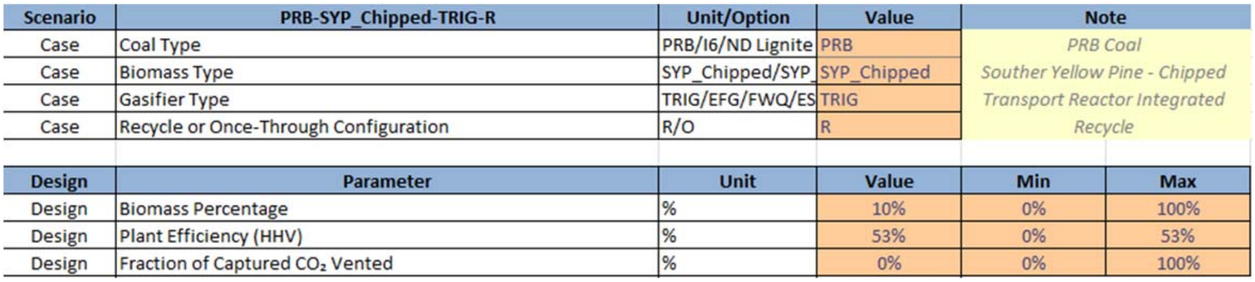
Figure 2-10: Scenario Editor Inputs Section



Select the scenario based on the options

Only the available options will be displayed

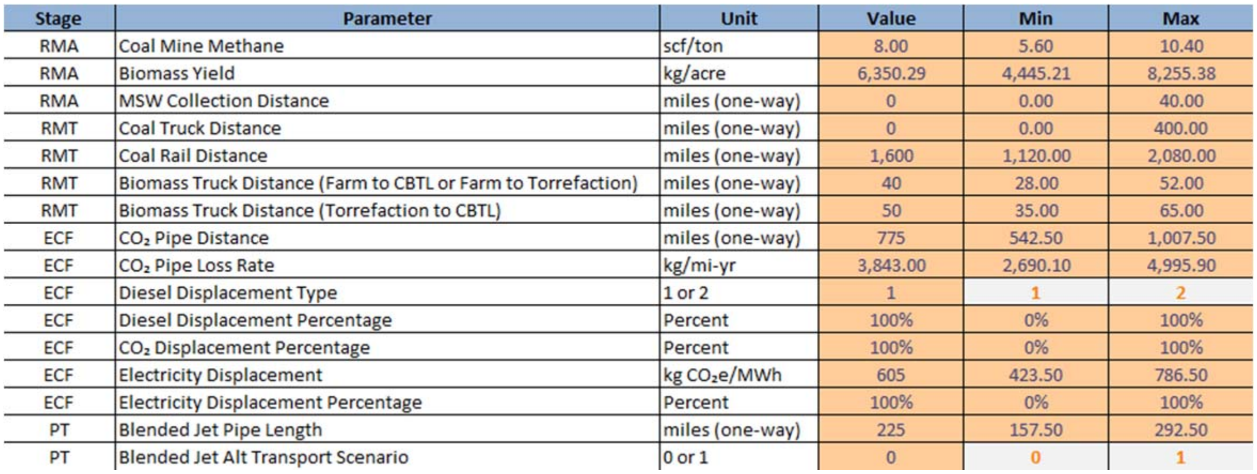
Figure 2-11: Model Scenario and Design Selections



Scenario	PRB-SYP_Chipped-TRIG-R	Unit/Option	Value	Note
Case	Coal Type	PRB/I6/ND Lignite	PRB	*PRB Coal*
Case	Biomass Type	SYP_Chipped/SYP_	SYP_Chipped	*Souther Yellow Pine - Chipped*
Case	Gasifier Type	TRIG/EFG/FWQ/ES	TRIG	*Transport Reactor Integrated*
Case	Recycle or Once-Through Configuration	R/O	R	*Recycle*

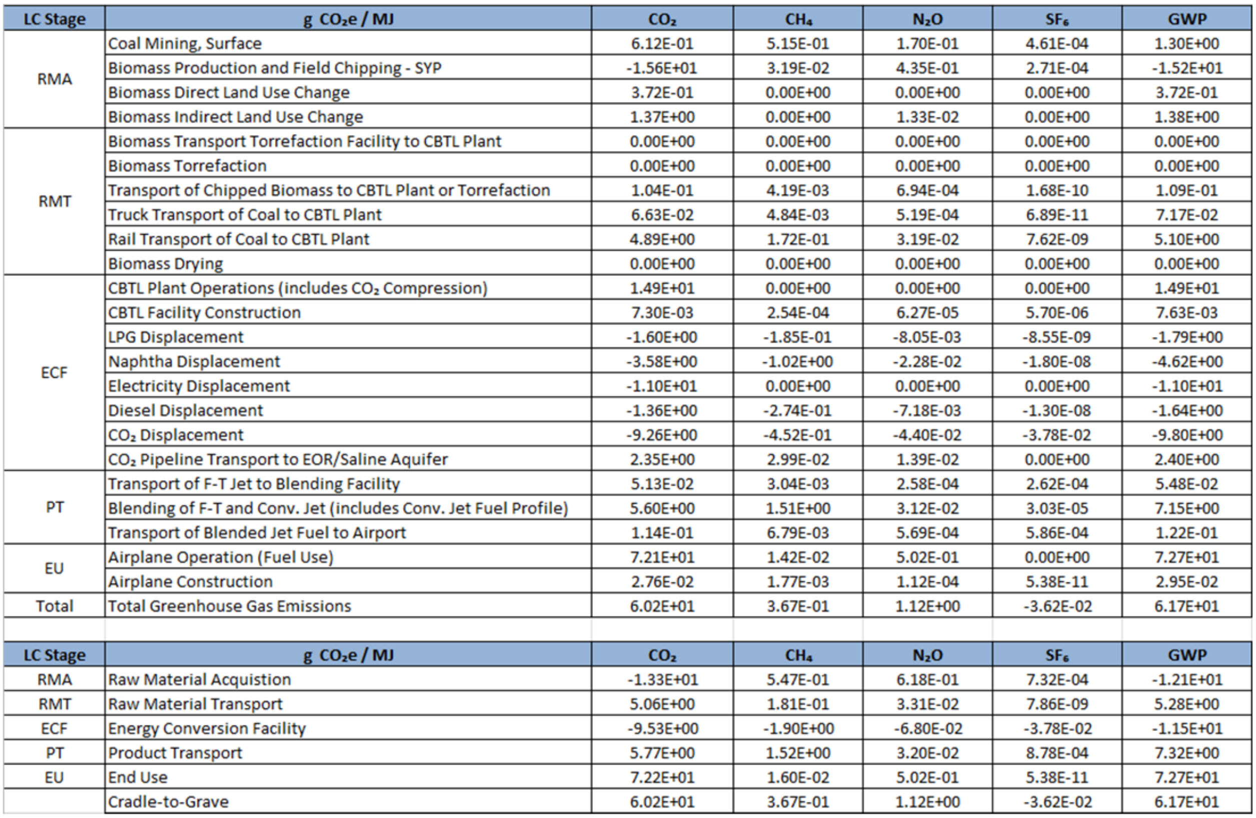
Design	Parameter	Unit	Value	Min	Max
Design	Biomass Percentage	%	10%	0%	100%
Design	Plant Efficiency (HHV)	%	53%	0%	53%
Design	Fraction of Captured CO_2 Vented	%	0%	0%	100%

Figure 2-12: Model Life Cycle Parameters Section



Stage	Parameter	Unit	Value	Min	Max
RMA	Coal Mine Methane	scf/ton	8.00	5.60	10.40
RMA	Biomass Yield	kg/acre	6,350.29	4,445.21	8,255.38
RMA	MSW Collection Distance	miles (one-way)	0	0.00	40.00
RMT	Coal Truck Distance	miles (one-way)	0	0.00	400.00
RMT	Coal Rail Distance	miles (one-way)	1,600	1,120.00	2,080.00
RMT	Biomass Truck Distance (Farm to CBTL or Farm to Torrefaction)	miles (one-way)	40	28.00	52.00
RMT	Biomass Truck Distance (Torrefaction to CBTL)	miles (one-way)	50	35.00	65.00
ECF	CO_2 Pipe Distance	miles (one-way)	775	542.50	1,007.50
ECF	CO_2 Pipe Loss Rate	kg/mi-yr	3,843.00	2,690.10	4,995.90
ECF	Diesel Displacement Type	1 or 2	1	1	2
ECF	Diesel Displacement Percentage	Percent	100%	0%	100%
ECF	CO_2 Displacement Percentage	Percent	100%	0%	100%
ECF	Electricity Displacement	kg CO_2e/MWh	605	423.50	786.50
ECF	Electricity Displacement Percentage	Percent	100%	0%	100%
PT	Blended Jet Pipe Length	miles (one-way)	225	157.50	292.50
PT	Blended Jet Alt Transport Scenario	0 or 1	0	0	1

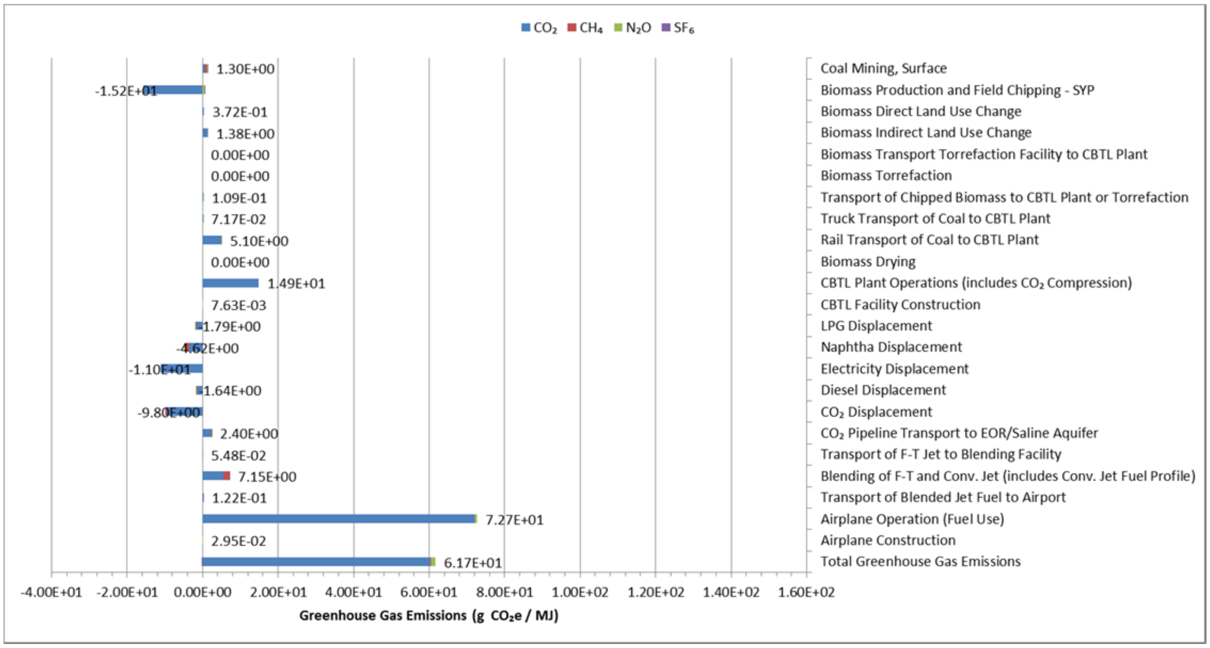
Figure 2-13: Model Output Data Table



LC Stage	g CO_2e / MJ	CO_2	CH_4	N_2O	SF_6	GWP
RMA	Coal Mining, Surface	6.12E-01	5.15E-01	1.70E-01	4.61E-04	1.30E+00
	Biomass Production and Field Chipping - SYP	-1.56E+01	3.19E-02	4.35E-01	2.71E-04	-1.52E+01
	Biomass Direct Land Use Change	3.72E-01	0.00E+00	0.00E+00	0.00E+00	3.72E-01
	Biomass Indirect Land Use Change	1.37E+00	0.00E+00	1.33E-02	0.00E+00	1.38E+00
RMT	Biomass Transport Torrefaction Facility to CBTL Plant	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
	Biomass Torrefaction	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
	Transport of Chipped Biomass to CBTL Plant or Torrefaction	1.04E-01	4.19E-03	6.94E-04	1.68E-10	1.09E-01
	Truck Transport of Coal to CBTL Plant	6.63E-02	4.84E-03	5.19E-04	6.89E-11	7.17E-02
	Rail Transport of Coal to CBTL Plant	4.89E+00	1.72E-01	3.19E-02	7.62E-09	5.10E+00
	Biomass Drying	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
ECF	CBTL Plant Operations (includes CO_2 Compression)	1.49E+01	0.00E+00	0.00E+00	0.00E+00	1.49E+01
	CBTL Facility Construction	7.30E-03	2.54E-04	6.27E-05	5.70E-06	7.63E-03
	LPG Displacement	-1.60E+00	-1.85E-01	-8.05E-03	-8.55E-09	-1.79E+00
	Naphtha Displacement	-3.58E+00	-1.02E+00	-2.28E-02	-1.80E-08	-4.62E+00
	Electricity Displacement	-1.10E+01	0.00E+00	0.00E+00	0.00E+00	-1.10E+01
	Diesel Displacement	-1.36E+00	-2.74E-01	-7.18E-03	-1.30E-08	-1.64E+00
	CO_2 Displacement	-9.26E+00	-4.52E-01	-4.40E-02	-3.78E-02	-9.80E+00
	CO_2 Pipeline Transport to EOR/Saline Aquifer	2.35E+00	2.99E-02	1.39E-02	0.00E+00	2.40E+00
PT	Transport of F-T Jet to Blending Facility	5.13E-02	3.04E-03	2.58E-04	2.62E-04	5.48E-02
	Blending of F-T and Conv. Jet (includes Conv. Jet Fuel Profile)	5.60E+00	1.51E+00	3.12E-02	3.03E-05	7.15E+00
	Transport of Blended Jet Fuel to Airport	1.14E-01	6.79E-03	5.69E-04	5.86E-04	1.22E-01
EU	Airplane Operation (Fuel Use)	7.21E+01	1.42E-02	5.02E-01	0.00E+00	7.27E+01
	Airplane Construction	2.76E-02	1.77E-03	1.12E-04	5.38E-11	2.95E-02
Total	Total Greenhouse Gas Emissions	6.02E+01	3.67E-01	1.12E+00	-3.62E-02	6.17E+01

LC Stage	g CO_2e / MJ	CO_2	CH_4	N_2O	SF_6	GWP
RMA	Raw Material Acquistion	-1.33E+01	5.47E-01	6.18E-01	7.32E-04	-1.21E+01
RMT	Raw Material Transport	5.06E+00	1.81E-01	3.31E-02	7.86E-09	5.28E+00
ECF	Energy Conversion Facility	-9.53E+00	-1.90E+00	-6.80E-02	-3.78E-02	-1.15E+01
PT	Product Transport	5.77E+00	1.52E+00	3.20E-02	8.78E-04	7.32E+00
EU	End Use	7.22E+01	1.60E-02	5.02E-01	5.38E-11	7.27E+01
	Cradle-to-Grave	6.02E+01	3.67E-01	1.12E+00	-3.62E-02	6.17E+01

Figure 2-14: Model Output Graph



2.3 Supporting Worksheets

In addition to the Dashboard tab, the CBTL GHG Optimization Tool contains a number of supporting tabs that contain information necessary for the model calculations. These tabs are described in

Table 2-1. There are some other tabs which are used for calculation purposes only and remain hidden from the user. Only values on the 'Dashboard' tab should be altered. Changing values on any of the other tabs may compromise the model results.

Table 2-1: F-T Black Box Model Worksheets

Tab Name	Description
Disclaimer	Model disclaimer
Dashboard	Input/Output interface for the model
UP Data	Background LCA calculations
UP Relationship	Relationships for UP parameters
UP Relationship Data	Feedstock LC GHG data
4.0 Plant I-O	Calculation of the CBTL plant I-O based on settings
Unit Reference	Reference values
Version	Version history

3 Modeling Approach and Assumptions

3.1 Technological Analysis and Process Model Overview

Results from the process model are intended to inform the economic and life cycle models, and also assist with refining key considerations for a development and demonstration/trial of the CBTL process, that is also being considered concurrent to this effort. The CBTL facility configuration considered in support of the technological analysis and process model design for the CBTL facility consider both biomass and coal feedstock supplies, as those would be processed through the CBTL facility into a suite of co-products, including F-T jet fuel, F-T diesel, F-T naphtha, F-T LPG, F-T electricity, and carbon dioxide.

The conceptual process designs for all of the CBTL facility scenarios considered here were based on systems level models for indirect coal liquefaction technology. Aspen Plus® simulation models for the CBTL facility scenarios were developed to determine the composition and flows of all of the major streams in the plants. Where appropriate, additional specialized software packages were used to extrapolate the performance of certain unit operations under site-specific conditions, such as validation of the gas turbine and steam cycle operating conditions and performance under the specific plant conditions and validation of simulation of operations like sour water stripping. These performance predictions were then incorporated into the Aspen Plus® systems models. The Aspen Plus® model results were validated against vendor data where possible and/or predictions from more detailed design models. Additional documentation of the process modeling is included in the referenced NETL studies (NETL, 2011, 2014a, 2014b, 2015a, 2015b).

Error! Reference source not found. through Error! Reference source not found. depict a high-level process flow diagram for each of the studies that was utilized for the cases contained in the CBTL GHG Optimization Tool. Not all of the configurations produce will produce all of the products (jet, diesel, naphtha, and LPG) due to different processing constraints from the original studies. Every configuration will produce jet and naphtha. The Zero S Diesel and CTL Baseline studies produce only diesel and naphtha. For the purposes of this tool, it was assumed that the configurations could produce an equivalent amount of jet fuel as the amount of diesel that was produced without any significant impact on facility operations or GHG emissions. Jet fuel and diesel have similar distillation ranges, thus it was assumed that only minor adjustments would be required in the product upgrading section of the facility. As this is considered a screening tool, this assumption was determined to be justified. If any of these cases are the basis for additional modeling, this assumption should be evaluated in more detail.

Figure 3-1: CCAT – TRIG PFD (NETL, 2015b)

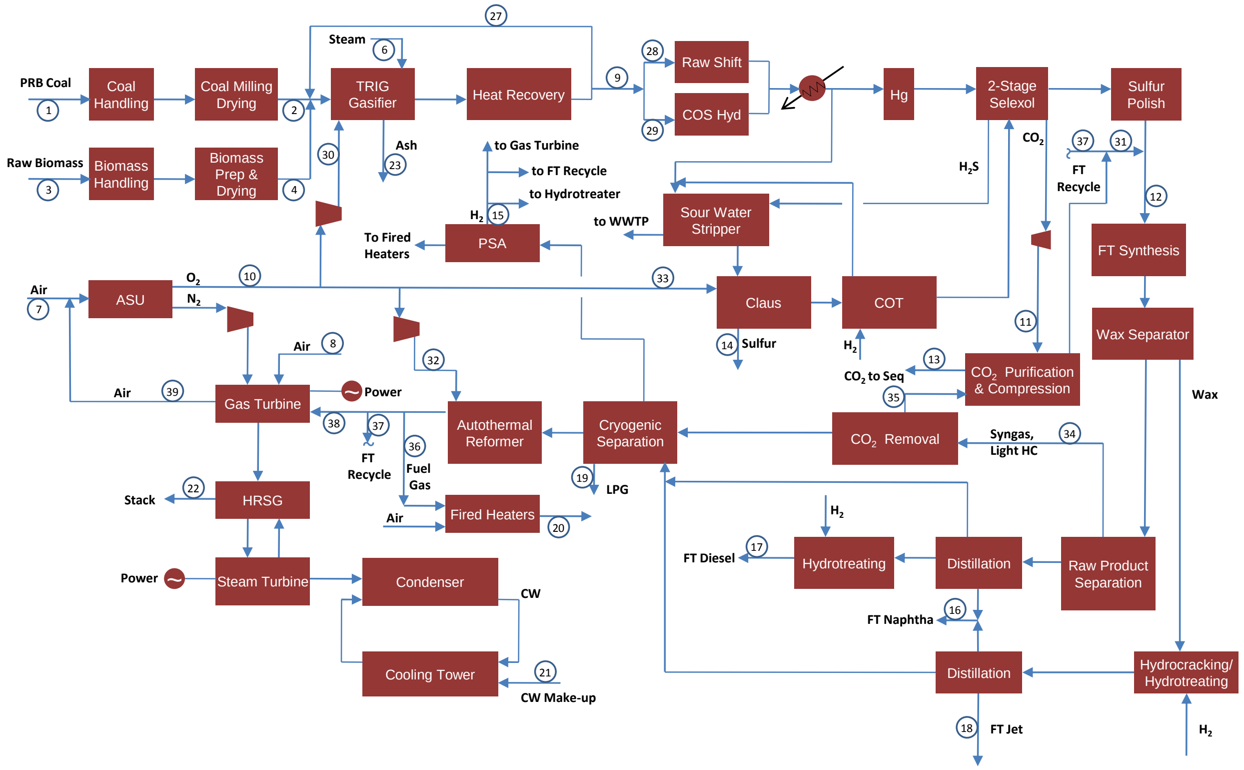


Figure 3-2: CCAT – EFG PFD (NETL, 2015a)

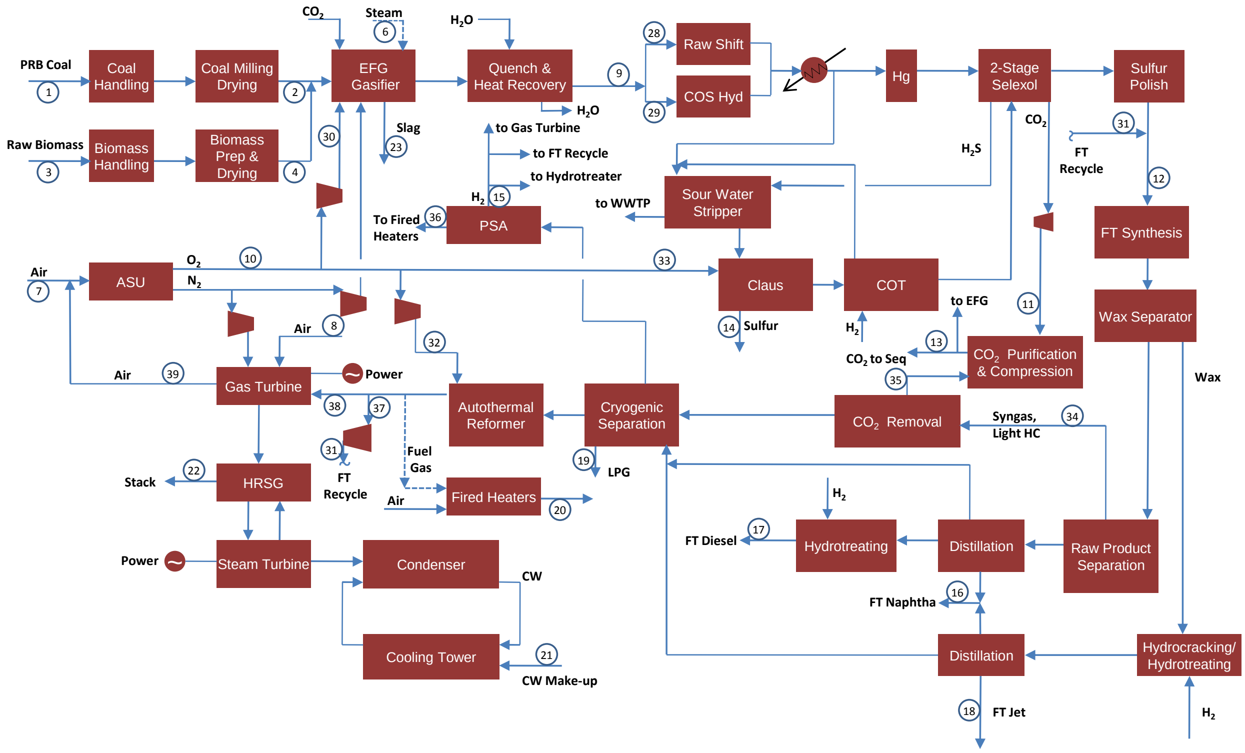


Figure 3-3: Zero Sulfur Diesel Recycle Case PFD (NETL, 2011)

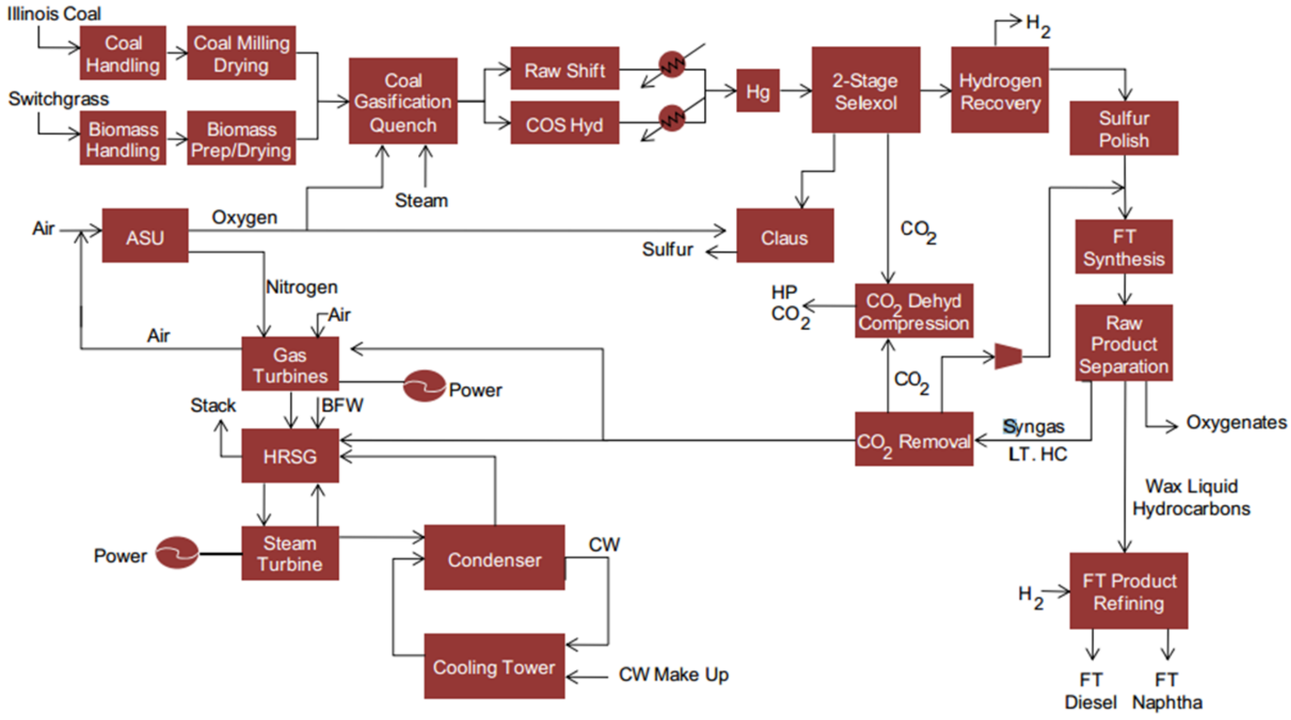


Figure 3-4: Zero Sulfur Diesel Once-Through Case PFD (NETL, 2011)

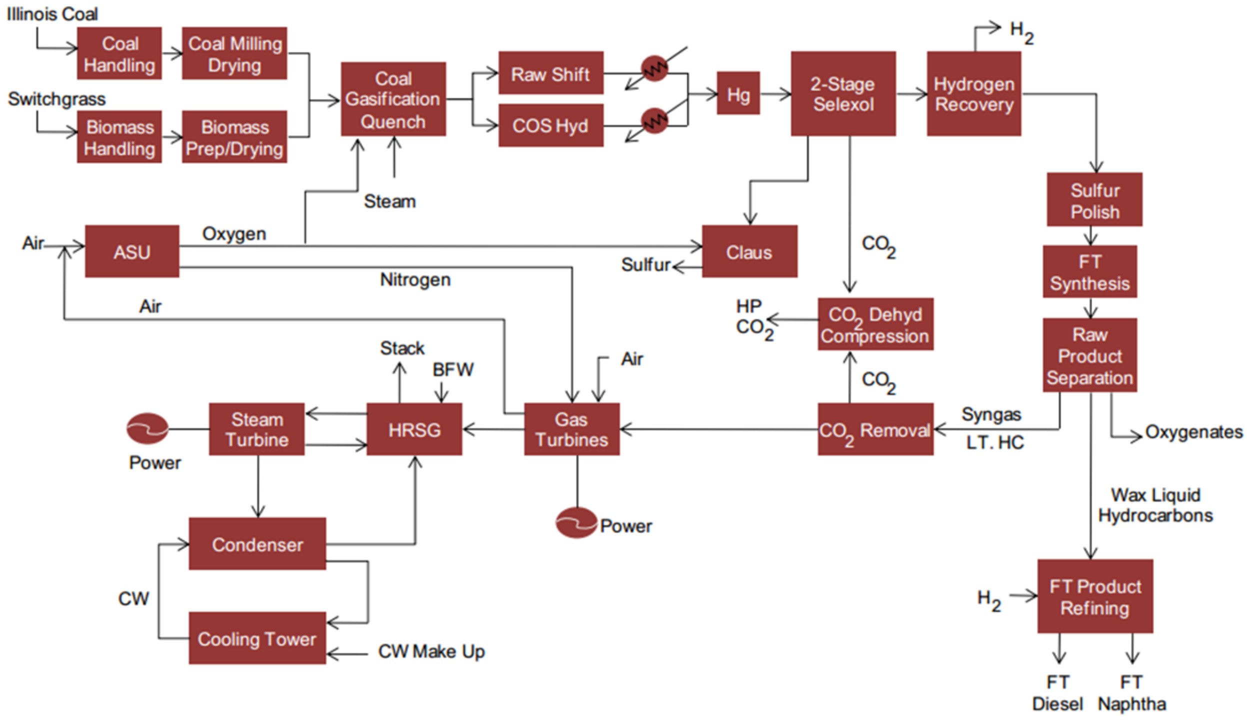
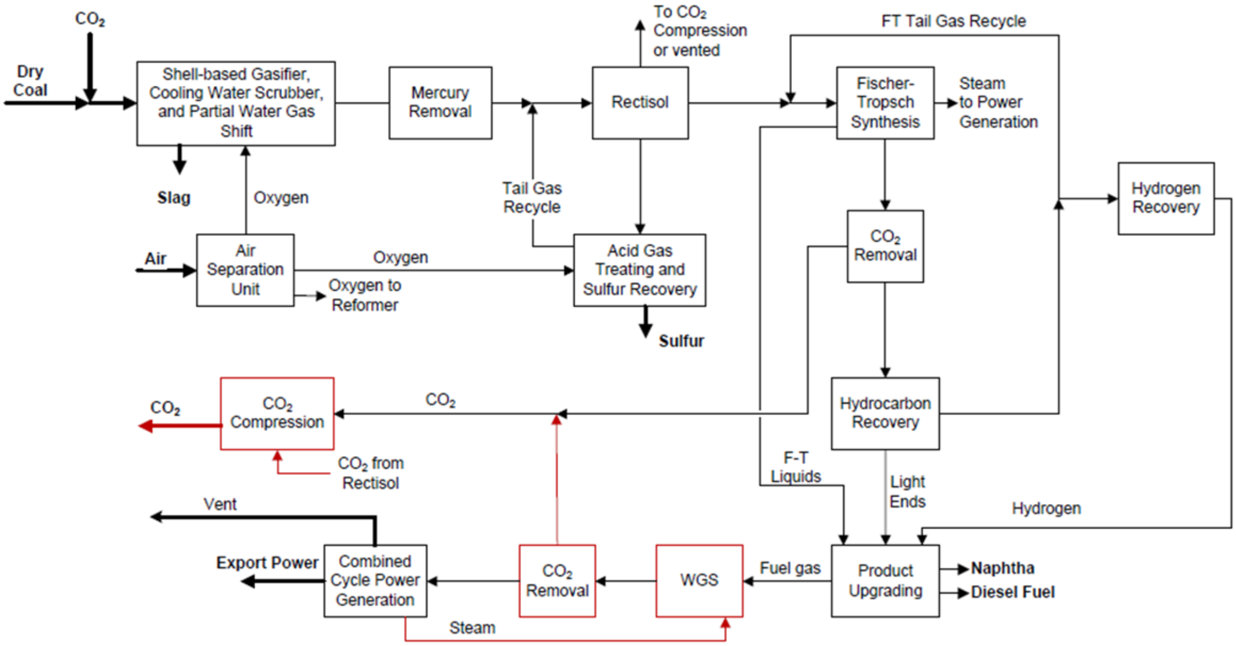


Figure 3-5: Coal-to-Liquids Baseline PFD (NETL, 2014b)



3.2 Coal, Biomass, and Gasifier Combinations Available

As previously noted, the coal and biomass combinations and gasifier types will be limited to the cases that NETL has previously modeled and published. Scenarios that have not been previously modeled and published by NETL will not be available for selection in the tool. The available configurations are displayed in

Table 3-1.

Two new feedstocks have been added that were not included in any of the reference studies – North Dakota Lignite coal and Municipal Solid Waste (MSW). The performance of North Dakota Lignite in the fuel production boundary (gasifier through F-T) will be approximated by utilizing PRB coal. Only the upstream acquisition emissions will be changed when North Dakota Lignite is selected as a feedstock. The performance of MSW in the fuel production boundary (gasifier through F-T) will be approximated by utilizing biomass. Only the upstream acquisition emissions will be changed when MSW is selected as a feedstock.

Table 3-1: Coal, Biomass, and Gasfier Combinations

Coal	Biomass	Gasifier	Recycle (R) or Once-Through (O)	Reference
Illinois No. 6	-	Shell	R	CTL Baseline
	-	Siemens	O	Zero S Diesel
	-	Siemens	R	Zero S Diesel
	Switchgrass	Siemens	O	Zero S Diesel
	Switchgrass	Siemens	R	Zero S Diesel
	MSW	Siemens	O	Zero S Diesel
	MSW	Siemens	R	Zero S Diesel
Montana Rosebud (PRB)	-	EFG	R	CCAT – EFG
	-	Siemens	O	Zero S Diesel
	-	Siemens	R	Zero S Diesel
	-	TRIG	R	CCAT – TRIG
	Southern Yellow Pine*	EFG	R	CCAT – EFG
	Southern Yellow Pine*	TRIG	R	CCAT – TRIG
	Switchgrass	Siemens	O	Zero S Diesel
	Switchgrass	Siemens	R	Zero S Diesel
	MSW	Siemens	O	Zero S Diesel
	MSW	Siemens	R	Zero S Diesel
ND Lignite	-	EFG	R	CCAT – EFG
	-	Siemens	O	Zero S Diesel
	-	Siemens	R	Zero S Diesel
	-	TRIG	R	CCAT – TRIG
	Southern Yellow Pine*	EFG	R	CCAT – EFG
	Southern Yellow Pine*	TRIG	R	CCAT – TRIG
	Switchgrass	Siemens	O	Zero S Diesel
	Switchgrass	Siemens	R	Zero S Diesel
	MSW	Siemens	O	Zero S Diesel
	MSW	Siemens	R	Zero S Diesel

***The model includes options for four preparations of Southern Yellow Pine – chipped, pelletized, torrefied, and torrefied/pelletized.**

3.3 Feedstock Data

The elemental composition of the feedstocks included in the CBTL GHG Optimization Tool are documented in the following tables.

Table 3-2: Analysis of Montana Rosebud PRB Sub-Bituminous Coal (NETL, 2014a)

Property	As Received	Dry Basis	As Fed
Proximate Analysis			
Moisture (%)	25.77	0.00	18.00
Ash (%)	8.19	11.04	9.05
Volatile Matter (%)	30.34	40.87	33.51
Fixed Carbon (%)	35.70	48.09	39.43
Total (%)	100.00	100.00	100.00
Ultimate Analysis			
C (%)	50.07	67.45	55.31
H (%)	3.38	4.56	3.74
O (%)	11.14	15.01	12.31
N (%)	0.71	0.96	0.79
S (%)	0.73	0.98	0.80
Cl (%)	0.01	0.01	0.01
Ash (%)	8.19	11.03	9.04
Moisture (%)	25.77	0.00	18.00
Total (%)	100.00	100.00	100.00
Heating Value			
HHV (Btu/lb)	8,564	11,516	9,443
LHV (Btu/lb)	8,252	11,096	9,079

Table 3-3:: Analysis of Illinois No. 6 Bituminous Coal (NETL, 2014b)

Property	As Received	Dry Basis	As Fed
Proximate Analysis			
Moisture (%)	11.12	0.00	6.00
Ash (%)	9.70	10.91	10.26
Volatile Matter (%)	34.99	39.37	37.00
Fixed Carbon (%)	44.19	49.72	46.74
Total (%)	100.00	100.00	100.00
Ultimate Analysis			
C (%)	63.75	71.72	67.42
H (%)	4.50	5.06	4.76
O (%)	6.89	7.75	7.29
N (%)	1.25	1.41	1.33
S (%)	2.51	2.82	2.65
Cl (%)	0.29	0.33	0.31
Ash (%)	9.70	10.91	10.26
Moisture (%)	25.77	0.00	18.00
Total (%)	100.00	100.00	100.00
Heating Value			
HHV (Btu/lb)	11,666	13,125	12,337
LHV (Btu/lb)	11,252	12,712	11,899

Table 3-4: Analysis of North Dakota Lignite Coal (NETL, 2012)

Property	As Received	Dry Basis
Proximate Analysis		
Moisture (%)	36.08	0.00
Ash (%)	26.52	41.48
Volatile Matter (%)	9.86	15.43
Fixed Carbon (%)	27.54	43.09
Total (%)	100.00	100.00
Ultimate Analysis		
C (%)	39.55	61.88
H (%)	2.74	4.29
O (%)	10.51	16.44
N (%)	0.63	0.98
S (%)	0.63	0.98
Cl (%)	0.00	0.00
Ash (%)	9.86	15.43
Moisture (%)	36.08	0.00
Total (%)	100.00	100.00
Heating Value		
HHV (Btu/lb)	6,617	10,427
LHV (Btu/lb)	6,364	10,032

Table 3-5: Analysis of Southern Pine Biomass (Non-Torrefied) (NETL, 2014a)

	As Received	Dry Basis	As Fed
Ultimate Analysis			
C (%)	30.55	53.88	44.18
H (%)	3.02	5.33	4.37
O (%)	22.25	39.25	32.19
N (%)	0.23	0.41	0.34
S (%)	0.02	0.04	0.03
Cl (%)	0	0	0
Ash (%)	0.62	1.09	0.89
Moisture (%)	43.3	0	18.00
Total (%)	100.00	100.00	100.00
Heating Value			
HHV (Btu/lb)	4,922	8,681	7,118
LHV (Btu/lb)	4,178	8,175	6,514

Table 3-6: Analysis of Torrefied Southern Pine Biomass (NETL, 2014a)

	As Received	Dry Basis	As Fed
Ultimate Analysis			
C (%)	59.89	63.52	59.89
H (%)	5.11	5.42	5.11
O (%)	28.36	30.08	28.36
N (%)	0.41	0.44	0.41
S (%)	0	0	0
Cl (%)	0	0	0
Ash (%)	0.51	0.54	0.51
Moisture (%)	5.72	0	5.72
Total (%)	100.00	100.00	100.00
Heating Value			
HHV (Btu/lb)	9,749	10,340	9,749
LHV (Btu/lb)	9,203	9,825	9,203

Table 3-7: Analysis of Switchgrass (NETL, 2014b)

	As Received	Dry Basis	As Fed to CBTL Facility
Ultimate Analysis			
C (%)	39.92	46.97	44.15
H (%)	4.86	5.72	5.37
O (%)	34.16	40.19	37.78
N (%)	0.73	0.86	0.80
S (%)	0.08	0.09	0.08
Cl (%)	0.00	0.00	0.00
Ash (%)	5.26	6.19	5.82
Moisture (%)	15.00	0.00	6.00
Total (%)	100.00	100.00	100.00
Heating Value			
HHV (Btu/lb)	6,851	8,060	7,576
LHV (Btu/lb)	6,405	7,536	7,084

3.4 Correlations for New Model Options

As noted in Section 1, the CBTL GHG Optimization Tool includes three new modeling options (biomass percentage, venting of captured CO_2, and adjustments to the plant efficiency). The correlations that were developed to enable those options is discussed below.

Biomass Feed Percentage:

To enable users to enter custom coal and biomass fractions, linear relationships were developed for the inputs and outputs of the facility. Relationships were derived for configurations that have at least one biomass case. These relationships are utilized in the model to calculate the feedstock inputs, liquid products, CO_2 emissions, CO_2 to pipeline, and export power for a custom biomass percentage. The upstream and downstream life cycle impacts are scaled according to the new plant inputs and outputs.

Captured CO_2 Venting:

Users can now choose to vent some or all of the captured CO_2 from the facility. The vented CO_2 is added to the existing stack emissions to produce a total CO_2 emission factor for the facility. The total export power is also affected by the percentage of captured CO_2 that the user chooses to vent because that fraction is no longer compressed to the pipeline pressure (2,200 psig). To determine the reduced compression auxiliary electricity load in the facility and the increase in export electricity from the facility, a linear relationship was developed for the compressor electricity requirement as a function of the CO_2 flow from existing cases previously modeled for CCAT and available in the *CCAT CBTL Jet Fuel Excel* model. The model utilizes the user-entered value for the vented fraction to calculate the new mass flow through the compressor for a given configuration, which combined with the power-flow relationship yields a new value for export electricity. From an LCA perspective, the venting of CO_2 increases the direct emissions from the facility, but also increases the export power displacement credit.

Plant Efficiency Adjustment:

The efficiency of a configuration is defined as the energy out of the facility (liquid fuels and electricity) divided by the energy in (coal and biomass), on a higher heating value (HHV) basis. This method of calculating efficiency is consistent with the cases that have been previously studied by NETL for CCAT available in the *CCAT CBTL Jet Fuel Excel* model (NETL, 2014a, 2015a, 2015b). It is assumed that the calculated efficiency is the currently optimal value for a configuration given currently available technology. All of the cases are based on Aspen models that have been run to optimize the efficiency of the facility. Therefore, users can only reduce the efficiency from the design point.

There are two potential changes that occur in the model when the user enters a new efficiency. The first is that the electricity export from the facility (numerator in the efficiency equation) is reduced until the user-desired efficiency is met. The basis for reducing the electricity export assumes that one of the three following reasons for a reduction in plant efficiency: (1) the power island is not operating at the design efficiency, (2) the auxiliary electricity loads are higher than designed, or (3) the steam flow (or quality) to the heat recovery steam generator (HRSG) is reduced to due to increased demands elsewhere in the plant.

If the plant does not produce net export electricity or reductions in the amount of export electricity are not sufficient to reach the target efficiency, the feedstock flows to the plant are increased accordingly. All facility configurations are assumed to produce approximately 50,000 bbl/day regardless of the user-entered efficiency. In other words, the liquid output from the facility is not available as a lever when adjusting the plant efficiency. Any increase to the feedstock is added in the proportion that the user has specified for that configuration (e.g. 10 percent Southern Yellow Pine pellets). From an LCA perspective, depending on the configuration, the electricity displacement credit will be reduced in magnitude and or the upstream feedstock impacts will increase in magnitude.

3.5 Environmental Model Overview

With respect to this study, quantification of life cycle GHG emissions focused on carbon dioxide (CO_2), methane (CH_4), nitrous oxide (N_2O), and sulfur hexafluoride (SF_6). These pollutants are generated during the production of alternative liquid fuels from coal and biomass. Hydrofluorocarbons and perfluorocarbons are not generated in large quantities during alternative liquid fuels production, and therefore were not considered further.

GHGs in this inventory are reported on a common mass basis of carbon dioxide equivalents (CO_2e) using the global warming potentials (GWP) of each gas from the 2013 Intergovernmental Panel on

Climate Change (IPCC) Fifth Assessment Report (AR5) (IPCC, 2013). The default GWP used is the 100-year time frame. **Table 1-2** shows the GWPs used for the GHGs inventoried in this study. Note that the AR5 GWP value used for fossil methane emissions was 30. There are no biogenic methane releases in the natural gas or coal models. The AR5 GWP for biogenic methane is 28.

The results of this analysis include only GHG emissions. GHGs in this inventory are reported on a common mass basis of carbon dioxide equivalents (CO_2e) using the global warming potentials (GWP) of each gas from the 2013 Intergovernmental Panel on Climate Change (IPCC) Fifth Assessment Report (AR5) (IPCC, 2013). The default GWP used is the 100-year time frame but, in some cases, results for the 20-year time frame are presented as well. **Table 2-1** shows the GWPs used for the GHGs inventoried in this study. The tool also provides results on the basis of the GWPs developed in the Fourth Assessment Report (AR4) (Forster et al., 2007). Note that the AR5 GWP value used for fossil methane emissions was 30. There are no biogenic methane releases in the natural gas or coal models. The AR5 GWP for biogenic methane is 28.

Table 3-8: IPCC AR4 and AR5 Global Warming Potentials (Forster, et al., 2007 and IPCC, 2013)

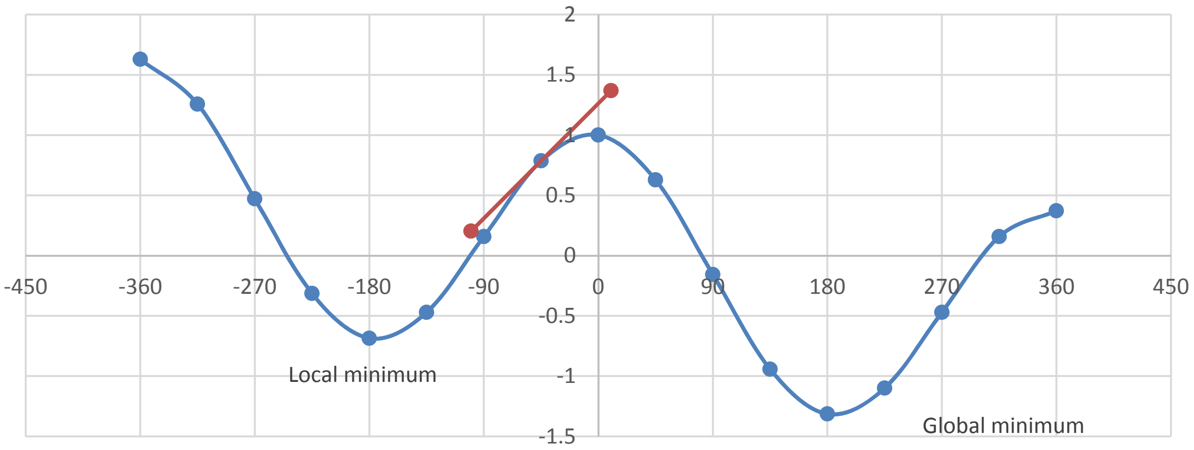
GHG	AR5 (IPCC 2013)		AR4 (IPCC 2007)	
	20-year	100-year (Default)	20-year	100-year
CO_2	1	1	1	1
CH_4	85	30	72	25
N_2O	264	265	289	298
SF_6	17,500	23,500	16,300	22,800

Five discrete life cycle stages were considered within the scope of the LCA presented here. These are represented in **Figure 3-6** and described below. **The optimization** algorithm used in this tool is the Microsoft Solver. It is the add-in comes with Excel (It might need manual activation). The tool's default solver engine uses the GRG Nonlinear method, which was developed by Leon Lasdon, of the University of Texas at Austin, and Allan Waren, of Cleveland State University.

The algorithm picks a set of trail input values (i.e., adjustable cells) and evaluates the results based on the constraints (i.e., minimums and maximums) and the target optimum cell (i.e., the target GHG value). Each trial is an iteration. As one can imagine, it will take an extremely long time and will use a lot of computer resources to exhaustively try all possible combinations in the variable space, especially when there are many variables.

To avoid this problem, this algorithm adjusts the input variables based on the trends of the results (i.e., whether it is closer to or further from the target values) for the next iteration. The algorithm measures the result change rate when the input is varied as the first derivative (**Figure 3-7**). When there are multiple variables, the algorithm keeps track of several partial derivatives measuring the rate of change in relation to each of the input values. These partial derivatives form the gradient of the function.

Figure 3-7: Illustration of Gradient, Local Minimum and Global Minimum



The gradients are the key components in guiding the algorithm to select new trial values. They are the clues for the algorithm to determine which and how much a variable should be changed. For example, if the optimum cell is being minimized (**Figure 3-7**) and its partial derivative in relation to one variable is a large negative number, while another partial derivate is near zero. The algorithm will probably change the value of the first variable on the next iteration. In other words, it evaluates the results based on changing variable values and searches along the solution curves.

If the preset iterations are reached and there's still no answer, the solver will still stop to prevent long execution time. It gives a faster convergence than the Evolutionary method. Even though there might be more than one satisfied solution in the solution space, the GRG Nonlinear method will most likely give the same solution due to its searching limitation (i.e., trapped in the local minimum in **Figure 3-7**). The Evolutionary method provides a better chance of escaping the local optimal results to find other solutions but it will take more iterations.

This tool tries to find the optimal solution to match the given GHG values and treat all parameters as independent. Since there can be more than one possible solution and there's no other way to set them apart (e.g., cost of each solution), all of those are satisfied solutions.

The tool uses the initial minimum and maximum values as constant boundaries during optimization and thus allow each variable to be changed within the provided range. Under the current setting, if users would like to fix a variable, users can make the value, min and max values of the variable to be the same. The algorithm will always use the variable value during the optimization.

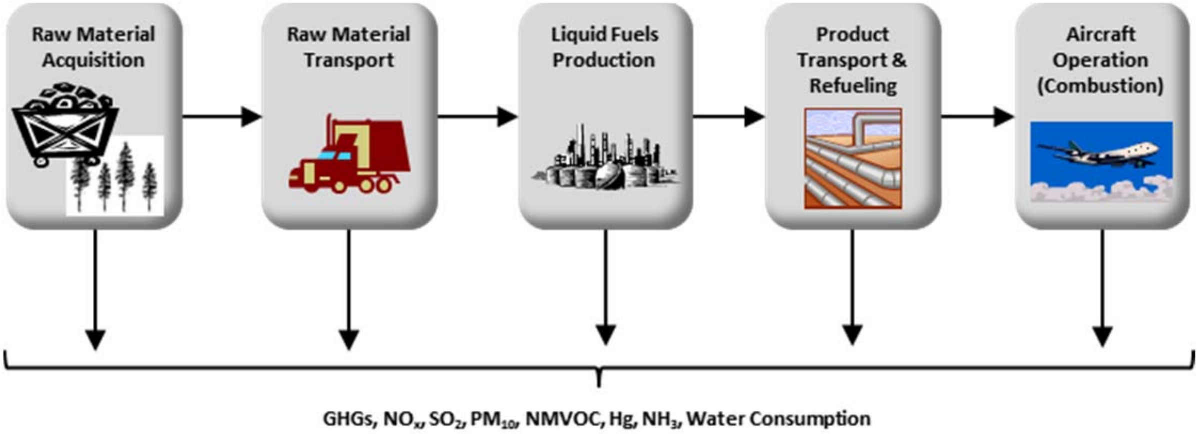
Please note that the maximum plant efficiency in the screening mode is formulated to be updated dynamically based on the biomass feed mass percentage and the fraction of vented captured CO_2 (Due to their dependencies). This can cause problems when all three design parameters are optimized at the same time as independent parameters. For example, the algorithm might pick a new biomass feed percentage which decreases the maximum plant efficiency in the process. However, the boundaries of plant efficiency has already been set as constants at the beginning of the optimization and therefore, the algorithm are allowed to select a value that is greater than the current decreased maximum plant efficiency.

To avoid this problem, the tool will find out the reasonable minimum plant efficiency for the selected case and use that as the upper bound (maximum) of the plant efficiency. This ensures that the algorithm will not select a plant efficiency value greater than its maximum value. A reasonable minimum plant efficiency is defined as the minimum value between the settings of 0% and 30% biomass feed percentage with 0% vented captured CO_2.

If users would like to change other solver settings, users can adjust the variables, constraints, and solving methods in Solver’s dialog menu after first running the optimization through the tool’s function. The problem will be kept and be able to access through Excel’s Solver menu (Under the DATA tab).

Figure 3-8 provides a more specific look at the processes that are included in each of the life cycle stages. This figure is specific to the scenarios already evaluated for CCAT, which are based on inputs of Montana Rosebud coal and Southern Pine biomass, but can be generalized for any type of coal and biomass. Not all of the configurations produce will produce all of the products (jet, diesel, naphtha, and LPG) due to different processing constraints from the original studies. Every configuration will produce jet and naphtha.

Figure 3-6: Life Cycle Stages Schematic



Source: Adapted From (Aviation Fuel Life Cycle Assessment Working Group, 2011)

Raw Material Acquisition (RMA): Raw material acquisition includes all construction and operations activities associated with the extraction of coal from a coal mine, and the production and harvesting of biomass. RMA also includes land use requirements and GHG emissions associated with land use change, that result from the conversion of land from existing conditions, in support of relevant RMA activities.

Raw Material Transport (RMT): Raw material transport includes construction and operations activities associated with the transport of coal and biomass from the downstream boundary of RMA to the energy conversion facility. RMT includes construction and operation of trains and trucks used for the transport of feedstock, but does not include construction of main line rails or roadways. For scenarios that include torrefaction, torrefaction facility construction and operations are also considered within the boundaries of RMT.

Energy Conversion (EC): Energy conversion is the process by which feedstock is converted into product fuels. EC includes construction and operations activities associated with this conversion process, as well as carbon management. As such, EC considers construction and operation of the CBTL facility and carbon dioxide transport pipelines.

Product Transport (PT): Product transport includes the construction and operations activities associated with the transport of product jet fuel from the downstream boundary of the CBTL facility to the point of end use. This includes select pipelines and, for sensitivity analysis, trucks used for the transport of blended jet fuel. Within this study, PT also includes upstream emissions associated with the production and transport of conventional petroleum jet fuel, which is blended with F-T jet fuel within this life cycle stage.

End Use (EU): End use includes the construction and operation of a jet airplane, which consumes blended jet fuel produced within the scope of the LCA.

Additional details on the specific assumptions and background data for each of the major processes can be found in the reports that NETL has prepared for CCAT (NETL, 2014a, 2015a, 2015b).

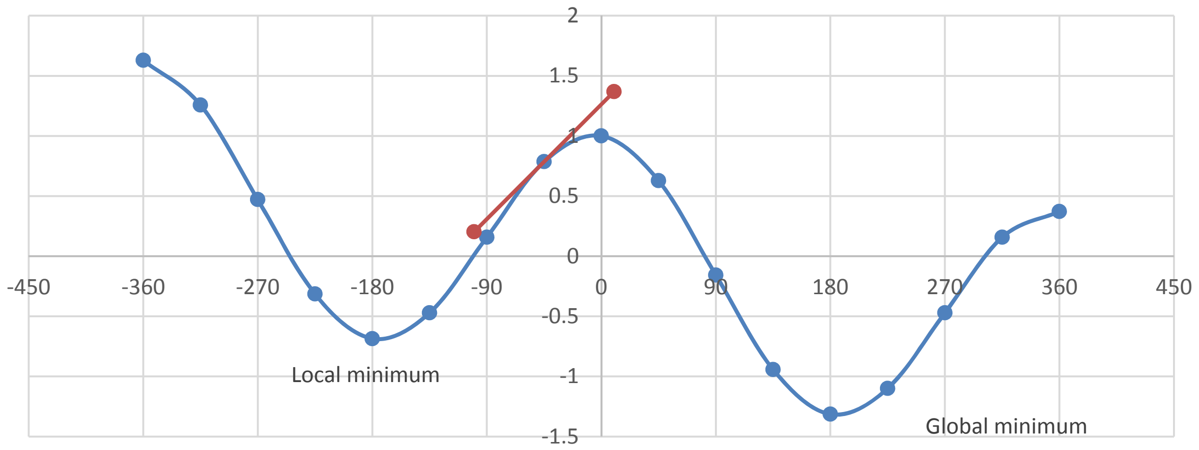
3.6 Optimization

The optimization algorithm used in this tool is the Microsoft Solver. It is the add-in comes with Excel (It might need manual activation). The tool's default solver engine uses the GRG Nonlinear method, which was developed by Leon Lasdon, of the University of Texas at Austin, and Allan Waren, of Cleveland State University.

The algorithm picks a set of trail input values (i.e., adjustable cells) and evaluates the results based on the constraints (i.e., minimums and maximums) and the target optimum cell (i.e., the target GHG value). Each trial is an iteration. As one can imagine, it will take an extremely long time and will use a lot of computer resources to exhaustively try all possible combinations in the variable space, especially when there are many variables.

To avoid this problem, this algorithm adjusts the input variables based on the trends of the results (i.e., whether it is closer to or further from the target values) for the next iteration. The algorithm measures the result change rate when the input is varied as the first derivative (**Figure 3-7**). When there are multiple variables, the algorithm keeps track of several partial derivatives measuring the rate of change in relation to each of the input values. These partial derivatives form the gradient of the function.

Figure 3-7: Illustration of Gradient, Local Minimum and Global Minimum



The gradients are the key components in guiding the algorithm to select new trial values. They are the clues for the algorithm to determine which and how much a variable should be changed. For example, if the optimum cell is being minimized (**Figure 3-7**) and its partial derivative in relation to one variable is a large negative number, while another partial derivate is near zero. The algorithm will probably change the value of the first variable on the next iteration. In other words, it evaluates the results based on changing variable values and searches along the solution curves.

If the preset iterations are reached and there's still no answer, the solver will still stop to prevent long execution time. It gives a faster convergence than the Evolutionary method. Even though there might be more than one satisfied solution in the solution space, the GRG Nonlinear method will most likely give the same solution due to its searching limitation (i.e., trapped in the local minimum in **Figure 3-7**). The Evolutionary method provides a better chance of escaping the local optimal results to find other solutions but it will take more iterations.

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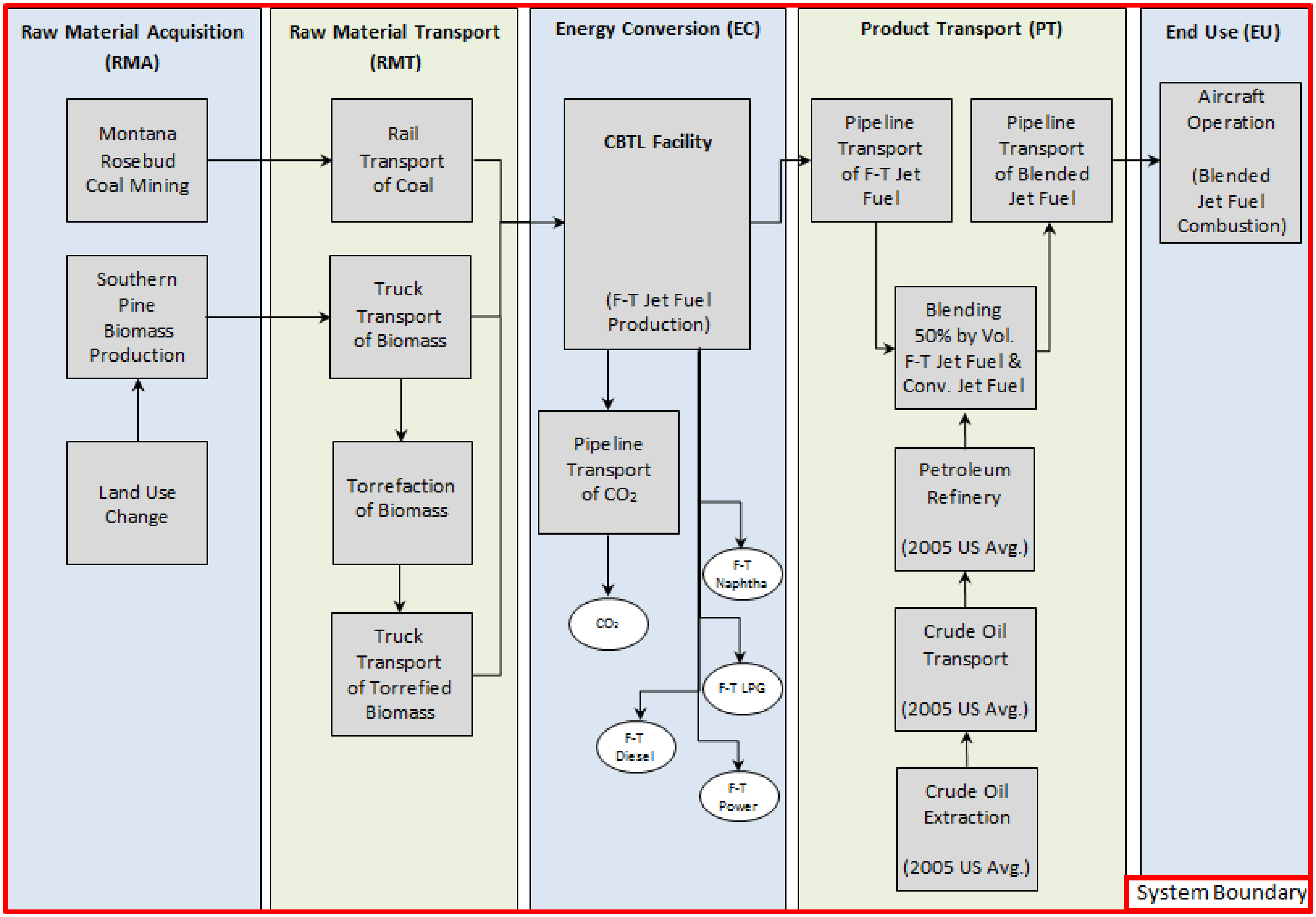
The tool uses the initial minimum and maximum values as constant boundaries during optimization and thus allow each variable to be changed within the provided range. Under the current setting, if users would like to fix a variable, users can make the value, min and max values of the variable to be the same. The algorithm will always use the variable value during the optimization.

Please note that the maximum plant efficiency in the screening mode is formulated to be updated dynamically based on the biomass feed mass percentage and the fraction of vented captured CO_2 (Due to their dependencies). This can cause problems when all three design parameters are optimized at the same time as independent parameters. For example, the algorithm might pick a new biomass feed percentage which decreases the maximum plant efficiency in the process. However, the boundaries of plant efficiency has already been set as constants at the beginning of the optimization and therefore, the algorithm are allowed to select a value that is greater than the current decreased maximum plant efficiency.

To avoid this problem, the tool will find out the reasonable minimum plant efficiency for the selected case and use that as the upper bound (maximum) of the plant efficiency. This ensures that the algorithm will not select a plant efficiency value greater than its maximum value. A reasonable minimum plant efficiency is defined as the minimum value between the settings of 0% and 30% biomass feed percentage with 0% vented captured CO_2.

If users would like to change other solver settings, users can adjust the variables, constraints, and solving methods in Solver's dialog menu after first running the optimization through the tool's function. The problem will be kept and be able to access through Excel's Solver menu (Under the DATA tab).

Figure 3-8: Study System Boundary, System Expansion



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