energies

Hybrid Solid Oxide Fuel Cell/Gas Turbine Model Development for Electric Aviation

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Simulation Package

Bryan Research & Engineering's ProMax 5.0 is a chemical process simulation package that was used to model this hybrid SOFC-GT aviation power system. It is built on top of Microsoft Visio and Excel, giving it a familiar user interface and lending to its ease of use. ProMax is typically used in the upstream (production), midstream (gas processing and conditioning, cryogenic separation, etc.), and downstream (crude oil refining) sectors of the oil and gas industry. Within the last two years, BR&E has expanded ProMax's application in Sustainable Hydrogen Technologies and Carbon Capture Storage/Utilization by developing prebuilt models and classes covering steam methane reforming (SMR), water-gas shift (WGS) optimization, CO_2 removal for compression and sequestration, ammonia production, ammonia cracking and membrane separation, and electrolysis with proton exchange membrane (PEM) fuel cells for energy storage. The model outlined below contains the first SOFC model built in ProMax, to date.

Detailed Model Development

1. Top Level Inputs and Key Features

The first top level inputs needed are the Equation of State (EOS) and component definitions. These are specified in the "Active Environment" window found in the "General" section within the ProMax tab.

While a large selection of general and specialized EOSs are available, the main two options for this type of model are either **Peng-Robinson** or **SRK**.

Once the EOS is defined, the user clicks into the "Components" tab in the same window to specify the chemical species used in the model.

Table S1. Top level inputs.

Parameter	Value
Equation of State	Peng-Robinson
Chemical Components	n-Dodecane (simple jet fuel surrogate) CH_4; H_2; CO (fuel reforming products) CO_2; H_2O (SOFC and combustion products) O_2; N_2 (simplified air surrogate)

Jet fuels are typically made from mixtures of 40+ hydrocarbon components that combine to produce fuel with desired C:H ratios and LHV-values. Jet-A, for instance, has a large subset of hydrocarbon components that produce a C:H ratio of 12:23 and typically has an LHV of 18,500 Btu/lb [43,031 kJ/kg]. Simplified jet fuel surrogate streams can be created by mixing hydrocarbons together and using "Simple Solvers" to vary composition/component flow rates until a desired C:H and LHV combination are achieved. These solvers can be added to virtually any process stream value and serve as a key feature in this model.

To add a solver, right click on any input value within a process stream and choose the "Create Simple Solver…" option. The user then paths in variables needed and writes in the function ProMax will use to close in on the necessary value. See the following example where a solver was used to change the molar flowrate of the "m-Xylene" process stream until the resultant jet fuel stream has the 12:23 ratio required of Jet-A.

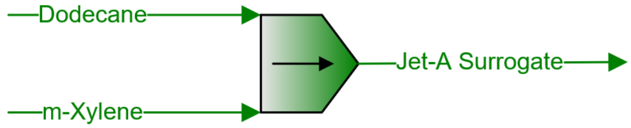


Figure S1. ProMax process stream setup for Jet-A Surrogate model.

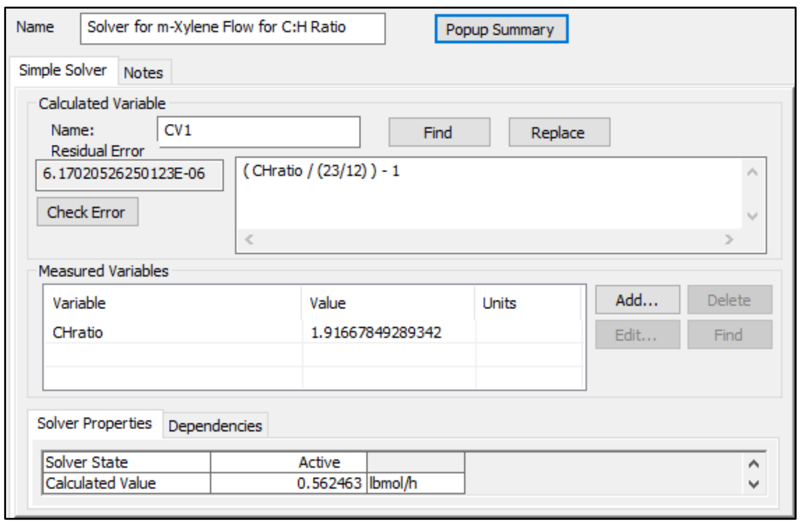


Figure S2. ProMax Simple Solver window with user-defined equation for C:H ratio.

This solver was used in tandem with Promax's scenario tool to analyze LHV values when various BTEX components were mixed into a 1 mol/s n-Dodecane stream while achieving the targeted 12:23 Jet-A ratio. The results were as follows:

Table S2. Jet-A Surrogate candidates.

BTEX Component	Molar Flowrate (lbmol/hr)	LHV (Btu/lb)
Benzene	0.5453	18,621.5
Toluene	0.5538	18,607.5
Ethylbenzene	0.5624	18,607.7
o-Xylene	0.5624	18,594.9
m-Xylene	**0.5624**	**18,546.4**
p-Xylene	0.5624	18,547.9

Here, ProMax solver identified the molar ratio of n-dodecane and m-xylene to act as a Jet-A surrogate that meets the C:H specifications with a slightly elevated LHV. A third hydrocarbon component could be added to the model with cascading solvers to close in on the exact LHV without changing the C:H ratio. Examples like this show how and why ProMax solvers are integral to the simulation environment.

2. Hybrid SOFC/GT Flowsheet and Unit Specifications

When building out a process in ProMax, users can opt to input required process stream properties and unit operation values as each stream and block are added, or they can specify values once the entire flowsheet is built. In either case, the following highlights the values and specifications for each unit included in this model.

Process Inputs

Fuel Feed:

- For model simplification, pure n-dodecane was used as the jet fuel surrogate in this study. This made is easier to validate the jet fuel steam reformer as n-dodecane reforming has been cited in open literature.
- Temperature = 25°C
- Pressure should be set to match what the reformer and SOFC are operating at. For aerospace modeling, the operating pressure range is defined by current altitude and the air compression ratio.

This pressure should not prove critical since a physical system would likely use an atomizer to efficiently disperse fuel into the reformer. This fact combined with the small mass flow rates meant model pressures simply needed to be high enough to not drop the pressure of the recycled anode gas.

- A solver was used to change the fuel flow rate to achieve the desired fuel utilization (U_f) in the SOFC based on Eq[14] from the main text.

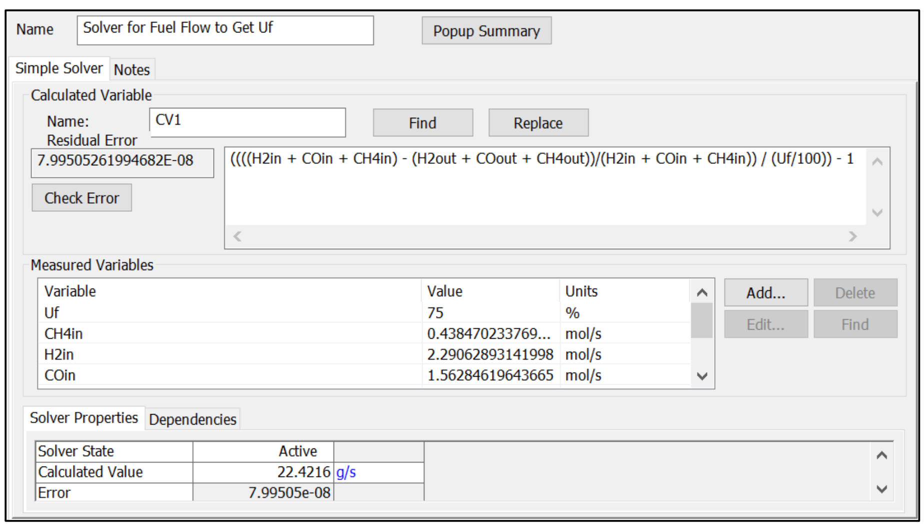


Figure S3. Fuel Feed solver used to achieve specified U_f – 'in' vs 'out' is relative to SOFC reactor.

Steam:

- This stream was only used to initially charge the system with the water required in the reforming process. There is more than enough steam produced in the SOFC anode for n-dodecane reforming, so recycling enough of the anode exhaust allows users to zero-out this process stream.
- Temperature was arbitrary and was set to 700°C to ensure 100% vapor when first getting the simulation to converge.
- Pressure was set to reflect what the reformer was operating at for initial runs.
- A solver was used at startup to target a specific O:C ratio in the reformer. An O:C operating range of 1.8 – 3.0 was chosen based on results from literature. This solver was set to "Disabled" after initial convergence.

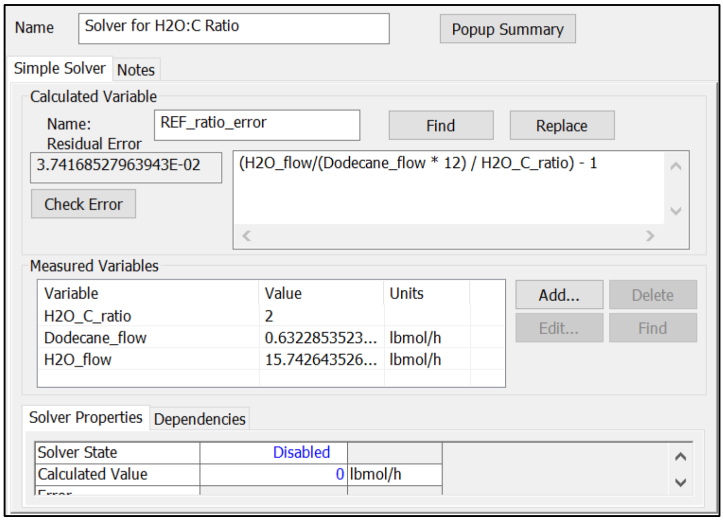


Figure S4. Steam solver used to get a first pass model convergence within desired O:C range.

<u>Outside Air:</u>

- A simplified air composition of 79 mol% N_2 and 21 mol% O_2 was used.
- Temperature and pressure of this stream was set to reflect ambient conditions for commercial aircraft flight path altitudes. The data shown in this paper was based on a 36,000′ – cruise altitude – condition.

Table S3. Ambient air conditions as a function of altitude.

Altitude (ft)	Temperature (°C)	psia	atm
0	15	14.7	1.00
8,000	-0.8	10.92	0.74
30,000	-44.4	4.364	0.30
36,000	-56.3	3.297	0.22
42,000	-56.5	2.471	0.17

- A solver was used to change the air flow rate needed to achieve an SOFC current density of 1.25 A/cm^2 (1,250 mA/cm^2) for all runs.

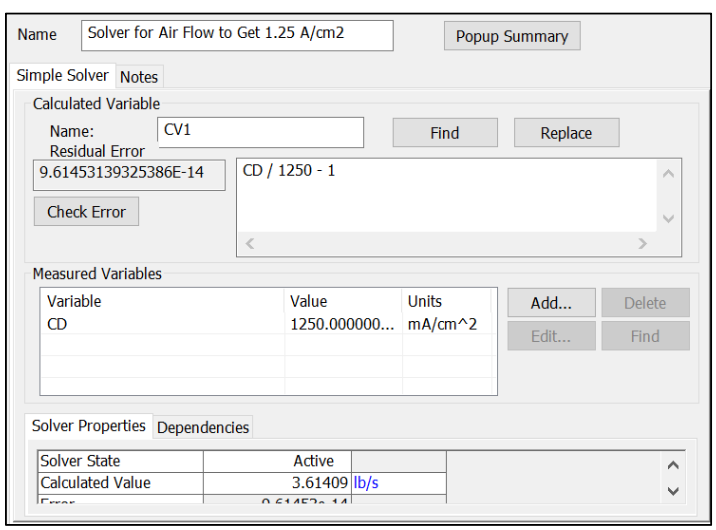


Figure S5. Outside Air solver used to get flow rate required for target SOFC current density.

Fuel Spray:

- This process stream was included to provide additional chemical energy upstream of the combustor for two main purposes: 1) many turbines have turbine inlet temperature (TIT) requirements for efficient operation and 2) there must be sufficient energy remaining in the process stream after expansion to satisfy the Second Law of Thermodynamics in the cathode air heat exchanger.

It should be noted that any amount of additional fuel requirement drastically decreases total system efficiency.

- Temperature and pressure were set to reflect the Fuel Feed stream properties since it would be drawn from the same fuel tank.
- A solver was used to change this flowrate to meet either a desired TIT or TET (turbine exit temperature).

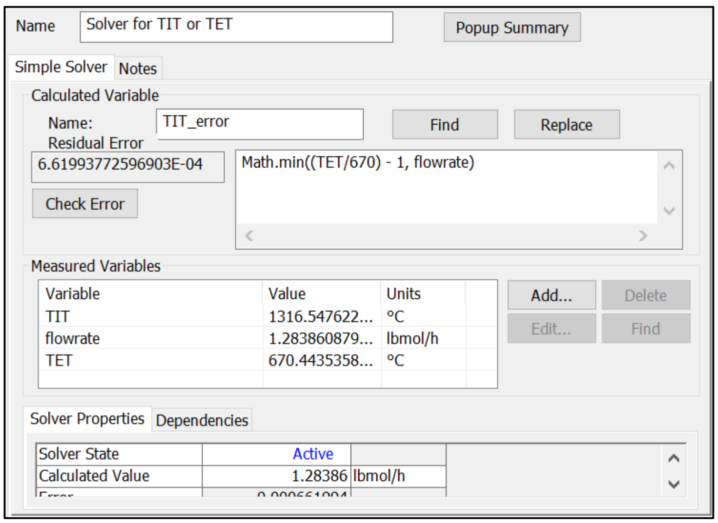


Figure S6. Fuel Spray solver used to get flow rate required for target TIT or TET.

ProMax Blocks (Units)

External Reformer (C12 REF):

- Reactor type = Gibbs Minimization
- Gibbs Set = General
- Pressure Drop = 0 psi
- Temp Change = 0 °C
- Linear Constraint set on "Dodecane" with a Change of 0.01

This limited the n-dodecane conversion to 99%. Literature did reference conditions in which 100% conversion was achieved in steam reforming, but we did not want to make that assumption in this study.

If a multi-component jet fuel surrogate was used, a method would need to be used to limit the combined conversion of all sub-components to the 99% set for n-dodecane.

SOFC:

- Reactor type = Gibbs Minimization
- Gibbs Set = General
- Pressure Drop = 0 psi
- Temp Change – the average operating SOFC temperature is set on the stream leaving the reactor block (800°C for the case shown), therefore the temperature change field is not accessible in this reactor block once that specification was set.

- Linear Constraint set on "O2" with a Simple Specifier set in the Change field.

Simple Specifiers are like Solvers, but they do not rely on methods to converge on a value. They reference static values and use equations to immediately determine and assign a value.

This Specifier uses the desired air utilization user-value to set the O2 conversion in the SOFC.

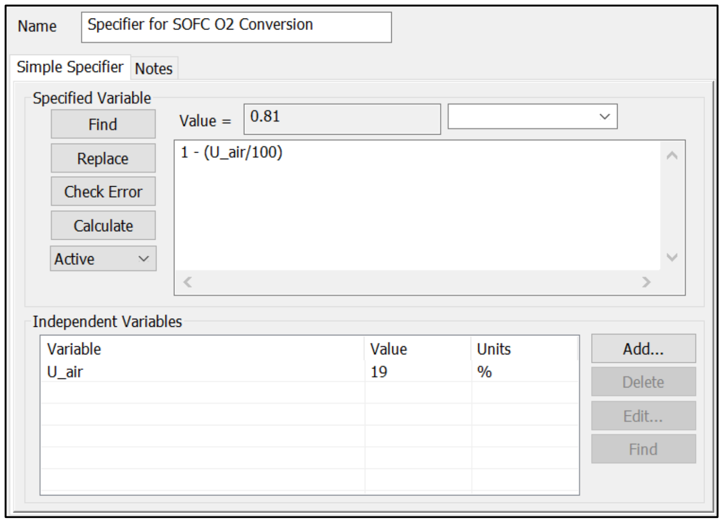


Figure S7. Oxygen Conversion specifier used to operate the SOFC at the desired air utilization.

<u>Combustor:</u>

- Reactor Type = Gibbs Minimization
- Gibbs Set = Burner
- Pressure Drop = 0 psi
- By not connecting an energy stream to the combustor, ProMax assumes it will operate in an adiabatic setting and convert all exothermic energy to sensible heat, increasing the temperature of the outlet process stream.
- Combustion analyses on the Fuel Spray and unrecycled anode exhaust (stream 2) showed an average of 3x the required O_2 for complete combustion depending on the U_f and U_{air}.

It is possible this ratio of air to combustible fuel causes a dilution and therefore hinds combustion, but the reported simulation assumed this was not the case.

<u>Turbine:</u>

- Adiabatic efficiency set to 81%.

This value came from the assumption that there would be two sets of blades in series – high and low pressure – each with efficiencies of 90%.

- TIT and TET could either float if a specific simulation case proved to have enough energy leaving the turbine – again, ensuring the 2nd Law of Thermodynamics is not violated in the CAHx – or they were controlled by the Fuel Spray flow solver.
- Exit pressure was back calculated from the plane exhaust and therefore becomes a function of ambient air pressure at a given altitude, condenser dP, and CAHx dP.

<u>Compressor:</u>

- Adiabatic efficiency set to 90%.
- Compression ratio would be static across the flight envelope.

For sensitivity and performance analyses, outlet pressure can be varied to see the effect that operating pressure has on the entire system.

Compression ratio should remain the same when comparing one altitude to another. We set the compression ratio to 16 when comparing cases.

- Air mass flow rate through the compressor increases as altitude decreases since there is an inverse relationship between altitude and ambient air density.

Turbogenerator:

- This was an empty box on the flowsheet to provide a visual with the calculations performed in a User Value Set in the background.
- Turbine Duty (kW) were subtracted from Compressor Duty (kW) to get Net Available Power (kW). This was then multiplied by a generator efficiency to get the Turbogenerator electricity production (kW).
- Turbogenerator Efficiency set to 90% for all runs.

Heat Exchangers:

- CAHx

Double-sided heat exchanger with 3% dP on each process stream.

Used to preheat the Cathode Air to within a 250 – 50°C dT vs the specified SOFC operating temperature.

20°C Minimum End Approach Temperature on hot inlet vs cold outlet was used as a lowest acceptable case for plausible designs.

- HX1

Single-sided heat exchanger with 5% dP to simulate SOFC cathode pressure drop.

Used to convert SOFC Heat Generation to sensible heat added to the SOFC exhaust.

SOFC Heat Generation is the difference between the SOFC Duty and SOFC Power with 10% loss to environment assumption.

- REF Heat

Single-sided heat exchanger with a 3% dP.

Used to provide heat needed in the endothermic n-dodecane reforming process.

- CNDSR

Doubled-sided heat exchanger with 3% dP on each process stream.

Special consideration needed to ensure H2O Recovery stream operates above the ice formation temperature.

Water Recovery:

- CNDSR heat exchanger combined with a 0 dP Flash unit to condense and separate water out of the plane exhaust.
- H2O Recovery stream temperature should change with altitude to ensure operation above ice formation temperature.

"Degrees above Solids (Ice) Formation" can be calculated with the "Freeze Out, Hydrate, H2O Dew Point" analysis in the Analyses tab within the H2O Recovery process stream.

- H2O Recovery pressure set to reflect ambient air pressures as a function of altitude, shown in Table S3.

3. ProMax User Value Sets

User Value Sets (UVSs) are generatable groups within which users can define properties or variables not available in ProMax. User values are commonly used in a few ways: 1) can be referenced by Simple Specifiers/Solvers in the flowsheet for a variety of reason (e.g. converging on process targets, setting multiple streams to the temperature/pressure, etc.), 2) can pull values from the flowsheet to perform background calculations, and 3) to display process data in flowsheet property tables through the moniker builder. This model contained 5 UVSs in which all three of these functions were leveraged to create a user-friendly interface.

Process Values UVS:

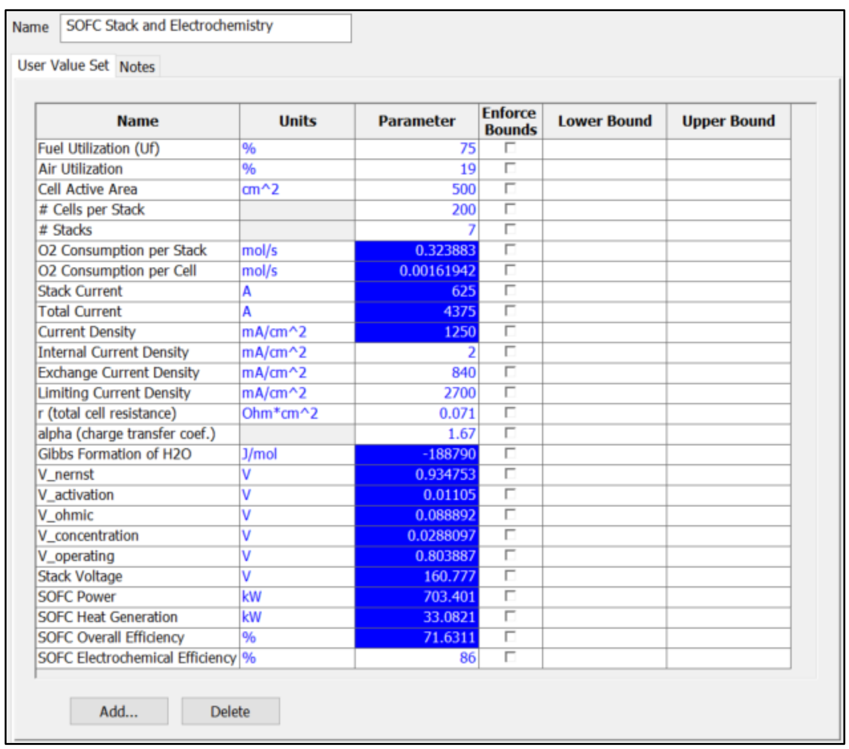
- Reformer O:C Target used by the Steam process stream during startup and initial convergence.
- Reformer O:C used a Simple Specifier to pull in and display the actual O:C ratio at the end of each converged simulation.
- Cathode dP used to set the HX1 dP to 5%.
- Heat Exchanger dPs used to set all other heat exchangers dPs to 3%.
- Thermal Losses to Environment used to derate the sensible heat added to the cathode exhaust in HX1 by 10%.

SOFC Conversions UVS:

- CH4 Conversion used Simple Specifier to display CH4 single-pass conversion.
- H2 Conversion used Simple Specifier to display H2 single-pass conversion.
- CO Conversion used Simple Specifier to display CO single-pass conversion.
- Air Utilization used Simple Specifier to display achieved U_{air}.
- Fuel Utilization used Simple Specifier to display achieved U_f.

SOFC Stack and Electrochemistry UVS:

This UVS was too extensive to list out all values and info. It contained the U_f and U_{air} targets, physical SOFC stack sizes and configurations, internal electrochemical static values, voltage and current calculations, and stack power and efficiency calculations.



Name: SOFC Stack and Electrochemistry

User Value Set | Notes

Name	Units	Parameter	Enforce Bounds	Lower Bound	Upper Bound
Fuel Utilization (Uf)	%	75			
Air Utilization	%	19			
Cell Active Area	cm^2	500			
# Cells per Stack		200			
# Stacks		7			
O2 Consumption per Stack	mol/s	0.323883			
O2 Consumption per Cell	mol/s	0.00161942			
Stack Current	A	625			
Total Current	A	4375			
Current Density	mA/cm^2	1250			
Internal Current Density	mA/cm^2	2			
Exchange Current Density	mA/cm^2	840			
Limiting Current Density	mA/cm^2	2700			
r (total cell resistance)	Ohm*cm^2	0.071			
alpha (charge transfer coef.)		1.67			
Gibbs Formation of H2O	J/mol	-188790			
V_nernst	V	0.934753			
V_activation	V	0.01105			
V_ohmic	V	0.088892			
V_concentration	V	0.0288097			
V_operating	V	0.803887			
Stack Voltage	V	160.777			
SOFC Power	kW	703.401			
SOFC Heat Generation	kW	33.0821			
SOFC Overall Efficiency	%	71.6311			
SOFC Electrochemical Efficiency	%	86			

Add... | Delete

Figure S8. SOFC Stack and Electrochemistry UVS; blue cells contain Simple Specifiers for background calculations.

Turbomachinery Calculations UVS:

- Turbogenerator Efficiency set to 90% and used to calculate generator electricity.

- Turbine Power Generated used Simple Specifier to pull in TRBN Duty.
- Compressor Power Consumed used Simple Specifier to pull in COMP Duty.
- Available Power used Simple Specifier to calculate difference between turbine and compressor powers.
- Turbogenerator Power used Simple Specifier to calculate electricity multiplying available power to turbogenerator efficiency.

System Power and Efficiency UVS:

- Hybrid System Power used Simple Specifier to calculate combine generated electricity.
- Hybrid System Efficiency used Simple Specifier to calculate combined system efficiency based on generated electricity and total chemical energy added to the system.

Table S4. ProMax n-Dodecane External Reformer and SOFC inlet and outlet process streams.

ProMax Process Stream Values

Process Streams		**REFin**	**SynGas**	**Cathode Air**	**Anode**	**Cath Ex**
Composition	**Status:**	**Solved**	**Solved**	**Solved**	**Solved**	**Solved**
Phase: **Total**	**From Block:**	**MIX-100**	**C12 REF**	**CAHX**	**Div-1**	**HX1**
	To Block:	**C12 REF**	**MIX-101**	**MIX-101**	**Recycle Split**	**MIX-102**
Mole Fraction		**%**	**%**	**%**	**%**	**%**
Dodecane		1.7017	0.0136	0*	0.0121	0
CH4		0.0001	6.3143	0*	0.0001	0
H2		8.6650	22.7928	0*	8.8078	0
CO		6.4066	14.0291	0*	6.5119	0
CO2		40.7766	33.7118	0*	41.4823	0
H2O		42.4500	23.1384	0*	43.1858	0
O2		0	0	21*	0	16.6227
N2		0	0	79*	0	83.3773
Molar Flow		**lbmol/h**	**lbmol/h**	**lbmol/h**	**lbmol/h**	**lbmol/h**
Dodecane		0.9392	0.0094	0*	0.0094	0
CH4		0.0001	4.3453	0*	0.0001	0
H2		4.7824	15.6852	0*	6.8266	0
CO		3.5359	9.6543	0*	5.0472	0
CO2		22.5055	23.1993	0*	32.1516	0
H2O		23.4291	15.9230	0*	33.4720	0
O2		0	0	61.6931*	0	46.2698
N2		0	0	232.084*	0	232.084
Properties						
	Units					
Temperature	°F	1148.86	1148.86	1202*	1382	1510.38
Pressure	psig	29.3919	29.3919	31.6330*	29.3919	29.3166*
Mole Fraction Vapor	%	100	100	100	100	100
Mole Fraction Light Liquid	%	0	0	0	0	0
Molecular Weight	lb/lbmol	30.4608	24.4301	28.8503	28.0584	28.6759
Mass Density	lb/ft^3	0.0777881	0.0623630	0.0748829	0.0625761	0.0596508
Molar Flow	lbmol/h	55.1921	68.8165	293.777	77.5070	278.353
Mass Flow	lb/h	1681.19	1681.19	8475.56	2174.72	7982.03
Vapor Volumetric Flow	ft^3/h	21612.5	26958.2	113184	34753.2	133813
Liquid Volumetric Flow	gpm	2694.54	3361.02	14111.3	4332.87	16683.1
Std Vapor Volumetric Flow	MMSCFD	0.502668	0.626754	2.67561	0.705904	2.53514
Std Liquid Volumetric Flow	sgpm	4.21232	5.11225	19.5623	5.41508	18.6986
Compressibility		1.00013	1.00052	1.00095	1.00023	1.00077
Specific Gravity		1.05173	0.843508	0.996127	0.968783	0.990104
Enthalpy	Btu/h	-5.867E+06	-5.503E+06	2.424E+06	-8.180E+06	2.970E+06
Mass Enthalpy	Btu/lb	-3489.72	-3273.06	286.019	-3761.55	372.083
Mass Cp	Btu/(lb*°F)	0.420278	0.419152	0.270519	0.388689	0.279584
Ideal Gas CpCv Ratio		1.18385	1.24080	1.34136	1.22282	1.32927
Dynamic Viscosity	cP	0.0357026	0.0359852	0.0390885	0.0409182	0.0432815
Kinematic Viscosity	cSt	28.6527	36.0227	32.5871	40.8214	45.2966
Thermal Conductivity	Btu/(h*ft*°F)	0.0454580	0.0619019	0.0366208	0.0531900	0.0418510
Net Ideal Gas Heating Value	Btu/ft^3	190.321	165.986	0	46.0361	0
Net Liquid Heating Value	Btu/lb	2045.76	2351.91	0	279.959	0

Gross Ideal Gas Heating Value	Btu/ft^3	227.158	195.533	0	72.2725	0
Gross Liquid Heating Value	Btu/lb	2504.77	2810.88	0	634.801	0