Mathematical Analysis of High-Temperature Co-Electrolysis of CO2 and O2 Production in a Closed-Loop Atmosphere Revitalization System

Michael G. McKellar Manohar S. Sohal Carl M. Stoots Lila Mulloth Bernadette Luna Morgan B. Abney

March 2010



The INL is a U.S. Department of Energy National Laboratory operated by Battelle Energy Alliance

DISCLAIMER

This information was prepared as an account of work sponsored by an agency of the U.S. Government. Neither the U.S. Government nor any agency thereof, nor any of their employees, makes any warranty, expressed or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness, of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. References herein to any specific commercial product, process, or service by trade name, trade mark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the U.S. Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the U.S. Government or any agency thereof.

Mathematical Analysis of High-Temperature Coelectrolysis of CO2 and O2 Production in a Closed-Loop Atmosphere Revitalization System

Michael G. McKellar Manohar S. Sohal Carl M. Stoots Idaho National Laboratory

Lila Mulloth
Bernadette Luna
NASA Ames Research Center

Morgan B. Abney
NASA Marshall Space Flight Center

March 2010

Idaho National Laboratory
High Temperature Electrolysis
Idaho Falls, Idaho 83415

http://www.inl.gov

Prepared for the
National Aeronautics and Space Administration
Under DOE Idaho Operations Office
Contract DE-AC07-05ID14517

High Temperature Electrolysis

Mathematical Analysis of High-Temperature Co-electrolysis of CO₂ and O₂ Production in a Closed-Loop Atmosphere Revitalization System

INL/EXT-10-19726

March 2010

Approved by:	
Mulad S. M. Kella	8/30/10
Michael G. McKellar	Date
Author	8/30/10
Carl M. Stoots	Date
Reviewer for J. Herring	0. /2 /
(c) 11(g)	8/30/10
J. Stephen Herring	Date
Approver	

SUMMARY

NASA has been evaluating two closed-loop atmosphere revitalization architectures based on Sabatier and Bosch carbon dioxide, CO₂, reduction technologies. The CO₂ and steam, H₂O, co-electrolysis process is another option that NASA has investigated. Utilizing recent advances in the fuel cell technology sector, the Idaho National Laboratory, INL, has developed a CO₂ and H₂O co-electrolysis process to produce oxygen and syngas (carbon monoxide, CO and hydrogen, H₂ mixture) for terrestrial (energy production) application. The technology is a combined process that involves steam electrolysis, CO₂ electrolysis, and the reverse water gas shift (RWGS) reaction. A number of process models have been developed and analyzed to determine the theoretical power required to recover oxygen, O₂, in each case. These models include the current Sabatier and Bosch technologies and combinations of those processes with high-temperature co-electrolysis. The cases of constant CO2 supply and constant O₂ production were evaluated. In addition, a process model of the hydrogenation process with co-electrolysis was developed and compared. Sabatier processes require the least amount of energy input per kg of oxygen produced. If co-electrolysis replaces solid polymer electrolyte (SPE) electrolysis within the Sabatier architecture, the power requirement is reduced by over 10%, but only if heat recuperation is used. Sabatier processes, however, require external water to achieve the lower power results. Under conditions of constant incoming carbon dioxide flow, the Sabatier architectures require more power than the other architectures. The Bosch, Boudouard with co-electrolysis, and the hydrogenation with co-electrolysis processes require little or no external water. The Bosch and hydrogenation processes produce water within their reactors, which aids in reducing the power requirement for electrolysis. The Boudouard with co-electrolysis process has a higher electrolysis power requirement because carbon dioxide is split instead of water, which has a lower heat of formation. Hydrogenation with co-electrolysis offers the best overall power performance for two reasons: it requires no external water, and it produces its own water, which reduces the power requirement for co-electrolysis.

CONTENTS

SUN	MAR	Y		vi
1.	INT	RODUC	CTION	1
2.	PRO	CESS N	MODELS	3
	2.1	Bosch	Process Models	3
	2.2	Sabati	ier Process Model	7
	2.3		ectrolysis Integrated Process Models 1-D Co-Electrolysis Model Implementation of Co-Electrolysis Model into HYSYS Sabatier Process with Co-Electrolysis Boudouard Process with Co-electrolysis Hydrogenation process with co-electrolysis	
		2.3.3	Try drogonation process with or crossory is	1
3.	RES	ULTS		18
	3.1	Oxyge	en Production at 1 kg/day	18
	3.2	Proces	ssing Carbon Dioxide at 1 kg/day	21
	3.3	Carbo	on Balance	23
4.	SOL	ID OXI	DE CELLS	24
	4.1	Solid	Oxide Cell Components	24
	4.2	Possib	ole Causes of Degradation in SOEC	26
		4.2.1	SOEC versus SOFC Stacks	
		4.2.2	Air/Oxygen Electrode	
		4.2.3	Air/O ₂ -Electrode Side Bond Layer	
		4.2.4	Electrolyte	
		4.2.5 4.2.6	Steam/H ₂ -Electrode	
		4.2.7	Interconnect	
		4.2.7	Summary of Stack Degradation	
		4.2.9	Degradation Measurements	
5.	CON	ICLUSI	ONS AND RECOMMENDATIONS	31
6.	REF	ERENC	CES	32
App	endix A	A Kaw l	Process Model Data	A-1

FIGURES

Figure 1	Sabatier process for atmosphere revitalization	l
Figure 2	Bosch process for atmosphere revitalization	1
Figure 3	Co-electrolysis process for atmosphere revitalization	2
Figure 4	Currently considered CO2 reduction process for closed-loop life support, by NASA	3
Figure 5	Process flow diagram of Bosch process	5
Figure 6	Process flow diagram of Bosch reactor	5
Figure 7	Process flow diagram of electrolysis module	6
Figure 8	Process flow diagram of Bosch process at sub-atmospheric conditions	6
Figure 9	Process flow diagram of Bosch process with single compressor	7
Figure 10	Process flow diagram of base Sabatier process	8
Figure 11	Process flow diagram external to the electrolysis module	12
Figure 12	Process flow diagram for electrolysis module	13
Figure 13	Process flow diagram of Sabatier process with co-electrolysis	15
Figure 14	Process flow diagram of Sabatier process with co-electrolysis without heat recuperation	16
Figure 15	Process flow diagram of Boudouard process with co-electrolysis	17
Figure 16	Process flow diagram of hydrogenation process with co-electrolysis	18
Figure 17	(a) Solid oxide electrolysis cell (SOEC); (b) solid oxide fuel cell (SOFC) operating in reverse compared to an SOEC [Guan, et al. 2006]	25
Figure 18	Ceramatec solid oxide cell/stack construction; (scanning electron microscopy figure on the right taken from Carter et al. 2008)	25
Figure 19	Area-specific resistance of a 25-cell stack as a function of time for a 1,000-hour test [O'Brien et al. 2007]	30
Figure 20	Hydrogen production rates during 1,000-hour long-term test [O'Brien et al. 2007]	30
	TABLES	
Table 1	Results for the production of 1 kg/day of oxygen	19
Table 2	Equipment for the production of 1 kg/day of oxygen, part 1	20
Table 3	Equipment for the production of 1 kg/day of oxygen, part 2	21
Table 4	Results for the processing of 1 kg/day of carbon dioxide	22
Table 5	Equipment for the processing of 1 kg/day of carbon dioxide, part 1	22
Table 6	Equipment for the processing of 1 kg/day of carbon dioxide, part 2	23
Table 7	Carbon balance for producing 1 kg/day of oxygen	24
Table 8	Carbon balance for processing 1 kg/day of carbon dioxide	
Table 9	Commonly used materials in SOFC/SOEC [Gazzari 2007]	26



Mathematical Analysis of High-Temperature Coelectrolysis of CO2 and O2 Production in a Closed-Loop Atmosphere Revitalization System

1. INTRODUCTION

NASA has been evaluating mainly two closed-loop atmosphere revitalization architectures based on Sabatier and Bosch CO₂ reduction technologies. Schematics of the Sabatier and Bosch concepts are shown in Figures 1 and 2 respectively.

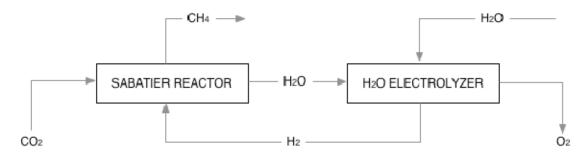


Figure 1 Sabatier process for atmosphere revitalization

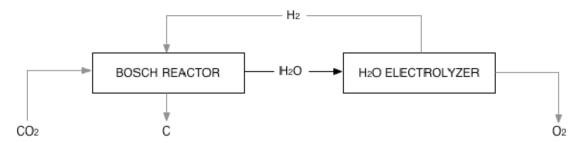


Figure 2 Bosch process for atmosphere revitalization

The CO2 and H2O co-electrolysis process is another option that NASA has investigated in the past. [1] Utilizing recent advances in the fuel cell technology sector, INL has developed a CO2 and H2O co-electrolysis process to produce oxygen and syngas (CO and H2 mixture) for terrestrial (energy production) application. The technology is a combined process that involves steam electrolysis, CO2 electrolysis, and the reverse water gas shift (RWGS) reaction. INL has also built and tested an inline methanation reactor to study direct methanation of co-electrolysis products. Schematic of the CO2 and H2O co-electrolysis concept in conjunction with the methanation reactor is shown in Figure 3.

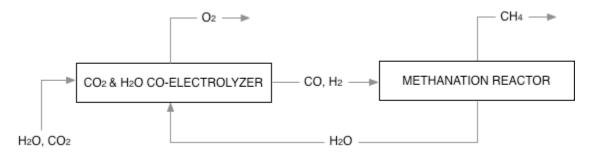


Figure 3 Co-electrolysis process for atmosphere revitalization

The co-electrolysis and methanation processes process have potential, direct application in development of NASA's future human and robotic missions. Co-electrolysis has a significant advantage over separate electrolysis of H2O and CO2 in terms of electrical efficiency. Compared to pure CO2 electrolysis, co-electrolysis using a solid-oxide cell utilizes considerably less electrical energy (only as much as the H2O electrolysis alone) since the CO production in co-electrolysis occurs mainly due to RWGS. The Bosch process offers complete loop closure in terms of water recovery. However, the low-efficiency process (approximately 10% conversion per pass) and the need for solid carbon handling add complications to the process implementation in a space environment.

The Sabatier and co-electrolysis processes are more efficient and manageable in a space cabin, but bring the disadvantage of partial loop closure since additional water supply is needed to compensate for hydrogen loss as methane, CH₄. The extent of loop closure can be increased if the byproducts of Sabatier and co-electrolysis processes, methane or syngas, can be utilized by power-generation systems within or external to the life support architecture in exchange for the products of combustion (water and CO₂). A mathematical analysis is being performed under this project to evaluate INL's co-electrolysis process as a CO₂ reduction option in NASA's atmosphere revitalization scheme in comparison to Sabatier and Bosch processes.

The results of a mathematical analysis are presented in this report to evaluate INL's co-electrolysis process as a CO₂ reduction option in NASA's atmosphere revitalization scheme in comparison to Sabatier and Bosch processes.

In a potential, closed-loop atmosphere revitalization architecture, the co-electrolysis unit will receive compressed CO₂ from a compressor. One example of NASA's potential atmosphere revitalization architecture is shown in Figure 4.

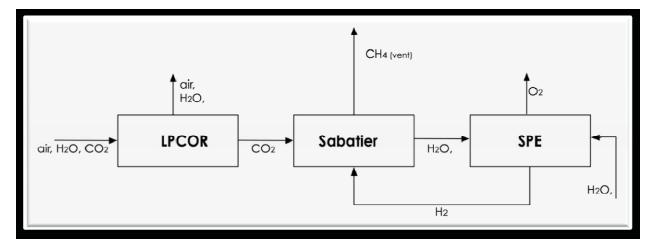


Figure 4 Currently considered CO2 reduction process for closed-loop life support, by NASA

The metabolic CO₂ from the cabin is removed and compressed using the LPCOR (Low-Power CO₂ Removal) technology and is delivered to a Sabatier reactor. Products of the Sabatier reaction (CH₄ and H₂O) are separated, H₂O is directed to an SPE (solid polymer electrolyte) water electrolysis unit, and CH₄ is vented (or stored for fuel). The oxygen from the electrolysis unit is released to the cabin and the H₂ is recycled to the Sabatier reactor.

If the Sabatier and SPE processes are replaced with the CO₂ and H₂O co-electrolysis process in the atmosphere revitalization scheme, additional downstream processors have to be implemented to recover and recycle H₂ from the products of electrolysis. That includes a Sabatier or Bosch reactor to produce and recycle H_2O .

2. PROCESS MODELS

The process models for this mathematical analysis were developed using Hyprotech's HYSYS.Plant v2.2.2 (Build 3806) process modeling software. HYSYS.Plant inherently ensures mass and energy balances across all components and it includes thermodynamic data for all chemical species. The software realistically models components such as pumps, compressors, turbines, and heat exchangers. It also models chemical equilibrium and kinetic reactions. The models described in this report were developed assuming steady state operation with chemical equilibrium reactions.

2.1 Bosch Process Models

The process flow diagram for the traditional Bosch process is shown in Figure 5. Carbon dioxide is compressed to 25 psia, the reaction pressure, and mixed with hydrogen and a recycle stream. The mixed stream is heated through a recuperating heat exchanger to the reaction temperature of 650°C and enters the Bosch reactor. The Bosch reactor is simulated with two reactors, see Figure 6. The first reactor is a Gibbs reactor within which the Gibbs free energy of selected products and reactants are minimized to estimate the most likely equilibrium products composition. The reactants and products that were selected for the Gibbs reactor are water, methane, carbon monoxide, carbon dioxide and hydrogen. The Gibbs reaction is primarily the reverse water gas shift reaction with some methanation.

$$CO_2 + H_2 \leftrightarrow CO + H_2O$$
 (4.2e+4 kJ/kgmole) (1)

$$CO + 3H_2 \leftrightarrow CH_4 + H_2O$$
 (-2.1e+5 kJ/kgmole) (2)

The next reactor is a chemical equilibrium reactor which simulates the Boudouard reaction.

$$2CO \leftrightarrow CO_2 + C$$
 (-8.6e+4 kJ/kgmole) (3)

Tabular chemical equilibrium data were used for this process. The Gibbs reaction is endothermic but the Boudouard reaction is more exothermic resulting in an overall Bosch reaction that is exothermic.

The molar flow of CO into the Bosch reactor was compared to the molar flow of carbon created to determine the % carbon conversion per pass. The approach temperature to the Boudouard reaction was adjusted to artificially limit the % pass conversion to 10% to be consistent with experimental data. Solid carbon and a gas stream exit the Bosch reactor. The gas stream is cooled and preheats the stream into the reactor within the recuperating heat exchanger. The water in the gas stream is condensed by ambient cooling. The water is mixed with a small amount of incoming water and then electrolyzed to produce hydrogen and oxygen. The resulting gas stream exiting the water condenser is recycled with the incoming carbon dioxide and hydrogen streams. This recycle stream is made up of hydrogen, methane, carbon monoxide, carbon dioxide and some water. The ratio of hydrogen to carbon dioxide was set to 2.1 by adjusting the incoming water stream. The composition of the recycle stream was adjusted to provide the recycle flow to combined hydrogen and carbon dioxide flow ratio to nearly 14. The hydrogen to carbon dioxide ratio and recycle flow values were selected based on experimental work performed by NASA.

The SPE electrolysis process is modeled as a conversion reactor that splits 100% of the water coming in based on the following equation, Figure 7.

$$2H_2O \rightarrow 2H_2 + O_2$$
 (2.4e+5 kJ/kgmole) (4)

The HYSYS calculates the power necessary to split the water. A component splitter follows to separate the oxygen from the hydrogen. The electrolysis process conditions are set to near ambient conditions.

Figure 8 is the process flow diagram of a second, slightly modified Bosch process. The Bosch reactor in this case is operated at sub-atmospheric conditions. The electrolysis process is operating at atmospheric conditions. Pumps are used instead of compressors through the process.

The final modification to the basic Bosch process is the replacement of the three compressors with one compressor for a third Bosch process model, illustrated in Figure 9. This version was motivated by a desire to reduce the number of equipment needed.

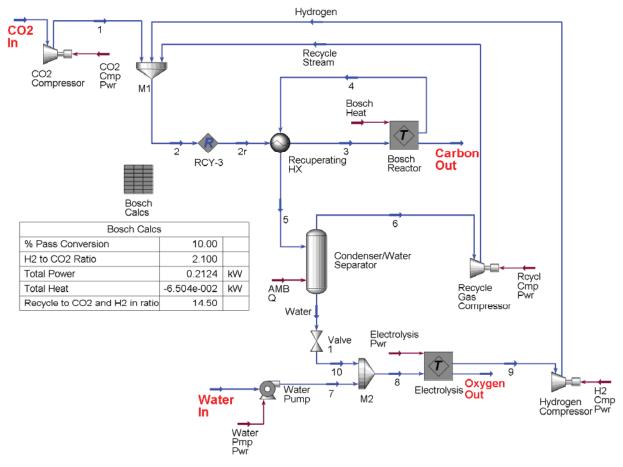


Figure 5 Process flow diagram of Bosch process

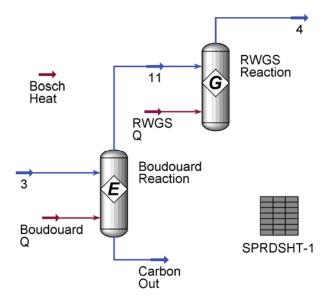


Figure 6 Process flow diagram of Bosch reactor

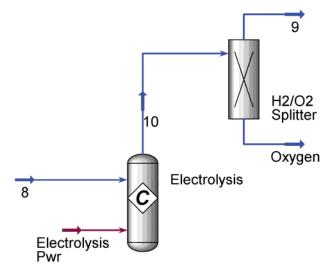


Figure 7 Process flow diagram of electrolysis module

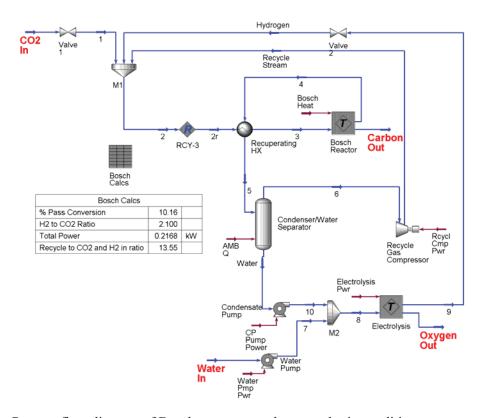


Figure 8 Process flow diagram of Bosch process at sub-atmospheric conditions

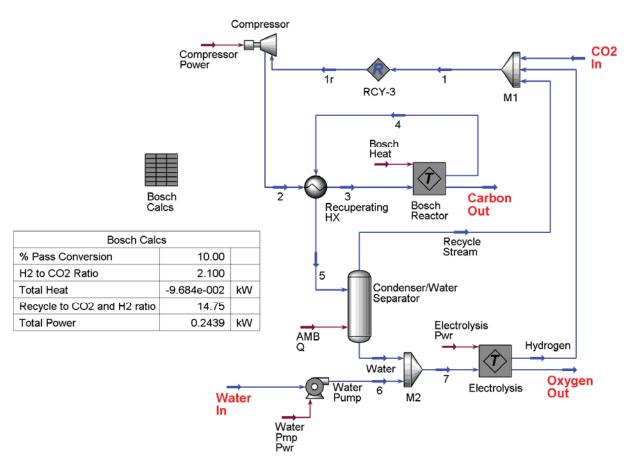


Figure 9 Process flow diagram of Bosch process with single compressor

2.2 Sabatier Process Model

The traditional Sabatier process is shown in Figure 10. In coming carbon dioxide mixes with hydrogen from the electrolysis unit and passes through the Sabatier reactor at the reaction pressure of 11.5 psia. The overall Sabatier reaction is simulated by using two equilibrium reactors, a higher temperature reactor at 565°C and a lower temperature reactor at 240°C. Heat recuperation occurs at the inlet and outlet of the total reactor and between the two equilibrium reactors. The equilibrium reactors calculate the outlet compositions based on the default tabulated methanation data within the HYSYS.Plant software. The outlet stream is cooled and water condensed within the water knockout tank. The condensate is combined with fresh water before passing through the electrolysis process. The condensate contains trace amount of carbon dioxide which will not adversely affect the electrolyzer. The gas stream exiting the water knockout tank is compressed to atmospheric conditions and released. The composition of this stream is primarily methane with some carbon dioxide and water and trace amounts of hydrogen. The Sabatier model uses the same electrolysis model as described in section 2.1. The optimal hydrogen to carbon dioxide ratio has been found to be 3.5; this ratio is set in test operations with the Sabatier reactor. In the model the 3.5:1 ratio was achieved by adjusting the water inlet.

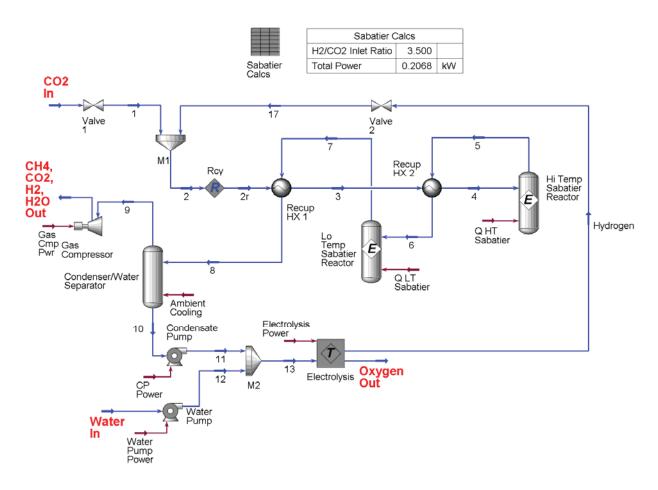


Figure 10 Process flow diagram of base Sabatier process

2.3 Co-Electrolysis Integrated Process Models

2.3.1 1-D Co-Electrolysis Model

Co-electrolysis is a process by which both steam and carbon dioxide may be electrolyzed in a high temperature ~800°C process using solid oxide electrolysis cells. A one-dimensional chemical equilibrium model has been developed for analysis of steam/carbon dioxide co-electrolysis. This model can be used to predict open-cell and operating potentials, electrolyzer outlet compositions, and outlet temperatures for specified inlet gas flow rates, current densities, cell area-specific resistance, and thermal boundary conditions.

The Nernst potential for the co-electrolysis system can be calculated as a function of temperature using the Nernst equation for either steam-hydrogen or for CO₂-CO, provided the equilibrium composition of the components is used in the evaluating the equation. Therefore, prior to applying the Nernst equation, the electrolyzer-inlet equilibrium composition must be determined at the operating temperature. The chemical equilibrium co-electrolysis model determines the equilibrium composition of the system as follows.

The overall water gas shift reaction that occurs during heat-up from the cold unmixed inlet conditions to the hot mixed pre-electrolyzer state can be represented as:

$$y_{0,CO} CO + y_{0,CO2} CO_2 + y_{0,H2} H_2 + y_{0,H2O} H_2O \rightarrow y_{1,CO} CO + y_{1,CO2} CO_2 + y_{1,H2} H_2 + y_{1,H2O} H_2O$$
 (5)

where the $y_{0,j}$ values represent the cold inlet mole fractions of CO, CO₂, H₂, and H₂O, respectively, that are known from specification of the individual component inlet gas flow rates. The unknown equilibrium mole fractions of the four species at the electrolyzer temperature, prior to electrolysis, are represented by the $y_{I,j}$ values. There are three governing chemical balance equations for carbon, hydrogen, and oxygen corresponding to Eqn. (5):

$$y_{0,CO} + y_{0,CO2} = y_{1,CO} + y_{1,CO2}$$
 (6)

$$2y_{0,H2} + 2y_{0,H2O} = 2y_{1,H2} + 2y_{1,H2O}$$
(7)

$$y_{0,CO} + 2y_{0,CO2} + y_{0,H2O} = y_{1,CO} + 2y_{1,CO2} + y_{1,H2O}$$
 (8)

The final equation invokes the equilibrium constant for the shift reaction:

$$K_{eq}(T) = \frac{y_{1,CO2}y_{1,H2}}{y_{1,CO}y_{1,H2O}}$$
(9)

completing a system of four equations and four unknowns. Simultaneous solution of this system of equations yields the hot inlet composition.

Once the hot inlet equilibrium composition is determined, the open-cell Nernst potential can be calculated from:

$$V_{N} = \frac{-\Delta G_{f,H_{2}O}(T)}{2F} - \frac{R_{u}T}{2F} \ln \left[\left(\frac{y_{1,H_{2}O}}{y_{1,H_{2}}y_{o2}^{1/2}} \right) \left(\frac{P}{P_{std}} \right)^{-1/2} \right] = \frac{-\Delta G_{f,CO_{2}}(T)}{2F} - \frac{R_{u}T}{2F} \ln \left[\left(\frac{y_{1,CO_{2}}}{y_{1,CO}y_{o2}^{1/2}} \right) \left(\frac{P}{P_{std}} \right)^{-1/2} \right]$$
(10)

where y_{O2} is the mole fraction of oxygen on the air-sweep side of the cells ($y_{O2} \sim 0.21$). Note that the Nernst equation for either steam-hydrogen or CO₂-CO yields the same result for the equilibrium system. The electrolyzer outlet composition can be determined similarly, after accounting for electrochemical reduction of the system. The chemical balance equation for oxygen must be modified to account for oxygen removal from the CO₂/steam mixture. Accordingly, the oxygen balance equation becomes:

$$y_{1,CO} + 2y_{1,CO2} + y_{1,H2O} = y_{2,CO} + 2y_{2,CO2} + y_{2,H2O} + \Delta n_0$$
 (11)

where Δn_O is the relative molar rate of monatomic oxygen removal from the CO₂/steam mixture given by:

$$\Delta n_O = \frac{I_e}{2F\dot{N}_{Tot}} \tag{12}$$

In this equation, I_e is the total ionic current, $I_e = i \cdot A_{cell} \cdot N_{cells}$, \dot{N}_{Tot} is the total molar flow rate on the CO_2 /steam side, including any inert gas flows, and F is the Faraday number. Finally, using the modified oxygen balance equation, the post-electrolyzer equilibrium composition (state 2) can be determined as a function of temperature from simultaneous solution of three chemical balance equations and the equilibrium constant equation.

In general, the electrolyzer outlet temperature is unknown. The magnitude of any temperature change associated with electrolyzer operation depends both on the operating conditions (operating voltage, inlet composition, gas flow rates, etc.) and on the thermal boundary condition. If the electrolyzer operating voltage is below the thermal neutral voltage, the endothermic reaction heat requirement dominates and the stack will tend to cool off. If the operating voltage is above thermal neutral, ohmic heating dominates and the stack tends to heat up.

If adiabatic electrolyzer operation is assumed, the outlet temperature can be determined as a function of operating voltage from simultaneous solution of the energy equation and the chemical balance and equilibrium constant equations. Alternately, if isothermal operation is assumed, the outlet composition can be determined independently of the energy equation and the heat required to maintain isothermal operation can be calculated as a function of operating voltage.

For pure-steam or pure-CO₂ electrolysis, the thermal neutral voltage is given by

$$V_{m,j}(T) = \frac{\Delta H_{R,j}(T)}{2F} \tag{13}$$

where $\Delta H_{R,j}(T)$ is the enthalpy of reaction for electrolysis of pure component j (H₂O or CO₂) at temperature T. At 800°C, $V_{tmH2O} = 1.29$ V and $V_{tmCO2} = 1.46$ V. For co-electrolysis, the thermal neutral voltage can range anywhere between the respective pure-component values, depending on inlet composition, oxygen utilization, and temperature (via the equilibrium constant, $K_{eq}(T)$). There is no simple explicit relation for the multi-component thermal neutral voltage. In general, the thermal neutral voltage for co-electrolysis will be closer to the pure-steam value if the inlet composition is dominated by steam and hydrogen. Conversely, if the inlet composition is dominated by CO₂ and CO, the co-electrolysis thermal neutral voltage will be closer to the pure-CO₂ value. At an operating temperature of 800°C, with syngas-production-relevant inlet compositions for co-electrolysis (i.e., ~2-to-1 steam/hydrogen vs CO₂), a thermal neutral voltage value of ~1.34 V is typical. The energy equation for the co-electrolysis process can be written as:

$$\dot{Q} - \dot{W} = \sum_{P} \dot{N}_{i} \left[\Delta H_{f_{i}}^{o} + H_{i}(T_{P}) - H_{i}^{o} \right] - \sum_{R} \dot{N}_{i} \left[\Delta H_{f_{i}}^{o} + H_{i}(T_{R}) - H_{i}^{o} \right]$$
(14)

where \dot{Q} is the external heat transfer rate to or from the electrolyzer, \dot{W} is the rate of electrical work supplied to the electrolyzer, \dot{N}_i is the molar flow rate of each reactant or product, $\Delta H_{f_i}^o$ is the standard-state enthalpy of formation of each reactant or product and $H_i(T) - H_i^o$ is the sensible enthalpy for each reactant or product. Applying the energy equation in this form, all reacting and non-reacting species in the inlet and outlet streams are accounted for, including inert gases, process steam, hydrogen (introduced to maintain reducing conditions on the steam/hydrogen electrode), CO_2 , and any excess unreacted process gases.

In general, determination of the outlet temperature from Eqn. (14) is an iterative process. The heat transferred during the process must first be specified (e.g., zero for the adiabatic case). The temperature-dependent enthalpy values of all species must be available from curve fits or some other database. The cathode-side hot electrolyzer-inlet molar composition and flow rates of steam, hydrogen, CO_2 , CO, and any inert carrier gases such as nitrogen (if applicable) have already been determined from specification of the cold inlet flow rates of all components and from Eqns. (6 – 10). The inlet flow rate of the sweep gas (e.g., air or steam) on the anode side must also be specified. At this point, the total electrolyzer-inlet enthalpy given by the second summation on the right-hand side of Eqn. (14) can be evaluated.

The current density, active cell area, and number of cells are then specified, yielding the total ionic current, I_e . Care must be taken to insure that the specified inlet gas flow rates and total ionic current are compatible. The minimum required inlet steam and CO_2 molar flow rates must satisfy the following constraint:

$$\dot{N}_{H_2O} + \dot{N}_{CO_2} \ge \frac{I_e}{2F} \tag{15}$$

to avoid oxygen starvation. Note that the oxygen contribution from the CO_2 is only counted once, since we want to avoid creation of carbon soot, which could foul the cells.

Evaluation of the electrolyzer-outlet total enthalpy, the first summation in Eqn. (14), requires the product temperature, but the product temperature is generally unknown and is determined from solution of the energy equation, so an iterative solution must be applied. The iterative solution process proceeds as follows. Based on a guessed value of electrolyzer outlet temperature, T_P , and the specified current, the electrolyzer outlet composition can be determined as described previously, allowing for evaluation of the total enthalpy of the products.

The remaining term in the energy equation is the electrical work, which is the product of the per-cell operating voltage and the total ionic current. The operating voltage corresponding to the specified current density is obtained from:

$$V_{op} = \overline{V}_N + i \times ASR(T) \tag{16}$$

The stack area-specific resistance, ASR(T), quantifies the loss mechanisms in the operating cell. It must be estimated, based on experimental data or an appropriate model, and specified as a function of temperature. The operating-cell mean Nernst potential, \overline{V}_N , accounting for the variation of gas composition and temperature across the operating cell, can be obtained from an integrated form of the steam-hydrogen-based (or the CO_2 -CO-based) Nernst equation:

$$\overline{V}_{N}(T_{P}) = \frac{1}{2F(T_{P} - T_{R})(y_{2,O_{2}} - y_{1,O_{2}})[y_{2,H_{2}}(T_{P}) - y_{1,H_{2}}]} \times \int_{T_{R}}^{T_{P}} \int_{y_{1,O_{2}}}^{y_{2,O_{2}}} \int_{y_{1,H_{2}}}^{y_{2,O_{2}}} \Delta G_{R,H_{2}O}(T) + R_{u}T \ln \left(\frac{1 - y_{H_{2}} - y_{0,CO_{2}} - y_{N_{2}}}{y_{H_{2}}y_{O_{2}}^{1/2}}\right) dy_{H_{2}} dy_{O_{2}} dT \tag{17}$$

Note that the variable in this equation is the unknown product temperature, T_P , which appears both explicitly and implicitly in the upper integration limits. The steam mole fraction has been expressed in the integrand numerator in terms of the hydrogen mole fraction. The mole-fraction subscripts 0, 1, 2 again refer to the cold inlet, hot electrolyzer inlet, and the hot electrolyzer outlet states, respectively. Mole fractions at states 0 and 1 are fully defined. The state-2 mole fractions are based on the specified current density and the guessed value for T_P .

Once the mean Nernst potential is evaluated based on a guessed value for T_P , the operating voltage can be determined and the energy equation can be evaluated. The final converged solution for T_P must simultaneously satisfy the chemical balance Eqns. (6, 7, 11), the equilibrium constant Eqn. (6), and the energy Eqn. (14), subject to Eqns. (16 – 17).

The solution methodology described above can be applied to any specified electrolyzer heat loss or gain. For adiabatic operation, Q = 0. Alternately, if the heat loss or gain from the operating electrolyzer is known from a separate heat transfer analysis for a given operating point, the value of that heat loss or gain would be used.

For isothermal electrolyzer operation, once the inlet flow rates, current density, and operating temperature are specified, an iterative solution is not necessary and the triple integral of Eqn. (17) reduces to a double integral with known upper limits of integration. The energy Eqn. (14) can be solved directly for the heat required to maintain isothermal operation at any operating point.

The model allows for accurate determination of co-electrolysis outlet temperature, composition (anode and cathode sides), mean Nernst potential, operating voltage and electrolyzer power based on specified inlet gas flow rates, heat loss or gain, current density, and cell ASR(T). Alternately, for isothermal operation, it allows for determination of outlet composition, mean Nernst potential, operating voltage, electrolyzer power, and the isothermal heat requirement for specified inlet gas flow rates, operating temperature, current density and ASR(T).

2.3.2 Implementation of Co-Electrolysis Model into HYSYS

Implementation of the model in HYSYS was done in a way that took advantage of as many built-in features of the systems-analysis code as possible. Figure 11 provides a process flow diagram (PFD) representing the implementation of the model in HYSYS. The user-specified cold inlet process-gas stream enters at the left. This stream is equilibrated at the desired electrolyzer inlet temperature by means of an equilibrium reactor module that supports the shift reaction, Eqn. (5). The hot shifted stream and the heated sweep-gas stream enter the electrolysis module. This electrolysis module was developed previously for pure steam electrolysis [11]. At this level of the model, the user may specify whether the electrolysis process will be isothermal or adiabatic. If the process is isothermal, the temperature of the process outlet stream must be specified, otherwise, the outlet temperature is determined by iteration using an embedded adjust logical (shown as the A within the diamond) until the process heat is zero. Also at this level, an embedded spreadsheet is used to input the electrolysis variables, (i.e. current density, number of cells, cell area, area specific resistance, etc.).

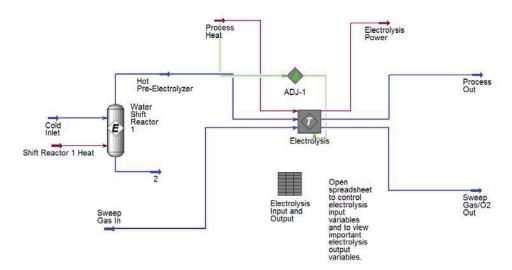


Figure 11 Process flow diagram external to the electrolysis module

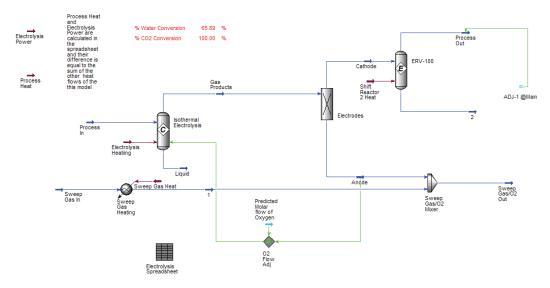


Figure 12 Process flow diagram for electrolysis module

The process flow diagram for the electrolysis module is shown in Figure 12. The hot shifted process stream enters a conversion reactor where the steam and/or carbon dioxide are electrolytically reduced. The conversion reactor unit includes both the steam and carbon dioxide reduction reactions. Based on the percent conversion of the steam and CO₂, the reactor will calculate the heat of reaction. The percent conversion of steam and/or CO₂ is determined by the amount of oxygen generated using Eqn. (9). This value of the molar flow rate of produced oxygen is stored in a dummy stream. A logical adjust is used to change the percent conversion of steam and carbon dioxide until the oxygen molar flow rate leaving the conversion reactor is the same as the calculated value. The oxygen is split from the rest of the reacted process-gas components by means of a component splitter unit (labeled Electrodes). The split oxygen combines with the sweep gas. The remaining components are passed through a second shift reactor to determine the outlet equilibrium composition.

As previously mentioned, the outlet temperature of both the process and sweep streams are specified but allowed to adjust if adiabatic conditions are desired. An embedded spreadsheet is used to evaluate the mean Nernst potential, Eqn. (17). Assuming a functional relationship for the Gibbs energy of formation, the definite integral was simplified analytically and this simplified version was programmed into the spreadsheet. The HYSYS calculation proceeds as follows: having defined the electrolysis variables, the amount of oxygen production is calculated in the spreadsheet using Eqn. (12). Based on an assumed outlet temperature, HYSYS proceeds to calculate all the thermodynamics and chemical reactions of the process resulting in outlet compositions for the process and sweep streams. With these now defined, the spreadsheet can calculate the mean Nernst potential by evaluating the simplified triple integral, Eqn. (17). The operating voltage is obtained from Eqn. (16) and the electrolysis power is calculated by multiplying the operating voltage with the total current. HYSYS inherently assures that the energy balance, Eqn. (14) is satisfied, which allows the process heat to be calculated by summing the electrolysis power with the total enthalpy differences from the electrolysis process and from the second shift reactor. If the outlet temperature is specified to be the same as the inlet temperature (isothermal operation), the calculation is complete and the process heat is known. If the process is specified to be adiabatic, the outlet temperature is adjusted until the process heat is zero. The process flow sheet automatically assures mass and energy balances.

2.3.3 Sabatier Process with Co-Electrolysis

The Sabatier process model was modified by removing the electrolysis module and replacing it with the co-electrolysis module. The overall process was modified as well in that water is mixed with the incoming carbon dioxide before the co-electrolysis process, see Figure 13. Recycled water is combined with incoming water and heated to a higher temperature through the low temperature recuperating heat exchanger. Carbon dioxide is mixed with the water and some hydrogen and carbon monoxide from exit side of the co-electrolysis process. About 10% of the molar composition of the inlet stream into the electrolysis process is hydrogen and carbon monoxide. The purpose of this is to provide reducing conditions at the hydrogen side of the solid oxide electrolysis cells. The heat from the exothermic Sabatier reactor further heats the stream to a vapor which is passed through a gas circulator to the high temperature recuperating heat exchanger. Although the heat transfer from the Sabatier reactors is not shown directly on the process flow diagram, an embedded spreadsheet was used to sum the heats of both Sabatier reactors and that sum is the heat that is used for the Sabatier heater. The gas is heated to over 700°C but needs to be further heated to the electrolysis temperature of 800°C through a high temperature electric heater. The gases as they enter the electrolysis unit shift composition due to these temperatures. The metals that make up the solid oxide electrolyzer cells act as a catalyst for this water gas shift reaction. This is simulated in the model by using a Gibbs reactor. The products leaving the co-electrolysis unit are primarily hydrogen and carbon monoxide, but some water and carbon dioxide remain. The oxygen also exits the electrolysis module in another stream. Both stream are at 800°C and are therefore used as the heat source for the high temperature recuperating heat exchanger. The oxygen stream is further cooled to near ambient conditions in the low temperature recuperating heat exchanger which warms the incoming water. A little over 10% of the hydrogen and carbon dioxide stream is mixed with the incoming water and carbon dioxide, the remaining 90% go through the Sabatier reactor where it is converted to methane and water. The water is condensed in the condenser/separator and mixed with fresh water. The methane with some hydrogen and water vapor is discharged out the vapor side of the condenser/separator. The hydrogen flow to the combined inlet carbon dioxide and carbon monoxide flow was set to 3.5 by adjusting the water in flow.

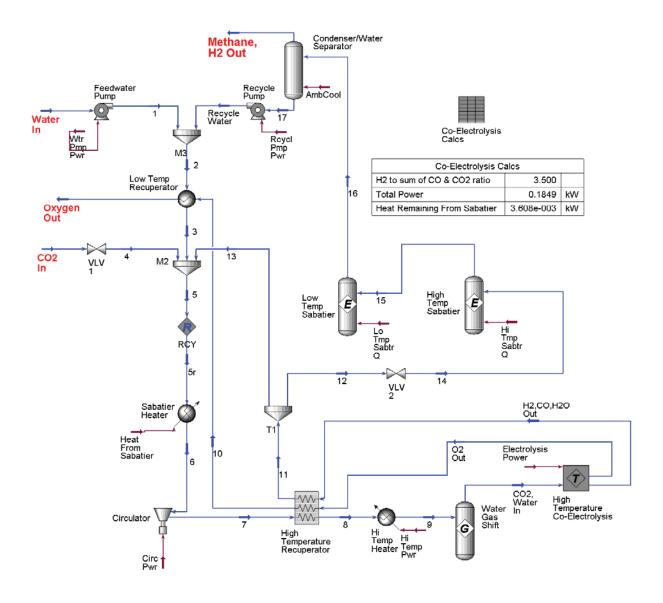


Figure 13 Process flow diagram of Sabatier process with co-electrolysis

The combined Sabatier and co-electrolysis process was modified to remove heat recuperation to determine the maximum amount of power that would be needed to make the process work, see Figure 14. Water, carbon dioxide and the syngas stream (carbon monoxide and hydrogen) from the electrolysis unit are combined, compressed through the circulator, and electrically heated to electrolysis temperatures before passing through the electrolyzer. The syngas passes through the Sabatier reactors to make methane and water. The water is condensed and mixed with incoming water and the methane with some hydrogen is discarded. The oxygen exiting the electrolyzer is cooled by an ambient cooler.

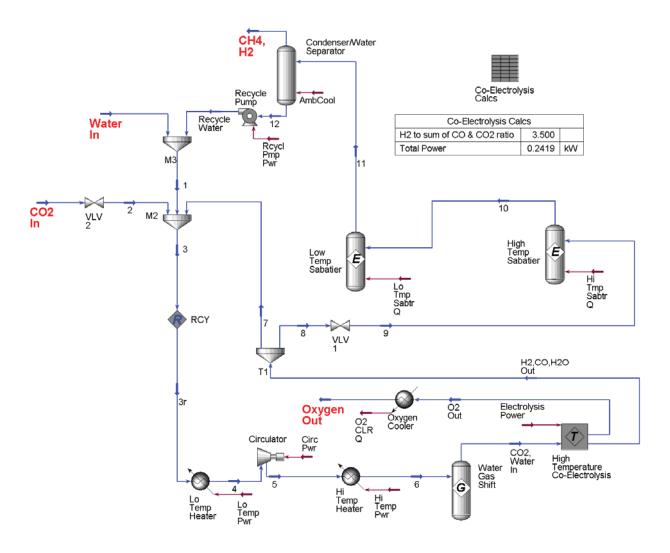


Figure 14 Process flow diagram of Sabatier process with co-electrolysis without heat recuperation

2.3.4 Boudouard Process with Co-electrolysis

The Bosch process was modified by removing the water gas shift reactor and combined with the high-temperature co-electrolysis process, see Figure 15. Incoming carbon dioxide is compressed to the Boudouard reaction pressure of 25 psia and heated by the hot oxygen product from the electrolysis unit. This stream is mixed with carbon dioxide from the Boudouard reactor and some carbon monoxide from the co-electrolysis unit to react a stream that is 10% carbon monoxide and 90% carbon dioxide. The carbon monoxide is used to provide reducing conditions at the carbon monoxide side of the solid oxide electrolysis cells. A high temperature recuperating heat exchanger heats the stream to nearly 700°C and is further heated to 800°C by an electric heater. The carbon dioxide is electrolyzed to carbon monoxide and oxygen in the electrolyzer. The outlet composition of the carbon side of the electrolyzer is 90% carbon monoxide and 10% carbon dioxide. The conversion reactor within the electrolysis unit was set to convert 88.8% of the carbon dioxide to prevent the full electrolysis of the carbon dioxide. In an actual carbon dioxide electrolysis process this is done to prevent the formation of carbon within the unit. If too much current is applied to the electrolysis cells, the carbon monoxide will split, forming oxygen and solid

carbon. The carbon could impair the cells. The carbon monoxide passes through the Boudouard reactor where solid carbon and carbon dioxide are formed at a temperature of 350°C. In this process no water or hydrogen is used and no methane is produced.

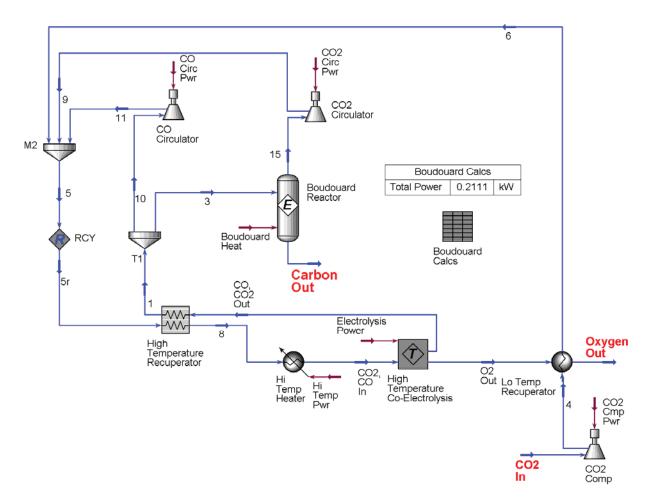


Figure 15 Process flow diagram of Boudouard process with co-electrolysis

2.3.5 Hydrogenation process with co-electrolysis

Hydrogenation is a process by which carbon monoxide and hydrogen are in equilibrium with water and carbon. Equilibrium data for the hydrogenation process were integrated into a HYSYS equilibrium reactor to simulate the process.

$$CO + H_2 \leftrightarrow C + H_2O \tag{18}$$

The hydrogenation process was combined with high-temperature co-electrolysis to develop an alternative oxygen producing process, see Figure 16. Compressed carbon dioxide is heated by cooling the hot oxygen exiting the co-electrolysis unit. The exit gas stream from the hydrogenation reactor, which is about 50% hydrogen and 40% steam, is mixed with the carbon dioxide and heated to over 700°C by the syngas and water exiting the electrolysis unit. The gas is then heated to the electrolysis process temperature by an electric heater. Oxygen and a syngas stream (hydrogen and carbon dioxide) are

produced from the electrolysis unit. The syngas reacts in the hydrogenation reactor at a pressure of 25 psia and a temperature of 350°C to produce carbon and water. Ideally the hydrogen and water within this overall process are recycled and therefore there is no need to replenish either.

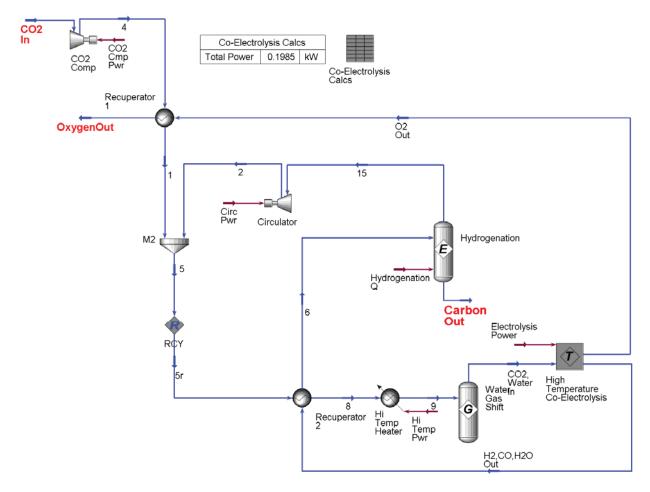


Figure 16 Process flow diagram of hydrogenation process with co-electrolysis

3. RESULTS

3.1 Oxygen Production at 1 kg/day

The scale of the process models were set at 1 kg/day of oxygen production to allow for comparison between processes. Table 1 shows the carbon dioxide and water inputs and the total power for the same rate of oxygen production. Tables 2 shows equipment lists of each component with the number of units and either power usage or duty need.

The highest flows of CO₂ are the Boudouard with co-electrolysis and Hydrogenation with co-electrolysis processes which also have no water input. The Bosch processes have slightly less CO₂ flows but also have small amounts of water. The lowest CO₂ flow rates are the Sabatier processes with and without co-electrolysis, but they also have the highest water flow rates. The CO₂ flow rate is affected by the rate of

water coming into the system. Both ultimately produce oxygen and therefore as the water flow rate into the process increases, the carbon dioxide flow rate decreases.

When considering total electrical power into the process, the Bosch process with one compressor has the highest value at 244 watts. A comparison between the 3 compressor and 1 compressor cases shows a power reduction of nearly 15%. The separate compression of the hydrogen, carbon dioxide and recycle streams reduces the compression power from 28.6 watts to 4.48. The Bosch process at sub-atmospheric conditions has a larger compression power need than the 3 compressor system, 10.3 watts compared to 5.87. However the overall power usage numbers are so close that the advantage of one system over the other is not clear. True pressure losses in both systems need to be determined. The Boudouard process with co-electrolysis compares well with Bosch process. The amount of power needed for the electrolysis processes are about the same. The Bosch process is electrolyzing water using the thermodynamically less efficient low temperature electrolysis. The Boudouard process is using the more efficient high-temperature electrolysis but is electrolyzing CO₂ which requires more power to split than water.

Table 1 Results for the production of 1 kg/day of oxygen

Table 1 Results for the production of 1	CO ₂ In	Water In	Total Electric Power
	(kg/day)	(kg/day)	(watts)
Bosch Process with 3 Compressors	1.310	0.033	212
Bosch Process with at Sub-atmospheric Conditions	1.310	0.035	217
Bosch Process with 1 Compressor	1.310	0.040	244
Sabatier Process	0.786	0.588	207
Sabatier Process with Co-Electrolysis with Recuperation	0.638	0.618	185
Sabatier Process with Co-Electrolysis without Recuperation	0.638	0.618	242
Boudouard with Co-Electrolysis	1.375	0.000	211
Hydrogenation with Co-Electrolysis	1.375	0.000	199

Table 2 Equipment for the production of 1 kg/day of oxygen, part 1

	Comp	oressors	Pumps		Heat Exchangers		Valves
	# of units	Power (watts)	# of units	Power (watts)	# of units	Duty (watts)	# of units
Bosch Process with 3 Compressors	3	5.87	1	3.02E-06	1	317.3	1
Bosch Process at Sub-atmospheric Conditions	1	10.3	2	6.72E-04	1	312.0	2
Bosch Process with 1 Compressor	1	37.4	1	3.38E-05	1	401.5	0
Sabatier Process	1	0.23	2	2.96E-04	0	0.0	2
Sabatier Process with Co-Electrolysis with Recuperation	1	0.42	2	2.17E-04	3	59.7	2
Sabatier Process with Co-Electrolysis without Recuperation	1	0.32	1	1.94E-04	1	9.1	2
Boudouard with Co-Electrolysis	3	0.79	0	0	2	18.4	0
Hydrogenation with Co-Electrolysis	2	1.33	0	0	2	29.4	0

The Sabatier process requires slightly less power than the Bosch processes due to lesser compression needs. The electrolysis power needs are the same. The Sabatier process with co-electrolysis has the least power need to produce 1kg/day of oxygen due to the 11% reduction of power within the electrolysis unit. Although an additional topping electric heater is needed to achieve electrolysis temperatures, this additional power is only 1 watt. However to achieve this power reduction, nearly 60 watts of recuperation need to occur. If recuperation is not present, the overall power increases by 31%.

The hydrogenation process with co-electrolysis has an overall power need that is second lowest with the Sabatier with co-electrolysis (with recuperation) having a lower power need. The Sabatier with co-electrolysis process has a lower power need than the Boudouard process with co-electrolysis, because water is produced within the process and is the primary component that is electrolyzed. Water electrolyzes at a lower power than carbon dioxide because the heat of formation is lower. When both carbon dioxide and water enter the co-electrolysis unit, power results indicate that the water probably is what is favored in the actual electrolysis process. As the water is depleted in the process and hydrogen is produced, the hydrogen shifts the carbon dioxide to carbon monoxide and water. The new shifted water is then further electrolyzed. In the case of the Boudouard with co-electrolysis, no water is present therefore the CO2 is directly split resulting in a higher power usage. With the case of the hydrogenation process, water is created and therefore the power requirement of the electrolysis process decreases. The hydrogenation process requires recuperation to achieve the lower power requirement, but the recuperation duty is about half of that of the Sabatier process with co-electrolysis and recuperation. The power requirement for the hydrogenation process could have been further reduced if the heat from the hydrogenation reactor had been recuperated as well.

Table 3 Equipment for the production of 1 kg/day of oxygen, part 2

	Cond	lensers	Reactors		Electrolyzer	Heaters	
	# of units	Duty (watts)	# of units	Duty (watts)	Power (watts)	# of units	Power (watts)
Bosch Process with 3 Compressors	1	-48.5	1	-16.6	207	0	0
Bosch Process at Sub-atmospheric Conditions	1	-53.3	1	-15.9	207	0	0
Bosch Process with 1 Compressor	1	-83.6	1	-13.3	206	0	0
Sabatier Process	1	-15.3	1	-28.9	207	0	0
Sabatier Process with Co-Electrolysis with Recuperation	1	-16.1	1	-33.1	183	1	1.07
Sabatier Process with Co-Electrolysis without Recuperation	1	-16.1	1	-51.7	183	2	58.2
Boudouard with Co-Electrolysis	0	0	1	-66.4	205	1	5.60
Hydrogenation with Co-Electrolysis	0	0	1	-54.2	192	1	5.40

3.2 Processing Carbon Dioxide at 1 kg/day

The data was adjusted so that the inlet flow of carbon dioxide was set to 1 kg/day. Tables 4, 5, and 6 show the adjusted data.

Power usage is lower for the Bosch cases than for the Sabatier cases when scaling to the carbon dioxide inlet flow. Although more oxygen is produced in the Sabatier cases, more power is needed to electrolyze the incoming water as well as the water generated by Sabatier reactor. Most of the water for the Bosch processes comes from carbon dioxide as it is processed through the Bosch reactor. The Boudouard with co-electrolysis process and the hydrogenation with co-electrolysis case have the lowest power usage to process 1 kg/day of carbon dioxide. However, they also have the lowest oxygen production. Both of these processes have no incoming water. The Boudouard process requires more power because carbon dioxide is directly split in the electrolysis unit. The hydrogenation reactor produces water that passes through the electrolysis unit with the carbon dioxide. Compression power requirements are low for all the Sabatier processes as well as the Boudouard and hydrogenation processes. Heat exchanger duties are highest with the Bosch processes due to the higher temperatures within the reactors. The Boudouard process with co-electrolysis and the hydrogenation process with co-electrolysis have no condensers. It is interesting to note that the Sabatier process with co-electrolysis requires more power than the base Sabatier process to convert 1kg/day of carbon dioxide, because the water requirement is higher.

Table 4 Results for the processing of 1 kg/day of carbon dioxide

	O ₂ Out	Water In	Total Electric Power
	(kg/day)	(kg/day)	(watts)
Bosch Process with 3 Compressors	0.763	0.025	162
Bosch Process with at Sub-atmospheric Conditions	0.763	0.027	165
Bosch Process with 1 Compressor	0.763	0.030	186
Sabatier Process	1.272	0.748	263
Sabatier Process with Co-Electrolysis with Recuperation	1.567	0.969	290
Sabatier Process with Co-Electrolysis without Recuperation	1.567	0.968	379
Boudouard with Co-Electrolysis	0.727	0.000	153
Hydrogenation with Co-Electrolysis	0.727	0.000	144

Table 5 Equipment for the processing of 1 kg/day of carbon dioxide, part 1

	Compressors		Pumps		Heat Exchangers		Valves
	# of units	Power (watts)	# of units	Power (watts)	# of units	Duty (watts)	# of units
Bosch Process with 3 Compressors	3	4.48	1	2.31E-06	1	242.2	1
Bosch Process at Sub-atmospheric Conditions	1	7.83	2	5.13E-04	1	238.2	2
Bosch Process with 1 Compressor	1	28.56	1	2.58E-05	1	306.5	0
Sabatier Process	1	0.29	2	3.77E-04	0	0.0	2
Sabatier Process with Co-Electrolysis with Recuperation	1	0.67	2	3.40E-04	3	93.5	2
Sabatier Process with Co-Electrolysis without Recuperation	1	0.50	1	3.03E-04	1	14.3	2
Boudouard with Co-Electrolysis	3	0.58	0	0.00E+00	2	13.4	0
Hydrogenation with Co-Electrolysis	2	0.96	0	0.00E+00	2	21.4	0

Table 6 Equipment for the processing of 1 kg/day of carbon dioxide, part 2

	Cond	Condensers		actors	Electrolyzer	Heaters	
	# of units	Duty (watts)	# of units	Duty (watts)	Power (watts)	# of units	Power (watts)
Bosch Process with 3 Compressors	1	-37.0	1	-12.7	158	0	0
Bosch Process at Sub-atmospheric Conditions	1	-40.7	1	-12.1	158	0	0
Bosch Process with 1 Compressor	1	-63.8	1	-10.1	158	0	0
Sabatier Process	1	-19.5	1	-36.8	263	0	0
Sabatier Process with Co-Electrolysis with Recuperation	1	-25.3	1	-51.8	287	1	1.68
Sabatier Process with Co-Electrolysis without Recuperation	1	-25.3	1	-81.1	287	2	91.27
Boudouard with Co-Electrolysis	0	0.0	1	-48.3	149	1	4.07
Hydrogenation with Co-Electrolysis	0	0.0	1	-39.4	139	1	3.92

3.3 Carbon Balance

A carbon balance was performed to determine where the carbon goes with each process. Both a constant oxygen production and constant carbon dioxide processing analyses were performed, see Tables 7 and 8.

For the Bosch processes and the Boudouard with co-electrolysis and the hydrogenation with co-electrolysis processes, the carbon exits as a solid. With the Sabatier processes, the exiting carbon is primarily methane. The Sabatier with standard electrolysis has also some carbon dioxide exiting.

When comparing the inlet with the outlet mole balance, all cases balance well except the Bosch. Some water was added to these cases to produce additional hydrogen for the Bosch processes. However a means to remove the hydrogen after the process was not provided which causes a mass imbalance. The water flow in for these cases was small and therefore the mass imbalance is small. When looking at the case with constant carbon dioxide flow, the difference is more pronounced.

Table 7 Carbon balance for producing 1 kg/day of oxygen

	Carbon In (gmole/hr)	Carbon Out (gmole/hr)					Carbon Out %			
Bosch Process with 3 Compressors	CO ₂	С	СО	CO ₂	CH ₄	Total	С	СО	CO ₂	CH ₄
Bosch Process at Sub-atmospheric Conditions	1.24	1.22	0.00	0.00	0.00	1.22	100%	0%	0%	0%
Bosch Process with 1 Compressor	1.24	1.25	0.000	0.00	0.00	1.25	100%	0%	0%	0%
Sabatier Process	1.24	1.22	0.000	0.00	0.00	1.22	100%	0%	0%	0%
Sabatier Process with Co-Electrolysis with Recuperation	0.744		0.00	0.095	0.650	0.744	0%	0%	13%	87%
Sabatier Process with Co-Electrolysis without Recuperation	0.604		0.00	0.00	0.604	0.604	0%	0%	0%	100%
Boudouard with Co-Electrolysis	0.604		0.00	0.00	0.604	0.604	0%	0%	0%	100%
Hydrogenation with Co-Electrolysis	1.30	1.30				1.30	100%	0%	0%	0%
Bosch Process with 3 Compressors	1.30	1.30				1.30	100%	0%	0%	0%

Table 8 Carbon balance for processing 1 kg/day of carbon dioxide

	Carbon In (gmole/hr)						Carbon Out %				
Bosch Process with 3 Compressors	CO ₂	С	СО	CO ₂	CH ₄	Total	С	СО	CO ₂	CH ₄	
Bosch Process at Sub-atmospheric Conditions	0.947	0.932	0.000	0.000	0.000	0.932	100%	0%	0%	0%	
Bosch Process with 1 Compressor	0.947	0.952	0.000	0.000	0.000	0.952	100%	0%	0%	0%	
Sabatier Process	0.947	0.933	0.000	0.000	0.000	0.933	100%	0%	0%	0%	
Sabatier Process with Co-Electrolysis with Recuperation	0.947	0.000	0.000	0.120	0.827	0.947	0%	0%	13%	87%	
Sabatier Process with Co-Electrolysis without Recuperation	0.947	0.000	0.000	0.000	0.947	0.947	0%	0%	0%	100%	
Boudouard with Co-Electrolysis	0.947	0.000	0.000	0.000	0.947	0.947	0%	0%	0%	100%	
Hydrogenation with Co-Electrolysis	0.947	0.947	0.000	0.000	0.000	0.947	100%	0%	0%	0%	
Bosch Process with 3 Compressors	0.947	0.947	0.000	0.000	0.000	0.947	100%	0%	0%	0%	

4. SOLID OXIDE CELLS

Most of the discussion on solid oxide cells included in this section is based on previous INL reports on solid oxide degradation by Sohal [2009a] and Sohal et al. [2009b].

4.1 Solid Oxide Cell Components

A solid oxide cell is a key component of the electrolysis system. It consists of three main components: an electrolyte and two electrodes (Figures 17 and 18). The electrolyte is a gas-tight ceramic membrane that can conduct ions and is sandwiched between two porous electrodes that can conduct electrons: the steam/hydrogen electrode (or anode in fuel cell mode) and the air/oxygen electrode (or cathode in the fuel cell mode). In the fuel cell mode, oxygen molecules dissociate at the oxygen electrode and combine with electrons coming from external electric power source to form oxygen ions. The oxygen ions conduct through the electrolyte and migrate towards the hydrogen electrode. The fuel (hydrogen or natural gas) is fed to the anode and reacts with the oxygen ions to form water and CO₂. If the fuel cell is operated in the electrolysis mode, the names and function of the electrodes are reversed as shown in Figure 17a.

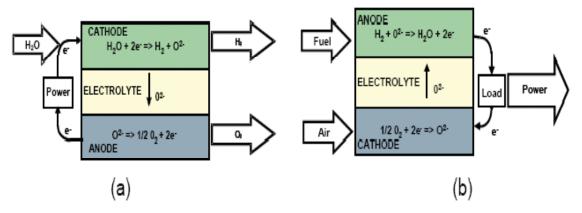


Figure 17 (a) Solid oxide electrolysis cell (SOEC); (b) solid oxide fuel cell (SOFC) operating in reverse compared to an SOEC [Guan, et al. 2006]

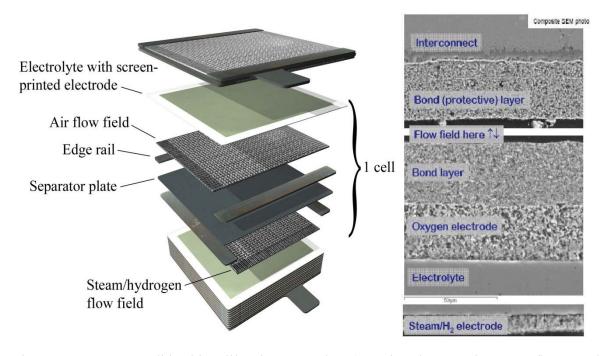


Figure 18 Ceramatec solid oxide cell/stack construction; (scanning electron microscopy figure on the right taken from Carter et al. 2008)

The most common materials currently used for the solid oxide cells are listed in Table 9 [Gazzarri 2007]. The electrolyte is a dense gas-tight ceramic layer, usually made from yttria stabilized zirconia (YSZ) with yttria content of 8 mol% to fully stabilize the electrolyte composition. The performance of the electrolyte depends on how well it can conduct oxide ions (O^-). The thinner the electrolyte, the higher its ion conductivity and the lower the cell's ohmic resistance. In an electrolyte supported cell, the electrolyte thickness is large (150-250 µm), which leads to relatively high ionic resistance. Therefore, if the mechanical strength can be provided by the steam/H₂ electrode, the electrolyte thickness can be reduced by a factor of ~10.

Table 9 Commonly used materials in SOFC/SOEC [Gazzari 2007]

Component	Material	Acronym
Steam/hydrogen electrode	Ni - Y _x Zr _{1-x} O _{2-x/2} (nickel-yttria stabilized zirconia)	Ni-YSZ
Electrolyte	Y _x Zr _{1-x} O _{2-x/2} (yttria stabilized zirconia)	YSZ
Air/oxygen electrode	$Sr_xLa_{1-x} MnO_{3-\delta} + Y_x Zr_{1-x} O_{2-x/2}$ (doped lanthanum manganite)	LSM-YSZ
Interconnect	Chromium based alloys/ceramics or stainless steel	SS

The most common anode material for SOFC is a porous cermet (<u>cer</u>amic-<u>met</u>al) made from Ni and YSZ. Electronically-conductive, gas-tight interconnect plates connect the individual cells to form a stack. The ionic conductivity of ceramics is highly dependent on the ceramic temperature. Thus, high operating temperatures are required to obtain sufficient overall conductivity in the solid oxide cell. YSZ exhibits acceptable conductivity in the 700–1,100°C temperature range, but if thermal cycling occurs, such as at start-up, the high operating temperature results in large thermal stresses in the cell components. Stresses can also be caused by large thermal gradients generated by the uneven distribution of electrochemical reaction sites. Finally, fabrication of the cell components also requires high temperatures that can cause detrimental residual stresses within the cell components.

In the fuel cell mode, the oxygen electrode is fed with air while the hydrogen electrode is fed with hydrogen or natural gas. Thus, the properties of the oxygen electrode should be such that it provides a component for oxygen gas to be easily reduced and similarly, the function of the hydrogen electrode is to oxidize the fuel gas. At the oxygen electrode, where electrons are supplied via the external electrical power, oxygen molecules are reduced to oxygen ions. The oxygen ions are conducted through the electrolyte to the hydrogen electrode. At the hydrogen electrode, oxygen ions oxidize the fuel gas which forms water and carbon dioxide, while the resulting free electrons are transported via the external circuit back to the oxygen electrode. The solid oxide electrolyte separates the reduction and oxidation reactions. Thus, in the electrolysis mode, the electrical energy is used to split hydrogen from steam. The electrolysis process is the reverse of the fuel cell process.

4.2 Possible Causes of Degradation in SOEC

At present, a complete understanding and reasonable agreement on the causes of degradation and electrochemical mechanisms behind them does not exist. Therefore, following write-up is not inclusive of all the available literature and all the phenomena relevant to degradation by any means.

Existing degradation data can be classified as (a) baseline progressive constant-rate degradation, (b) degradation corresponding to transients caused by thermal or redox (**red**uction and **ox**idation) cycling phenomena occurring in a cell, and (c) degradation resulting from a sudden incident or a failure/malfunction of a component or a control in a stack system. However, there is no clear evidence if different events lead to similar or drastically different electrochemical degradation mechanisms within a cell.

4.2.1 SOEC versus SOFC Stacks

The degradation mechanisms in a stack are not identical to that in a single cell. Also, degradation in a SOEC is not identical to that in a SOFC. Long-term, single-cell tests show that SOEC operation has greater degradation rates than that in SOFC mode. Some researchers observed that higher operating temperature increases degradation in SOEC, but higher current density does not increase degradation. However, Argonne National Laboratory (ANL) observed higher degradation in higher current flow regions of O₂-electrodes [Carter et al., 2008].

4.2.2 Air/Oxygen Electrode

It is understood that degradation of the O_2 -electrode is more severe than that of the H_2 -electrode. Therefore, it was proposed to focus initially on the degradation of the O_2 -electrodes in a stack. ANL examination of a SOEC operated by INL for $\sim 1,500$ hours showed that O_2 -electrode delaminated from the bond layer/electrolyte. However, the causes of the delamination can be termed as speculative because confirmative tests proving the fundamental cause(s) have not been performed. It is thought that high oxygen evolution in over-sintered regions can build up high pressure at that location. In SOEC mode, O_2 has to be pushed out, hence chances of delamination increase. Therefore, the high porosity of the O_2 -electrode is very important. Per ANL observations, the delamination occurs in cell areas with high current flows. It has also been suggested that chromium poisoning originating from the interconnects or the balance-of-plant pipes may get located at the interface or triple phase boundary (TPB). This can result in the bond layer getting separated from the O_2 -electrode. Deposition of impurities at the TPB and delamination can adversely impact the electrochemical reactions and ionic conductivity in the cell.

4.2.3 Air/O₂-Electrode Side Bond Layer

An O₂-electrode side protective bond layer is shown in Figure 18. Because, it is next to the O₂-electrode, it encounters similar electrochemical phenomena that lead to cell degradation. However, besides ANL's observations [Carter et al., 2008], no other studies or data are available that can demonstrate the bond layer's significance relative to the O₂-electrode in terms of overall cell degradation. ANL found an average of 1–8% (~30% maximum) Cr-contamination in bond layer, probably originating from interconnects. Cr contaminants were found in association with lanthanum strontium chromite (LSC). In O₂ bond layer, a secondary phase may form. However, there are conflicting opinions about severity of Cr contamination. ANL observed delamination and weak interface between the O₂-electrode and LSC bond layer, which can prevent solid state Cr from diffusing into the O₂-electrode. For this reason, the O₂-electrode can remain stable, but a weak interface is not desirable from an electrical conductivity point of view.

4.2.4 Electrolyte

In electrolytes, the main cause of degradation is loss of electrical/ionic conductivity. Müller et al. [2003] showed that during first 1,000 hours of testing, yttria and scandia doped zirconia (8 mol% Y_2O_3 Sc-ZrO₂/8YSZ) electrolytes showed ~23% of degradation. For the next 1,700 hours of testing, the decrease in conductivity was as high as 38%. An increase in tetragonal phase during annealing at the expense of cubic and monoclinic phases was detected for the 3YSZ samples. However, 3YSZ and 4YSZ samples showed much smaller decrease in conductivity after 2,000 hours of testing. Both Steinberger-Wilckens [2008] and Hauch [2007] reported the formation of impurities at the TPBs. A substantial amount of SiO₂ was detected at the Ni/YSZ H₂-electrode-electrolyte interface during electrolysis, while no Si was detected in other reference cells. These Si containing impurities were probably from albite glass sealing. ANL [Carter et al., 2008] observed that cubic, tetragonal, and monoclinic phases of ZrO₂ remained stable at the present Scandia doping level.

4.2.5 Steam/H₂-Electrode

Overall, many researchers agree that the contribution of a steam/H₂-electrode to SOEC degradation is much less than that of other cell components. ANL also observed Si as a capping layer on steam/H₂-electrode. It probably was carried by steam from the seals, which contain Si. SiO_x also emanates from interconnect plates. Mn also diffuses from interconnects, but the significance of Mn diffusion is unknown. Hauch [2007] observed contaminants containing Si to segregate to the innermost few microns of the H2-

electrode near the electrolyte. The impurities that diffused to and accumulated at the TPBs of the H₂-electrode are believed to be the main cause of performance degradation in SOECs [Hauch 2007]. In literature, it has been noted that steam content greater than 30% shows conductivity loss. Therefore, an optimum ratio of steam-H₂ mixture and steam utilization percentage needs to be determined.

4.2.6 Interconnect

Interconnects can be a source of serious degradation. Sr, Ti, and Si segregate and build-up at interfaces. Sr segregates to the interconnect—bond layer interface. Mn segregates to the interconnect surface. Si and Ti segregate to the interconnect-passivation layer interface. Cr contamination can originate from interconnects and it can interact with O_2 -electrode surface or even diffuse into the O_2 -electrode. Coated stainless steel interconnects have shown reduced degradation rates. GE observed higher degradation with stainless steel current collectors than with Au current collectors [Gaun et al. 2006].

4.2.7 Contaminants and Impurities

A hydrogen electrolysis plant or a laboratory-scale experiment is always connected to the pipes, gas storage tanks/cylinders, or other such equipment. These components can be a source of undesirable particles/chemicals, which can get deposited at different locations in a solid oxide electrolysis cells. It has been shown in previous sections that any foreign particles depositing at the triple phase boundary can lead to degradation in cell performance. The reactant gases can also have some undesirable impurities. It is understood that the balance of plant and gases are merely sources of impurities. The phenomenological causes of degradation depend on other electrochemical reasons.

Severe corrosion was encountered when glass seals were used, but appeared to be reasonably under control when the glass seals were replaced. Nickel from nickel mesh can volatize in high water content environments, move into the steel and make it austenitic, which will eventually corrode. Silica poisoning is a potential problem. Impure water can contain Si. Therefore, in SOEC, it is likely that high temperature steam interacting with balance-of-plant piping picks up Si and transports it elsewhere to form nonconductive scale. Iron can also diffuse into glass seals and cause electrical shorting. Mn diffuses from interconnect, but its effect on degradation is unknown. Phosphorus and arsenic can react and interact with the electrode containing Ni. They can form eutectics and enhance Ni mobility. This is a very low-level effect.

4.2.8 Summary of Stack Degradation

Main sources of degradation come from several cell components. Details about the following list of general observations and main sources of SOEC stack degradation have been discussed in earlier sections:

- Delamination of O_2 -electrode side bond layer from the O_2 -electrode,
- Bond layer on steam/H₂-electrode side is not degrading,
- Air and steam/H₂ flow fields (flow channels) are not degrading,
- Five cell components are suspect:
 - Bond layer on O₂-electrode-Cr poisoning and dissociation
 - O₂-electrode-microstructural changes and delamination
 - Loss of electrical/ionic conductivity of electrolyte
 - Interconnect-generation of contaminants

- Steam/H₂- electrode

This list is not all inclusive, but represents a majority opinion of participants who attended a degradation workshop in 2008 [Sohal 2009a].

4.2.9 Degradation Measurements

There are two common definitions for quantifying degradation given by Gemmen et al. [2008]. Area Specific Resistance (ASR) is defined in Equation (1). The ASR represents instantaneous degradation rate. Another degradation definition is termed as average degradation rate, $D\overline{R}(t)$. It is defined for a time period of (t-t₀). Thus for any cell voltage V(I_s, t), at a time t, average degradation rate, $D\overline{R}(t)$, is given by [Gemmen et al. 2008]:

$$D\overline{R}(t) = \frac{V(i_s, t_0) - V(i_s, t)}{V(i_s, t_0) \times (t - t_0)} 100.$$
(19)

ASR is best suited for comparing the performances of the same cell with two types of technologies such as one type of interconnect design with another. However, DR is more suitable for comparing cell performance with a stack performance of the same type of cells. To understand the degradation phenomena, a solid oxide electrolyzer needs to be operated and tested. Current density, voltage, area specific resistance (ASR), cell system temperature, reactants, and product flow rates are some of the commonly measured parameters during the tests. However, to understand the electrochemical behavior of the electrodes and electrolytes, their chemical microstructure has to be understood before and after an electrolysis operation. Also, the location of the impurities, for example, Ni, Cr, and their movement as a result of the electrolysis operation should be identified. The impact of the impurities movement on electrochemical performance of a single cell and a stack should also be determined by making relevant measurements.

Performance degradation results with a 25-cell SOEC stack tested for 1,000 hours at INL were presented by O'Brien et al. [2007] and are shown in Figures 19 and 20. Figure 19 plots the stack ASR as a function of time for the 1,000 hours. The furnace temperature was increased from 800 to 830 °C over an elapsed time of 118 hours, resulting in a sudden drop in ASR. The increase in ASR with time represents degradation in stack performance. The degradation rate decreases with time and is relatively low for the last 200 hours of the test. However, from the 118-hour mark to the end of the test, the ASR increased more than 40% over approximately 900 hours. Reduction of this performance degradation is an objective of ongoing research. Figure 20 shows the corresponding generation of hydrogen.

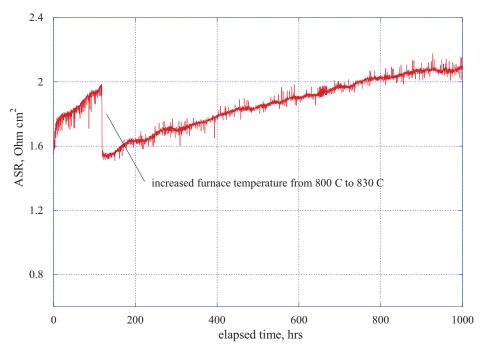


Figure 19 Area-specific resistance of a 25-cell stack as a function of time for a 1,000-hour test [O'Brien et al. 2007]

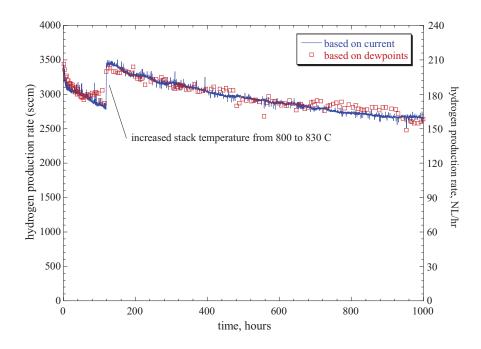


Figure 20 Hydrogen production rates during 1,000-hour long-term test [O'Brien et al. 2007]

5. CONCLUSIONS AND RECOMMENDATIONS

The energy of formation for water is less than for carbon dioxide. If water is added to one of the processes, the power to produce oxygen goes down for a given amount of oxygen. However, less carbon dioxide is processed. For applications which use these processes, not only is a reduction of energy important but also reduction of mass. The addition of water means an additional mass load of the water.

High temperature co-electrolysis is thermodynamically more efficient than low temperature electrolysis. However a means is needed to raise the temperature of the carbon dioxide and water to the electrolysis temperature of 800°C.

With this in mind the following conclusions may be made.

- The Bosch processes have higher power requirements when considering oxygen production alone but converts more carbon dioxide per power in.
- The Sabatier processes require less power when considering oxygen production alone, but require more water in.
- For pure oxygen production, the Sabatier process with co-electrolysis (and recuperation?) requires the least amount of power. However it also has the highest water requirement. When considering processing a given amount of carbon dioxide, this process has almost the highest power requirement.
- The Boudouard process with co-electrolysis compares with the base Bosch process when considering oxygen production, but processes carbon dioxide with less power.
- Hydrogenation with co-electrolysis has the best overall performance. For pure oxygen production it is second only to the Sabatier with co-electrolysis for the least amount of power needed. However it performs better than all of the processes for processing carbon dioxide.
- If co-electrolysis is used, heat recuperation is necessary to reduce power consumption.

The following recommendations should be considered:

- The Bosch processes need to be modeled without any water in to be more consistent with respect to the other models. By doing so, the carbon flow in will be more in balance with the carbon flow out.
- If a small amount of water is desired for the Bosch process, a hydrogen purge stream needs to be added to allow for a better mass balance.
- The models within the work have assumed steady state operation and chemical equilibrium within the reactors. The kinetics of the reactors need to be considered to model more realistic chemical reactions.

6. REFERENCES

- Carter, D. J. et al. (2008). "Determining Causes of Degradation in High Temperature Electrolysis Stacks," Presented at the Workshop on Degradation in Solid Oxide Electrolysis Cells and Strategies for its Mitigation, October 27, 2008, Fuel Cell Seminar & Exposition, Phoenix, AZ.
- Gazzarri, J. I. (2007). "Impedance Model of a Solid Oxide Fuel Cell for Degradation Diagnosis," Ph. D. Thesis, The University of British Columbia, Vancouver, Canada.
- Gemmen, R. S., Williams, M. C., and Gerdes, K. (2008). "Degradation Measurement and Analysis for Cells and Stacks," J. Power Sources, 184, 251-259.
- Guan, J. et al. (2006). "High Performance Flexible Reversible Solid Oxide Fuel Cell," GE Global Research Center Final Report for DOE Cooperative Agreement DE-FC36-04GO-14351.
- Hauch, A. (2007). "Solid Oxide Electrolysis Cells Performance and Durability," Ph.D. Thesis, Technical University of Denmark, Risø National Laboratory, Roskilde, Denmark.
- Müller, A.C., Weber, A., Herbstritt, D., and Ivers-Tiffée, E. (2003). "Long Term Stability of Yttria and Scandia doped Zirconia Electrolytes," Proceedings 8th International Symposium on SOFC, (Edited by) Singhal, S. C., Dokiya, M., PV 2003-07, The Electrochemical Society, 196-199.
- O'Brien, J. E., Stoots, C. M., Herring, J. S., and Hartvigsen, J. J. (2007). "Performance of Planar High-Temperature Electrolysis Stacks for Hydrogen Production from Nuclear Energy," Nuclear Technology, 158, 118-131.
- Sohal, M. S. (2009a). "Degradation in Solid Oxide Cells during High Temperature Electrolysis," INL Report INL/EXT-09-15617.
- Sohal, M. S. et al. (2009b). "Critical Causes of Degradation in Integrated Laboratory Scale Cells during High Temperature Electrolysis," INL Report INL/EXT-09-16004.
- Steinberger-Wilckens, R. (2008). "Degradation Issues in SOFCs," Presented at the Workshop on Degradation in Solid Oxide Electrolysis Cells and Strategies for its Mitigation, October 27, 2008, Fuel Cell Seminar & Exposition, Phoenix, AZ.

Appendix A Raw Process Model Data

Appendix A Raw Process Model Data

The models of the processes in Appendix A were developed using HYSYS.Plant Version 2.2.2 (Build 3806) from Hyprotech Ltd. on a desktop computer running Microsoft Windows XP Professional Version 2002 Service Pack 3.

A.1 Bosch Process with 3 Compressors

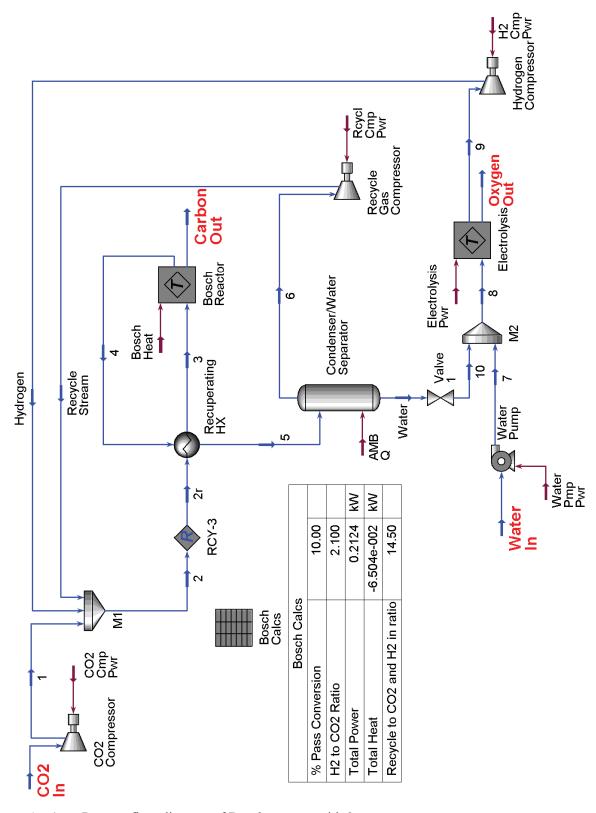


Figure A - 1 Process flow diagram of Bosch process with 3 compressors

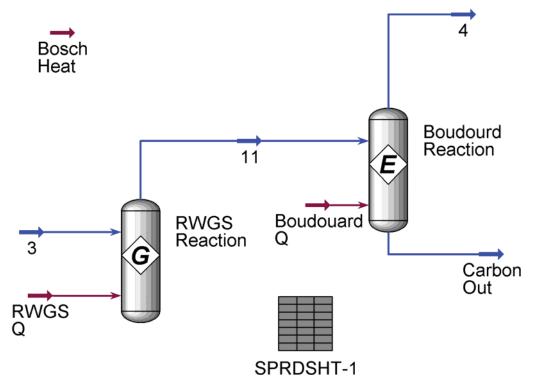


Figure A - 2 Process flow diagram of Bosch reactor

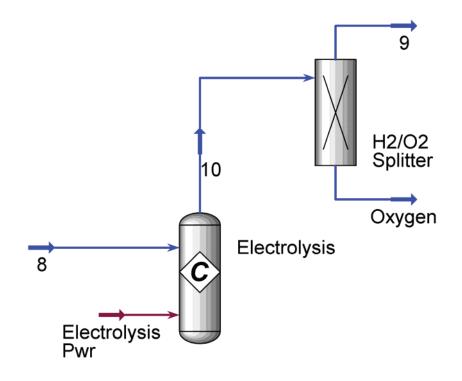


Figure A - 3 Process flow diagram of electrolysis module

2		INL		Case Name:	C:\NASA Final\Bosch 3-	Comp v_2.hsc			
3	HYPROTECH	Calgary, A	Alberta	Unit Set:	NASA2				
5	part of the same o	0,10,10,1		Date/Time:	Date/Time: Mon Aug 23 10:20:55 2010				
6									
8	Worki	ook:	Case (Main)					
9				Streams					
11	Name		CO2 In	1	Hydrogen	Recycle Stream	2		
12	Vapour Fraction		1.0000	1.0000	1.0000	1.0000	1.0000		
13	Temperature	(C)	21.111 '	45.103	91.537	34.609	37.371		
14 15	Pressure	(kPa)	131.00 ° 1.2404	172.37 ° 1.2404	172.37	172.37	172.37 53.317		
16	Molar Flow Mass Flow	(gmole/h) (kg/d)	1.2404	1.2404	2.6054 0.12633	49.471 20.826	53.317 22.262		
17	Liquid Volume Flow	(m3/h)	6.614e-005	6.614e-005	7.519e-005	1.917e-003	2.059e-003		
18	Heat Flow	(kW)	-0.1358	-0.1354	1.344e-003	-1.406	-1.540		
19		kJ/kgmole)	-3.940e+005	-3.931e+005	1857	-1.023e+005	-1.040e+005		
20	Name	(to/ttg/filoic/	2r	3	Carbon Out	4	5		
21	Vapour Fraction		1.0000	1.0000	1.0000 *	1.0000	1.0000		
22	Temperature	(C)	37.396 *	620.26 *	650.00	650.00	62.396		
23	Pressure	(kPa)	172.37 '	169.37	163.37	163.37	160.37		
24	Molar Flow	(gmole/h)	53.298	53.298	1.2214	52.001	52.001		
25	Mass Flow	(kg/d)	22.272 *	22.272	0.35208	21.920	21.920		
26	Liquid Volume Flow	(m3/h)	2.058e-003	2.058e-003	8.934e-006	1.963e-003	1.963e-003		
27	Heat Flow	(kW)	-1.543	-1.225	3.473e-003	-1.245	-1.563		
28	Molar Enthalpy (kJ/kgmole)	-1.042e+005	-8.276e+004	1.024e+004	-8.621e+004	-1.082e+005		
29	Name		6	Water	Water In	7	8		
30	Vapour Fraction		1.0000	0.0000	0.0000	0.0000	0.0000		
31	Temperature	(C)	25.000 *	25.000	21.111 *	21.112	24.897		
32	Pressure	(kPa)	157.37	157.37	101.32 '	107.32 '	107.32		
33	Molar Flow	(gmole/h)	49.471	2.5291	7.6325e-002	7.6325e-002	2.6054		
34	Mass Flow	(kg/d)	20.826	1.0936	3.3000e-002 *	3.3000e-002	1.1266		
35	Liquid Volume Flow	(m3/h)	1.917e-003	4.566e-005	1.378e-006	1.378e-006	4.704e-005		
36	Heat Flow	(kW)	-1.411	-0.2005	-6.057e-003	-6.057e-003	-0.2066		
37		kJ/kgmole)	-1.026e+005	-2.854e+005	-2.857e+005	-2.857e+005	-2.854e+005		
38	Name		Oxygen Out	9	10	CO2 Cmp Pwr	AMB Q		
39	Vapour Fraction		1.0000	1.0000	0.0000				
40 41	Temperature	(C)	24.996	24.897	25.011				
42	Pressure Molar Flow	(kPa)	101.32 1.3025	101.32 2.6054	107.32 2.5291				
43	Mass Flow	(gmole/h) (kg/d)	1.0003	0.12633	1.0936				
44	Liquid Volume Flow	(m3/h)	3.664e-005	7.519e-005	4.566e-005				
45	Heat Flow	(kW)	-3.500e-006	-3.110e-005	-0.2005	3.154e-004	-4.846e-002		
46		kJ/kgmole)	-9.675	-42.97	-2.854e+005	3.1346-004	-4.0406-002		
47	Name	, , , , , , , , , , , , , , , , , , , ,	Rcycl Cmp Pwr	H2 Cmp Pwr	Bosch Heat	Electrolysis Pwr	Water Pmp Pwr		
48	Vapour Fraction								
49	Temperature	(C)							
50	Pressure	(kPa)							
51	Molar Flow	(gmole/h)							
52	Mass Flow	(kg/d)							
53	Liquid Volume Flow	(m3/h)							
54	Heat Flow	(kW)	4.180e-003	1.375e-003	-1.658e-002	0.2065	3.025e-009		
55	Molar Enthalpy (kJ/kgmole)							
56 57				Composition					
58	Name		CO2 In	1	2	2r	3		
59	Comp Mole Frac (Carbon)		0.00000 *	0.00000	0.00000	0.00000 *	0.00000		
60	Comp Mole Frac (Oxygen)		0.00000 *	0.00000	0.00000	0.00000 *	0.00000		
61	Comp Mole Frac (H2O)		0.00000 *	0.00000	0.01859	0.01858 *	0.01858		
62	Comp Mole Frac (Methane))	0.00000 *	0.00000	0.19444	0.19380 ° 0.22911 °	0.19380		
63	Comp Mole Frac (CO)		0.00000 *	0.00000	0.22924	0.22911			
104	Comp Mole Frac (Hydroger	1)	0.00000 *	0.00000	0.40538	0.40554 *	0.40554		
64		,							
64 65	Comp Mole Frac (CO2) Hyprotech Ltd.	,	1.00000 *		0.15235		0.15297 Page 1 of 5		

68 Hyprotech Ltd. HYSYS.Plant v2.2.2 (Build 3806) Page 1 of
Licensed to: INL * Specified by user.

2	INL		Case Name:	C:\NASA Final\Bosch 3-	Comp v_2.hsc				
3	HYPROTECH Calgary,	Alberta	Unit Set:	NASA2					
5	CANADA		Date/Time:	Date/Time: Mon Aug 23 10:20:55 2010					
6				•					
7	Workbook:	Case (Main) (continue	(continued)					
9 10		Co	mposition (conti	position (continued)					
11	Name	Carbon Out	4	5	6	Recycle Stream			
12	Comp Mole Frac (Carbon)	1.00000	0.00000	0.00000	0.00000	0.00000			
13	Comp Mole Frac (Oxygen)	0.00000	0.00000	0.00000	0.00000	0.00000			
14 15	Comp Mole Frac (H2O)	0.00000	0.06769	0.06769	0.02003	0.02003			
15 16	Comp Mole Frac (Methane) Comp Mole Frac (CO)	0.00000	0.19936 0.23505	0.19936 0.23505	0.20955 0.24706	0.20955 0.24706			
17	Comp Mole Frac (Hydrogen)	0.00000	0.36555	0.36555	0.38423	0.38423			
18	Comp Mole Frac (CO2)	0.00000	0.13236	0.13236	0.13912	0.13912			
19	Name	Water	Water In	7	8	9			
20	Comp Mole Frac (Carbon)	0.00000	0.00000*	0.00000	0.00000	0.00000			
21	Comp Mole Frac (Oxygen)	0.00000	0.00000 *	0.00000	0.00000	0.00000			
22	Comp Mole Frac (H2O)	0.99989	1.00000 *	1.00000	0.99990	0.00000			
23	Comp Mole Frac (Methane)	0.00000	0.00000 *	0.00000	0.00000	0.00000			
24	Comp Mole Frac (CO)	0.00000	0.00000 *	0.00000	0.00000	0.00000			
25	Comp Mole Frac (Hydrogen)	0.00000	0.00000 *	0.00000	0.00000	0.99990			
26	Comp Mole Frac (CO2)	0.00010	0.00000 *	0.00000	0.00010	0.00010			
27	Name	Oxygen Out	Hydrogen	10					
28	Comp Mole Frac (Carbon)	0.00000	0.00000	0.00000					
29	Comp Mole Frac (Oxygen)	1.00000	0.00000	0.00000					
30	Comp Mole Frac (H2O)	0.00000	0.00000	0.99989					
31	Comp Mole Frac (Methane)	0.00000	0.00000	0.00000					
32	Comp Mole Frac (CO)	0.00000	0.00000	0.00000					
33	Comp Mole Frac (Hydrogen)	0.00000	0.99990	0.00000					
34	Comp Mole Frac (CO2)	0.00000	0.00010	0.00010					
35 36			Heat Exchange	rs					
37	Name	Recuperating HX							
38	Duty (kW)	0.3173							
39	Tube Inlet Temperature (C)	37.40 *							
40	Tube Outlet Temperature (C)	620.3 ⁻							
41	Shell Inlet Temperature (C)	650.0							
42	Shell Outlet Temperature (C)	62.40							
43	UA (W/C)	11.54							
44	LMTD (C)	27.49							
45 46	Minimum Approach (C)	25.00				L			
46 47			Compressors	<u> </u>					
48	Name	CO2 Compressor	Recycle Gas Compre	Hydrogen Compresso					
49	Feed Pressure (kPa)	131.0 *	157.4	101.3					
50	Product Pressure (kPa)	172.4 *	172.4	172.4					
51	Molar Flow (gmole/h)	1.240	49.47	2.605					
52	Energy (kW)	3.154e-004	4.180e-003	1.375e-003					
53	Adiabatic Efficiency	75 *	75 *	75 *					
54	Polytropic Efficiency	76	75	77					
55 56			Pumps						
57	Name	Water Pump							
58	Delta P (kPa)	6.000							
59	Energy (kW)	3.025e-009							
60	Feed Pressure (kPa)	101.3 *							
61	Product Pressure (kPa)	107.3 ⁻							
62	Molar Flow (gmole/h)	7.632e-002							
63	Adiabatic Efficiency (%)	75.00 *							
64									
65									
66	Hyprotech Ltd.	HY:	SYS.Plant v2.2.2 (Buil	d 3806)		Page 2 of 5			
	Licensed to: INI					* Specified by user			

Licensed to: INL *Specified by user.

_										
2	lan.	18.11			Case Name: C	:\NASA Final\Bosch 3	-Comp v_2	2.hsc		
3	HYPROTECH	INL Calgary, A	lberta		Unit Set: N	IASA2				
4 5		CANADA			Date/Time: Mon Aug 23 10:20:55 2010					
6	NA/ a vel ala	l	0 /\/	.:	(4:	-1\				
7	Workb	оок:	Case (IVIa	un) ((continue	a)				
9 10					Unit Ops					
11	Operation Name	Ope	ration Type		Feeds	Products		Ignored	Calc. Level	
12 13	CO2 Compressor	Compres	sor	CO2 Ir	n Cmp Pwr	1		No	500.0 *	
14 15	Recycle Gas Compressor	Compressor		6		Recycle Stream		No	500.0 *	
16	Hydrogen Compressor	Compressor		9	Cmp Pwr	Hydrogen		No	500.0 *	
17 18	Tryurogen Compressor	Compressor		H2 Cm	ıp Pwr	2		140	300.0	
19	M1			Hydrog	gen			No	500.0 *	
20 21				Recyc 10	le Stream	8				
22	M2	Mixer		7				No	500.0 *	
23 24	Recuperating HX	Heat Exc	hanger	2r		3		No	500.0 *	
24 25				5		5 Water				
26	Condenser/Water Separator	Separato	r	AMB C	2	6		No	500.0 *	
27 28	DOV 2	Desirate		2		AMB Q		NI-	2500 !	
29	RCY-3 ADJ-1	Recycle Adjust		2		2r		No No	3500 °	
30	ADJ-2	Adjust						No	3500 °	
31	Bosch Calcs	Spreadsh	eet					No	500.0 *	
32	Bosch Reactor		Sub-Flowsheet	3		4			2500 °	
33 34	BOSON NEGOTO	Ctandara	odb i lowsheet	Bosch 8	Heat	Carbon Out Oxygen Out		No		
35	Electrolysis	Standard	Sub-Flowsheet	_	olysis Pwr	9		No	2500 °	
36	Water Pump	Pump		Water		7		No	500.0 *	
37 38	Valve 1	Valve		Water	Pmp Pwr	10		No	500.0 *	
39										
40 41	Workb	ook:	Bosch R	eact	or (TPL1)					
42					Streams					
43 44	Name		2 @TDL 1	11		Carbon Out @TDI 1	Paudau	ard Q @TPL1	4 @TDI 1	
45	Name Vapour Fraction		3 @TPL1 1.00		1.0000	Carbon Out @TPL1 0.0000	Doddoda	ard Q @ IPL1	4 @TPL1 1.0000	
46	Temperature	(C)	620.		650.00	650.00			650.00 *	
47	Pressure	(kPa)	169.	_	166.37	163.37			163.37	
48	Molar Flow	(gmole/h)	53.2	98	53.222	1.2214			52.001	
49	Mass Flow	(kg/d)	22.2		22.272	0.35208			21.920	
50	Liquid Volume Flow	(m3/h)	2.058e-0		1.983e-003	8.934e-006			1.963e-003	
51	Heat Flow	(kW)	-1.2		-1.184	3.473e-003		5.826e-002	-1.245	
52 53	Molar Enthalpy (k. Name	J/kgmole)	-8.276e+0		-8.006e+004 osch Heat @TPL1	1.024e+004			-8.621e+004	
54	Vapour Fraction				osch neat @TPLT					
55	Temperature	(C)								
	Pressure	(kPa)								
56 57		(gmole/h)								
58	Mass Flow	(kg/d)								
59	Liquid Volume Flow	(m3/h)								
60	Heat Flow	(kW)	4.167e-0		-1.658e-002					
61 62	Molar Enthalpy (k	J/kgmole)					<u> </u>			
63										
64										
64 65										
66	Hyprotech Ltd.			HYSYS	.Plant v2.2.2 (Build	3806)			Page 3 of 5	
_	Linemand by INII		_							

Licensed to: INL Specified by user.

4							
2		INL		Case Name:	C:\NASA Final\Bosch 3	-Comp v_2.hsc	
3	HYPROTECH	Calgary, /	Alberta	Unit Set:	NASA2		
5		0,10,0,1		Date/Time:	Mon Aug 23 10:20:55 2	2010	
6 7 8	Workb	ook:	Bosch Re	eactor (TPL	1) (continue	d)	
9				Material Strea	ıms		
11	Name		3 @TPL1	11 @TPL1	Carbon Out @TPL1	4 @TPL1	
12	Comp Mole Frac (Carbon)		0.0000			0.00000	
13	Comp Mole Frac (Oxygen)		0.0000			0.00000	
14 15	Comp Mole Frac (H2O)		0.0185			0.06769	
15 16	Comp Mole Frac (Methane)	0.1938 0.2291			0.19936 0.23505		
17	Comp Mole Frac (Hydrogen)	Comp Mole Frac (CO) Comp Mole Frac (Hydrogen)			0.00000	0.36555	
18	Comp Mole Frac (CO2)				0.00000	0.13236	
19 20				Unit Ops			
21	Operation Name	Оре	eration Type	Feeds	Products	Ignored	Calc. Level
22				3 @TPL1	10 @TPL1		
23	RWGS Reaction @TPL1	Gibbs Re	eactor	RWGS Q @TPL1	11 @TPL1	No	500.0 *
24 25				11.07011	RWGS Q @TPL1		
25 26	Boudourd Reaction @TPL1	Equilibriu	ım Reactor	11 @TPL1 Boudouard Q @TPL1	Carbon Out @TPI 4 @TPL1	_1 No	500.0 *
27	boddodid Neaction @TFLT	Lquiibiic	iii iteactoi	Boddodaid & @IFEI	Boudouard Q @Ti		300.0
28	SPRDSHT-1 @TPL1	Spreadsl	neet			No	500.0 *
29	Manulaha	l::	Clootrol.	oio (TDL 0)			
30 31	Workd	оок:	Electroly	sis (TPL2)			
32 33				Streams			
34	Name		8 @TPL2	10 @TPL2	9 @TPL2	Oxygen @TPL2	Electrolysis Pwr @TF
35	Vapour Fraction		0.000			1.0000	
36	Temperature	(C)	24.89	7 24.897	24.897	24.996	
37	Pressure	(kPa)	107.3			101.32	
38 39	Molar Flow Mass Flow	(gmole/h)	2.605			1.3025	
40	Liquid Volume Flow	(kg/d) (m3/h)	1.126 4.704e-00			1.0003 3.664e-005	
41	Heat Flow	(kW)	-0.206			-3.500e-006	0.2065
42	Molar Enthalpy (k.	J/kgmole)	-2.854e+00	5 -31.87	-42.97	-9.675	
43 44				Material Strea	ims		
45	Name		8 @TPL2	9 @TPL2	10 @TPL2	Oxygen @TPL2	
46	Comp Mole Frac (Carbon)		0.0000			0.00000	
47 48	Comp Mole Frac (Oxygen)		0.0000			1.00000	
48 49	Comp Mole Frac (H2O) Comp Mole Frac (Methane)		0.9999			0.00000	
50	Comp Mole Frac (CO)		0.0000			0.00000	
51	Comp Mole Frac (Hydrogen)		0.0000			0.00000	
52	Comp Mole Frac (CO2)		0.0001	0.00010	0.00007	0.00000	
53 54				Unit Ops			
54 55 56	Operation Name	Ope	eration Type	Feeds	Products	Ignored	Calc. Level
56		,		8 @TPL2	17 @TPL2		
57 58	Electrolysis @TPL2	Conversi	ion Reactor	Electrolysis Pwr @TPL		No	500.0 *
58 59			10 @TPL2	Electrolysis Pwr @ 9 @TPL2	gIPL2		
60	H2/O2 Splitter @TPL2 Component Splitter		.0 W 11 CZ	Oxygen @TPL2	No	500.0 *	
61	SET-1 @TPL2 Set				No	500.0 °	
62	SET-2 @TPL2 Set				No	500.0 *	
63 64	SET-3 @TPL2 SET-4 @TPL2	Set Set				No No	500.0 °
65	SE1-4 WIFEZ	Set				140	500.0
66	Hyprotech Ltd.			HYSYS.Plant v2.2.2 (B	uild 3806)		Page 4 of 5
	Licensed to: INL						* Specified by user.

A-9

_										
1 2	INL			Case N	ame: C:\NAS	A Final\Bo	sch 3-Comp v	_2.hsc		
3	HYPROTESH Calgary,			Unit Set	:: NASA2	!				
4 5	CANADA			Date/Tir	Date/Time: Mon Aug 23 10:20:55 2010					
6	E acciditación	D	al							
7	Equilibriu	ım: B	oudo	uara						
9 10				STOICHI	OMETRY					
11	Component			Molecula	r Weight		5	Stoichiomet	ric Coefficient	
12 13		CO2				28.01 44.01				
14		Carbon				12.01			1	
15 16	Balance Error: 0	0.0000				Read	tion Heat: -	8.631e+004	kJ/kgmole	
17				BA	SIS				•	
18 19	Paris.	Dhann		Appr	oach		Min. Temp		Max. Temp	
20 21	Basis	Phase	urPhase		C)		(C)	3.15	(C) 3000.0	
22	Activity	PARAM			-21	3.15	3000.0			
23 24				PARAIN	EIERO					
25			,	Source : K	Vs. T Table					
26 27	Coeff A Coeff B			-21.68 2.078e+004	R2 T High				1.000000	
28	Coeff C			6.615e-002	T Low					
29 30	Coeff D			-3.643e-005						
31	Temperature		Keq			KCalc		Р	ercentage Error	
32 33	(C) 25.000 °			1.039e+021 '		1	.039e+021 *		1.641e-002	
34	127.00			2.026e+013 *			026e+013 *		-1.147e-002	
35 36	227.00 °			6.330e+008 * 6.290e+005 *			335e+008 * 287e+005 *		-7.829e-002 4.151e-002	
37	427.00 *			4500 '			4501 *		-2.620e-002	
38	527.00 *			111.0 *			110.8 *		0.1924	
39 40	627.00 *			6.210 *			6.211 *		-1.484e-002	
40 41	727.00 ° 827.00 °			0.6190 * 9.390e-002 *		-	0.6195 °		-8.445e-002 -5.988e-002	
42	927.00 *			1.950e-002			.951e-002 *		-5.029e-002	
43	1027.0 *			5.160e-003 *			.159e-003 *		2.623e-002	
44	1127.0 *			1.650e-003 *		1	.649e-003 °		4.861e-002	
45 46 47	Conversion	on: El	ectro	lysis						
48				STOICHI	OMETRY					
49 50	Component			Mole V				Stoichiom	etric Coeff.	
51	H2O					18.015			-2	
52	Hydrogen					2.016			2	
53	Oxygen					32.000			1	
54 55										
56	Balance Error: 0	0.0000				Rea	ction Heat: 2	.410e+005	kJ/kgmole	
56 57 58 59				BA	SIS				-	
58 59	Base Component: H2O		Conver	sion Percent:		,	Reaction	on Phase:	LiquidPhase	
60				PARAM						
62										
60 61 62 63 64										
64 65										
66	Hyprotech Ltd.		H	YSYS.Plant v2.	2.2 (Build 3806	3)			Page 5 of 5	
	Licensed to: INL								* Specified by user.	

A-10

A.2 Bosch Process with 3 Compressors with Sub Atmospheric Conditions

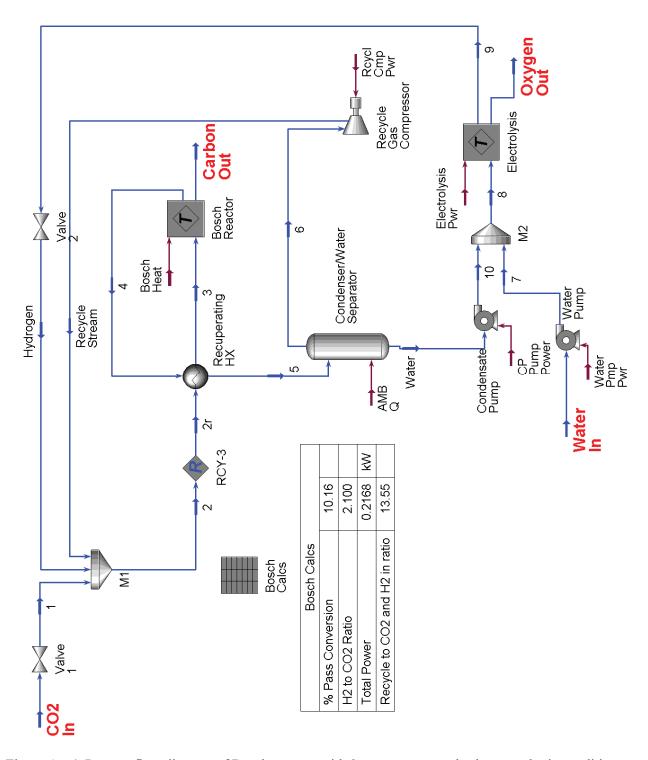


Figure A - 4 Process flow diagram of Bosch process with 3 compressors and sub atmospheric conditions

_									
2	Dec		Case Name:	C:\NASA Final\Bosch 3-	Comp sub atm.hsc				
3	INL Calgary,	Alberta	Unit Set:	NASA					
5	CANADA		Date/Time:	Date/Time: Mon Aug 23 10:24:41 2010					
6									
7	Workbook:	Case (Main	1)						
9			Streams	Streams					
11	Name	CO2 In	1	Hydrogen	Recycle Stream	2			
12	Vapour Fraction	1.0000	1.0000	1.0000	1.0000	1.0000			
13	Temperature (C)	21.111 *	20.569	24.882	47.245	45.592			
14	Pressure (kPa)	131.00 *	82.290 *	82.290	82.290	82.290			
15	Molar Flow (gmole/h)	1.2404	1.2404	2.6049	54.007	57.853			
16	Mass Flow (kg/d)	1.3102 *	1.3102	0.12614	19.464	20.900			
17	Liquid Volume Flow (m3/h)	6.614e-005	6.614e-005	7.517e-005	1.878e-003	2.019e-003			
18	Heat Flow (kW)	-0.1358	-0.1358	-1.361e-005	-1.361	-1.497			
19	Molar Enthalpy (kJ/kgmole)	-3.940e+005	-3.940e+005	-18.81	-9.072e+004	-9.314e+004			
20	Name	2r	3	Carbon Out	4 .0000	5			
21	Vapour Fraction	1.0000	1.0000	1.0000 *	1.0000	1.0000			
22	Temperature (C)	45.606 *	618.21 *	650.00	650.00	70.605			
23	Pressure (kPa)	82.290 *	79.290	73.290	73.290	70.290			
24	Molar Flow (gmole/h)	57.813	57.813	1.2478	56.531	56.531			
25	Mass Flow (kg/d)	20.915	20.915	0.35969	20.555	20.555			
26	Liquid Volume Flow (m3/h)	2.018e-003	2.018e-003	9.127e-006	1.923e-003	1.923e-003			
27	Heat Flow (kW)	-1.499	-1.187	3.548e-003	-1.206	-1.518			
28	Molar Enthalpy (kJ/kgmole)	-9.332e+004	-7.390e+004	1.024e+004	-7.681e+004	-9.667e+004			
29	Name	6	Water	Water In	7	8			
30	Vapour Fraction	1.0000	0.0000	0.0000	0.0000	0.0000			
31	Temperature (C)	25.000 *	25.000	21.111 *	21.112	24.883			
32	Pressure (kPa)	67.290	67.290	101.32 '	107.32 '	107.32			
33	Molar Flow (gmole/h)	54.007	2.5239	8.0951e-002	8.0951e-002	2.6049			
34	Mass Flow (kg/d)	19.464	1.0913	3.5000e-002 *	3.5000e-002	1.1263			
35 36	Liquid Volume Flow (m3/h)	1.878e-003	4.556e-005	1.461e-006	1.461e-006	4.703e-005			
37	Heat Flow (kW)	-1.371	-0.2001	-6.425e-003	-6.425e-003	-0.2065			
38	Molar Enthalpy (kJ/kgmole)	-9.141e+004	-2.854e+005	-2.857e+005	-2.857e+005	-2.854e+005			
39	Name	Oxygen Out 1.0000	1.0000	0.0000	AMB Q	Reycl Cmp Pwr			
40	Vapour Fraction								
41	Temperature (C) Pressure (kPa)	24.981 101.32	24.883 101.32	25.004 107.32					
42	, ,	1.3023	2.6049	2.5239					
43	Molar Flow (gmole/h) Mass Flow (kg/d)	1.0002	0.12614	1.0913					
44	Liquid Volume Flow (m3/h)	3.663e-005	7.517e-005	4.556e-005					
45	Heat Flow (kW)	-3.650e-006	-1.361e-005	-0.2001	-5.330e-002	1.025e-002			
46	Molar Enthalpy (kJ/kgmole)	-3.6506-006	-1.3616-005	-2.854e+005	-3.3306-002	1.0236-002			
47	Name (k5/kginole)	Bosch Heat	Electrolysis Pwr	Water Pmp Pwr	CP Pump Power				
48	Vapour Fraction		Liectrolysis P Wi						
49	Temperature (C)								
50	Pressure (kPa)								
51	Molar Flow (gmole/h)								
52	Mass Flow (kg/d)								
53	Liquid Volume Flow (m3/h)								
54	Heat Flow (kW)	-1.587e-002	0.2065	3.206e-009	6.693e-007				
55	Molar Enthalpy (kJ/kgmole)								
56 57			Composition						
58	Name	CO2 In	1	2	2r	3			
59	Comp Mole Frac (Carbon)	0.00000 *	0.00000	0.00000	0.00000 *	0.00000			
60	Comp Mole Frac (Oxygen)	0.00000	0.00000	0.00000	0.00000 *	0.00000			
61	Comp Mole Frac (H2O)	0.00000	0.00000	0.04339	0.04344 *	0.04344			
62	Comp Mole Frac (Methane)	0.00000	0.00000	0.07363	0.07339 *	0.07339			
63	Comp Mole Frac (CO)	0.00000	0.00000	0.21219	0.21244 *	0.21244			
64	Comp Mole Frac (Hydrogen)	0.00000	0.00000	0.53282	0.53236 *	0.53236			
65	Comp Mole Frac (CO2)	1.00000	1.00000	0.13797	0.13838 *	0.13838			
66	Hyprotech Ltd.		SYS.Plant v2.2.2 (Buil		0.10000	Page 1 of 5			
~~	rijprotoon Eta.	FIII		u 0000)		r ago i oi o			

68 Hyprotech Ltd. HYSYS.Plant v2.2.2 (Build 3806) Page 1 of
Licensed to: INL * Specified by user.

_								
1	NI NI		Case Name:	C:\NASA Final\Bosch 3	-Comp sub atm.hsc			
3	INL Calgary,	Alberta	Unit Set:	NASA				
4 5	CANADA		Date/Time:	Date/Time: Mon Aug 23 10:24:41 2010				
6								
7	Workbook:	Case (Main) (continue	ed)				
9								
10			mposition (cont					
11 12	Name	Carbon Out 1.00000	0.00000	5 0.00000	0.00000	Recycle Stream 0.00000		
13	Comp Mole Frac (Carbon) Comp Mole Frac (Oxygen)	0.00000	0.00000	0.00000	0.00000	0.00000		
14	Comp Mole Frac (H2O)	0.00000	0.08905	0.08905	0.04648	0.04648		
15	Comp Mole Frac (Methane)	0.00000	0.07535	0.07535	0.07887	0.07887		
16	Comp Mole Frac (CO)	0.00000	0.21715	0.21715	0.22730	0.22730		
17	Comp Mole Frac (Hydrogen)	0.00000	0.49920	0.49920	0.52253	0.52253		
18	Comp Mole Frac (CO2)	0.00000	0.11926	0.11926	0.12483	0.12483		
19	Name	Water	Water In	7	8	9		
20	Comp Mole Frac (Carbon)	0.00000	0.00000 *	0.00000	0.00000	0.00000		
21	Comp Mole Frac (Oxygen)	0.00000	0.00000 *	0.00000	0.00000	0.00000		
22	Comp Mole Frac (H2O)	0.99996	1.00000 *	1.00000	0.99996	0.00000		
23	Comp Mole Frac (Methane)	0.00000	0.00000 *	0.00000	0.00000	0.00000		
24	Comp Mole Frac (CO)	0.00000	0.00000 *	0.00000	0.00000	0.00000		
25	Comp Mole Frac (Hydrogen)	0.00000	0.00000 *	0.00000	0.00000	0.99996		
26	Comp Mole Frac (CO2)	0.00004	0.00000 *	0.00000	0.00004	0.00004		
27	Name	Oxygen Out	Hydrogen	10				
28	Comp Mole Frac (Carbon)	0.00000	0.00000	0.00000				
29	Comp Mole Frac (Oxygen)	1.00000	0.00000	0.00000				
30	Comp Mole Frac (H2O)	0.00000	0.00000	0.99996				
31	Comp Mole Frac (Methane)	0.00000	0.00000	0.00000				
32	Comp Mole Frac (CO)	0.00000	0.00000	0.00000				
33 34	Comp Mole Frac (Hydrogen)	0.00000	0.99996 0.00004	0.00000 0.00004				
35	Comp Mole Frac (CO2)	0.00000						
36			Heat Exchange	rs				
37	Name	Recuperating HX						
38	Duty (kW)	0.3120						
39	Tube Inlet Temperature (C)	45.61 ⁻						
40	Tube Outlet Temperature (C)	618.2 ⁻						
41	Shell Inlet Temperature (C)	650.0						
42	Shell Outlet Temperature (C)	70.60						
43	UA (kJ/C-h)	39.47						
44	LMTD (C)	28.45						
45 46	Minimum Approach (C)	25.00						
46 47			Compressors	;				
48	Name	Recycle Gas Compre						
49	Feed Pressure (kPa)	67.29						
50	Product Pressure (kPa)	82.29						
51	Molar Flow (gmole/h)	54.01						
52	Energy (kW)	1.025e-002						
53	Adiabatic Efficiency	75 °						
54	Polytropic Efficiency	76						
55			Pumps					
56 57	Name	Water Pump	Condensate Pump					
58	Delta P (kPa)	5.996	40.03					
59	Energy (kW)	3.206e-009	6.693e-007					
60	Feed Pressure (kPa)	101.3	67.29					
61	Product Pressure (kPa)	107.3	107.3					
62	Molar Flow (gmole/h)	8.095e-002	2.524					
63	Adiabatic Efficiency (%)	75.00 *	75.00 *					
64	, (10)				1			
65								
66	Hyprotech Ltd.	HYS	SYS.Plant v2.2.2 (Buil	d 3806)		Page 2 of 5		
_	Licensed to: INI					* Specified by user		

Licensed to: INL *Specified by user.

1					Case Name: C	:\NASA Final\Bosch 3-	Comp sub	atm.hsc		
3	HYPROTECH	INL Calgary, A	lberta		Unit Set: N	IASA				
5		CANADA			Date/Time: Mon Aug 23 10:24:41 2010					
6	184I-I-	•	0 (14		1 1	-15				
7	Workb	оок:	Case (IVIa	un)	(continue	a)				
9					Unit Ops					
11	Operation Name	Ope	ration Type		Feeds	Products		Ignored	Calc. Level	
12 13	Recycle Gas Compressor	Compres	sor	6	al Ones Design	Recycle Stream		No	500.0 *	
14				1	cl Cmp Pwr	2				
15	M1	Mixer		Rec	ycle Stream			No	500.0 *	
16 17				Hydi 10	rogen	8				
18	M2	Mixer						No	500.0 *	
19	Recuperating HX	Recuperating HX Heat Exchanger				3		No	500.0 *	
20 21				5		5 Water				
22	Condenser/Water Separator	Separato	r	AME	3 Q	6		No	500.0 *	
23		·				AMB Q				
24	RCY-3	Recycle		2		2r		No	3500 *	
25 26	ADJ-1 ADJ-2	Adjust Adjust						No No	3500 °	
27	ADJ-3	Adjust						No	3500 *	
28	Bosch Calcs	Spreadsh	eet					No	500.0 *	
29	Bosch Reactor	Standard	Sub-Flowsheet	3		4		No	2500 °	
30	DOSCIT REDUCE	Otaridard	Oub-1 lowsheet	_	ch Heat	Carbon Out		140	2000	
31 32	Electrolysis	Standard	Sub-Flowsheet	8 Flec	trolysis Pwr	Oxygen Out		No	2500 °	
33		_			er In	7				
34	Water Pump	Pump			er Pmp Pwr			No	500.0	
35 36	Condensate Pump	Pump		Wat		10		No	500.0 *	
37	Valve 1	Valve		CO2	Pump Power	1		No	500.0 *	
38	Valve 2	Valve		9		Hydrogen		No	500.0 *	
39										
40 41	Workb	ook:	Bosch R	eac	tor (TPL1)					
42 43					Streams					
44	Name		3 @TPL1		11 @TPL1	Carbon Out @TPL1	Boudou	ard Q @TPL1	4 @TPL1	
45	Vapour Fraction		1.00	00	1.0000	0.0000			1.0000	
46	Temperature	(C)	618.	-	650.00 *	650.00			650.00 *	
47 48	Pressure Malas Flavo	(kPa)	79.2		76.290	73.290			73.290	
49	Molar Flow Mass Flow	(gmole/h) (kg/d)	57.8 20.9		57.779 20.915	1.2478 0.35969			56.531 20.555	
50	Liquid Volume Flow	(m3/h)	2.018e-0	_	1.944e-003	9.127e-006			1.923e-003	
51	Heat Flow	(kW)	-1.1		-1.143	3.548e-003		5.951e-002	-1.206	
52	Molar Enthalpy (k.	J/kgmole)	-7.390e+0	_	-7.122e+004	1.024e+004			-7.681e+004	
53 54	Name		RWGS Q @TPL		Bosch Heat @TPL1					
54	Vapour Fraction Temperature	(C)								
55 56	Pressure	(kPa)								
57 58		(gmole/h)								
58	Mass Flow	(kg/d)								
59	Liquid Volume Flow	(m3/h)								
60 61	Heat Flow Molar Enthalpy (k.	(kW) J/kgmole)	4.364e-0	02	-1.587e-002					
62	molar Enthalpy (K	orkginole)	1							
63										
63 64										
					10 Pt - 1 - 2	2000)				
66	Hyprotech Ltd.			HYSY	'S.Plant v2.2.2 (Build	3806)			Page 3 of 5	

68 Hyprotech Ltd. HYSYS.Plant v2.2.2 (Build 3806) Page 3 of Licensed to: INL *Specified by user.

2		INL		Case Name:	C:\NASA Final\Bosch 3-	Comp sub a	atm.hsc	
3	HYPROTECH	Calgary, A	lberta	Unit Set:	NASA			
5	part of the same o	0,40,0,1		Date/Time:	Mon Aug 23 10:24:41 2	010		
6	M/ a ulula	!	Danah Da	4- ·· /TDL 4	\	-1\		
7 8	VVOIKD	оок:	Bosch Re	actor (TPL1) (continue	a)		
9 10				Material Strean	ns			
11	Name		3 @TPL1	11 @TPL1	Carbon Out @TPL1	Carbon Out @TPL1 4 @TPL1		
12	Comp Mole Frac (Carbon)		0.00000		1.00000		0.00000	
13 14					0.00000		0.00000	
15	Comp Mole Frac (H2O) Comp Mole Frac (Methane)		0.04344 0.07339		0.00000		0.08905	
16	Comp Mole Frac (CO)		0.21244		0.00000		0.21715	
17	Comp Mole Frac (Hydrogen)		0.53236		0.00000		0.49920	
18	Comp Mole Frac (CO2)		0.13838		0.00000		0.11926	
19 20				Unit Ops				
21	Operation Name	Ope	ration Type	Feeds	Products		Ignored	Calc. Level
22				3 @TPL1	10 @TPL1			
23	RWGS Reaction @TPL1	Gibbs Re	actor	RWGS Q @TPL1	11 @TPL1		No	500.0 *
24					RWGS Q @TPL1			
25				11 @TPL1	Carbon Out @TPL	.1		
26	Boudourd Reaction @TPL1	Equilibriu	m Reactor	Boudouard Q @TPL1	4 @TPL1		No	500.0 *
27					Boudouard Q @TF	PL1		
28 29	SPRDSHT-1 @TPL1	Spreadsh	eet				No	500.0 *
30 31	Workb	ook:	Electrolys	is (TPL2)				
32 33				Streams				
34	Name		8 @TPL2	10 @TPL2	9 @TPL2	Oxygen C	Out @TPL2	Electrolysis Pwr @TF
35	Vapour Fraction		0.0000		1.0000		1.0000	
	Vapour Fraction		0.0000		1.0000			
36	Temperature	(C)	24.883		24.883		24.981	
37	Temperature Pressure	(C) (kPa)		24.883				
37 38	Pressure Molar Flow ((kPa) (gmole/h)	24.883 107.32 2.6049	24.883 104.32 3.9072	24.883 101.32 2.6049		24.981 101.32 1.3023	
37 38 39	Pressure Molar Flow Mass Flow	(kPa) (gmole/h) (kg/d)	24.883 107.32 2.6049 1.1263	24.883 104.32 3.9072 1.1263	24.883 101.32 2.6049 0.12614		24.981 101.32 1.3023 1.0002	
37 38 39 40	Pressure Molar Flow Mass Flow Liquid Volume Flow	(kPa) (gmole/h) (kg/d) (m3/h)	24.883 107.32 2.6049 1.1263 4.703e-005	24.883 104.32 3.9072 1.1263 1.118e-004	24.883 101.32 2.6049 0.12614 7.517e-005		24.981 101.32 1.3023 1.0002 663e-005	
37 38 39 40 41	Pressure Molar Flow Mass Flow Liquid Volume Flow Heat Flow	(kPa) (gmole/h) (kg/d) (m3/h) (kW)	24.883 107.32 2.6049 1.1263 4.703e-005 -0.2065	24.883 104.32 3.9072 1.1263 1.118e-004 -1.726e-005	24.883 101.32 2.6049 0.12614 7.517e-005 -1.361e-005		24.981 101.32 1.3023 1.0002 663e-005 650e-006	
37 38 39 40 41 42	Pressure Molar Flow Mass Flow Liquid Volume Flow Heat Flow	(kPa) (gmole/h) (kg/d) (m3/h)	24.883 107.32 2.6049 1.1263 4.703e-005	24.883 104.32 3.9072 1.1263 1.118e-004 -1.726e-005 -15.90	24.883 101.32 2.6049 0.12614 7.517e-005 -1.361e-005		24.981 101.32 1.3023 1.0002 663e-005	
37 38 39 40 41 42	Pressure Molar Flow (Mass Flow Liquid Volume Flow Heat Flow Molar Enthalpy (k.)	(kPa) (gmole/h) (kg/d) (m3/h) (kW)	24.883 107.32 2.6049 1.1263 4.703e-005 -0.2065 -2.854e+005	24.883 104.32 3.9072 1.1263 1.118e-004 -1.726e-005 -15.90 Material Strean	24.883 101.32 2.6049 0.12614 7.5176-005 -1.361e-005 -18.81	-3.	24.981 101.32 1.3023 1.0002 663e-005 650e-006 -10.09	
37 38 39 40 41 42 43 44 45	Pressure Molar Flow Mass Flow Liquid Volume Flow Heat Flow Molar Enthalpy (k.)	(kPa) (gmole/h) (kg/d) (m3/h) (kW)	24.883 107.32 2.6049 1.1263 4.703e-005 -0.2065 -2.854e+005	24.883 104.32 3.9072 1.1263 1.118e-004 -1.726e-005 -15.90 Material Stream 9 @TPL2	24.883 101.32 2.6049 0.12614 7.517e-005 -1.361e-005 -18.81 15	-3.	24.981 101.32 1.3023 1.0002 663e-005 650e-006 -10.09	
37 38 39 40 41 42 43 44 45	Pressure Molar Flow Mass Flow Liquid Volume Flow Heat Flow Molar Enthalpy (ku	(kPa) (gmole/h) (kg/d) (m3/h) (kW)	24.883 107.32 2.6049 1.1263 4.703e-005 -0.2065 -2.854e+006	24.883 104.32 3.9072 1.1263 1.118e-004 -1.726e-005 -15.90 Material Stream 9 @TPL2	24.883 101.32 2.6049 0.12614 7.517e-005 -1.361e-005 -18.81 10 @TPL2 0.00000	-3.	24.981 101.32 1.3023 1.0002 663e-005 650e-006 -10.09 Out @TPL2 0.00000	
37 38 39 40 41 42 43 44 45 46 47	Pressure Molar Flow Mass Flow Liquid Volume Flow Heat Flow Molar Enthalpy (k.) Name Comp Mole Frac (Carbon) Comp Mole Frac (Oxygen)	(kPa) (gmole/h) (kg/d) (m3/h) (kW)	24.883 107.32 2.6049 1.1263 4.703e-005 -0.2065 -2.854e+005 8 @TPL2 0.00000 0.00000	24.883 104.32 3.9072 1.1263 1.118e-004 -1.726e-005 -15.90 Material Stream 9 @TPL2 0.00000 0.00000	24.883 101.32 2.6049 0.12614 7.517e-005 -1.361e-005 -18.81 15 10 @TPL2 0.00000 0.33331	-3.	24.981 101.32 1.3023 1.0002 663e-005 650e-006 -10.09 Dut @TPL2 0.00000 1.00000	
37 38 39 40 41 42 43 44 45 46 47	Pressure Molar Flow Mass Flow Liquid Volume Flow Heat Flow Molar Enthalpy (ku Name Comp Mole Frac (Carbon) Comp Mole Frac (Oxygen) Comp Mole Frac (H2O)	(kPa) (gmole/h) (kg/d) (m3/h) (kW)	24.883 107.32 2.6049 1.1263 4.703e-005 -0.2065 -2.854e+005 8 @TPL2 0.00000 0.00000	24.883 104.32 3.9072 1.1263 1.118e-004 -1.726e-005 -15.90 Material Strean 9 @TPL2 0.00000 0.00000 0.00000	24.883 101.32 2.6049 0.12614 7.517e-005 -1.361e-005 -18.81 10 @TPL2 0.00000	-3.	24.981 101.32 1.3023 1.0002 663e-005 650e-006 -10.09 20t @TPL2 0.00000 1.00000	
37 38 39 40 41 42 43 44 45 46 47 48	Pressure Molar Flow Mass Flow Liquid Volume Flow Heat Flow Molar Enthalpy (k.) Name Comp Mole Frac (Carbon) Comp Mole Frac (Oxygen)	(kPa) (gmole/h) (kg/d) (m3/h) (kW)	24.883 107.32 2.6049 1.1263 4.703e-005 -0.2065 -2.854e+005 8 @TPL2 0.00000 0.00000	24.883 104.32 3.9072 1.1263 1.118e-004 -1.726e-005 -15.90 Material Strean 9 @TPL2 0.00000 0.00000 0.00000 0.00000	24.883 101.32 2.6049 0.12614 7.517e-005 -1.361e-005 -18.81 15 10 @TPL2 0.00000 0.33331 0.00000	-3.	24.981 101.32 1.3023 1.0002 663e-005 650e-006 -10.09 Dut @TPL2 0.00000 1.00000	
37 38 39 40 41 42 43 44 45 46 47 48 49 50	Pressure Molar Flow Mass Flow Liquid Volume Flow Heat Flow Molar Enthalpy (ku Name Comp Mole Frac (Carbon) Comp Mole Frac (Oxygen) Comp Mole Frac (H2O) Comp Mole Frac (Methane)	(kPa) (gmole/h) (kg/d) (m3/h) (kW)	24.883 107.32 2.6049 1.1263 4.703e-005 -0.2065 -2.854e+005 8 @TPL2 0.00000 0.00000 0.99996 0.00000	24.883 104.32 3.9072 1.1263 1.118e-004 -1.726e-005 -15.90 Material Strean 9 @TPL2 0.00000 0.00000 0.00000 0.00000 0.00000	24.883 101.32 2.6049 0.12614 7.517e-005 -1.361e-005 -18.81 1S 10 @TPL2 0.00000 0.33331 0.00000 0.00000	-3.	24.981 101.32 1.3023 1.0002 663e-005 650e-006 -10.09 20tt @TPL2 0.00000 1.00000 0.00000	
37 38 39 40 41 42 43 44 45 46 47 48 49 50	Pressure Molar Flow Mass Flow Liquid Volume Flow Heat Flow Molar Enthalpy (k.) Name Comp Mole Frac (Carbon) Comp Mole Frac (Daygen) Comp Mole Frac (Methane) Comp Mole Frac (Methane) Comp Mole Frac (CO)	(kPa) (gmole/h) (kg/d) (m3/h) (kW)	24.883 107.32 2.6049 1.1263 4.703e-005 -0.2065 -2.854e+005 8 @TPL2 0.00000 0.00000 0.99996 0.00000	24.883 104.32 3.9072 1.1263 1.118e-004 -1.726e-005 -15.90 Material Strean 9 @TPL2 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.99996	24.883 101.32 2.6049 0.12614 7.517e-005 -1.361e-005 -18.81 15 10 @TPL2 0.00000 0.33331 0.00000 0.00000 0.00000	-3.	24.981 101.32 1.3023 1.0002 663e-005 650e-006 -10.09 0.00000 1.00000 0.00000 0.00000	
37 38 39 40 41 42 43 44 45 46 47 48 49 50	Pressure Molar Flow Liquid Volume Flow Heat Flow Molar Enthalpy Name Comp Mole Frac (Carbon) Comp Mole Frac (H2O) Comp Mole Frac (H2O) Comp Mole Frac (CO) Comp Mole Frac (CO) Comp Mole Frac (Hydrogen)	(kPa) (gmole/h) (kg/d) (m3/h) (kW)	24.883 107.32 2.6049 1.1263 4.703e-005 -0.2065 -2.854e+005 8 @TPL2 0.00000 0.00000 0.99996 0.00000 0.00000	24.883 104.32 3.9072 1.1263 1.118e-004 -1.726e-005 -15.90 Material Strean 9 @TPL2 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.99996	24.883 101.32 2.6049 0.12614 7.517e-005 -1.361e-005 -18.81 10 @TPL2 0.00000 0.33331 0.00000 0.00000 0.00000 0.00000	-3.	24.981 101.32 1.3023 1.0002 663e-005 663e-006 -10.09 0ut @TPL2 0.00000 1.00000 0.00000 0.00000 0.00000	
37 38 39 40 41 42 43 44 45 46 47 48 49 50	Pressure Molar Flow Liquid Volume Flow Heat Flow Molar Enthalpy Name Comp Mole Frac (Carbon) Comp Mole Frac (H2O) Comp Mole Frac (H2O) Comp Mole Frac (CO) Comp Mole Frac (CO) Comp Mole Frac (Hydrogen)	(kPa) (gmole/h) (kg/d) (m3/h) (kW) J/kgmole)	24.883 107.32 2.6049 1.1263 4.703e-005 -0.2065 -2.854e+005 8 @TPL2 0.00000 0.00000 0.99996 0.00000 0.00000	24.883 104.32 3.9072 1.1263 1.118e-004 -1.726e-005 -15.90 Material Strean 9 @TPL2 0.00000 0.00000 0.00000 0.00000 0.00000 0.099996 0.00004	24.883 101.32 2.6049 0.12614 7.517e-005 -1.361e-005 -18.81 10 @TPL2 0.00000 0.33331 0.00000 0.00000 0.00000 0.00000	-3.	24.981 101.32 1.3023 1.0002 663e-005 650e-006 -10.09 Dut @TPL2 0.00000 1.00000 0.00000 0.00000 0.00000 0.00000 0.00000	
37 38 39 40 41 42 43 44 45 46 47 48 49 50 51 52 53 54 55 56	Pressure Molar Flow Mass Flow Liquid Volume Flow Heat Flow Molar Enthalpy (Kulture) Name Comp Mole Frac (Carbon) Comp Mole Frac (Oxygen) Comp Mole Frac (H2O) Comp Mole Frac (Methane) Comp Mole Frac (CO) Comp Mole Frac (CO) Comp Mole Frac (CO) Comp Mole Frac (CO)	(kPa) (gmole/h) (kg/d) (m3/h) (kW) J/kgmole)	24.883 107.32 2.6049 1.1263 4.703e-005 -0.2065 -2.854e+005 8 @TPL2 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	24.883 104.32 3.9072 1.1263 1.118e-004 -1.726e-005 -15.90 Material Stream 9 @TPL2 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.99996 0.00004 Unit Ops	24.883 101.32 2.6049 0.12614 7.517e-005 -1.361e-005 -18.81 10 @TPL2 0.00000 0.33331 0.00000 0.00000 0.00000 0.66666 0.000003	-3.	24.981 101.32 1.3023 1.0002 663e-005 663e-006 -10.09 0ut @TPL2 0.00000 1.00000 0.00000 0.00000 0.00000	0.2065
37 38 39 40 41 42 43 44 45 46 47 48 49 50 51 52 53 54 55 56	Pressure Molar Flow Mass Flow Liquid Volume Flow Heat Flow Molar Enthalpy (Kulture) Name Comp Mole Frac (Carbon) Comp Mole Frac (Oxygen) Comp Mole Frac (H2O) Comp Mole Frac (Methane) Comp Mole Frac (CO) Comp Mole Frac (CO) Comp Mole Frac (CO) Comp Mole Frac (CO)	(kPa) (gmole/h) (kg/d) (m3/h) (kW) J/kgmole)	24.883 107.32 2.6049 1.1263 4.703e-005 -0.2065 -2.854e+005 8 @TPL2 0.00000 0.00000 0.09996 0.00000 0.00000 0.00000 0.00000	24.883 104.32 3.9072 1.1263 1.118e-004 -1.726e-005 -15.90 Material Strean 9 @TPL2 0.00000 0.00000 0.00000 0.00000 0.00000 0.99996 0.00004 Unit Ops	24.883 101.32 2.6049 0.12614 7.517e-005 -1.361e-005 -18.81 10 @TPL2 0.00000 0.33331 0.00000 0.00000 0.00000 0.06666 0.00003 Products 17 @TPL2 10 @TPL2	-3.	24.981 101.32 1.3023 1.0002 663e-005 650e-006 -10.09 Dut @TPL2 0.00000 1.00000 0.00000 0.00000 0.00000 0.00000 0.00000	0.2065
37 38 39 40 41 42 43 44 45 46 47 48 49 50 51 52 53 54 55 56 57 58	Pressure Molar Flow Mass Flow Liquid Volume Flow Heat Flow Molar Enthalpy (ku Name Comp Mole Frac (Carbon) Comp Mole Frac (Oxygen) Comp Mole Frac (H2O) Comp Mole Frac (Methane) Comp Mole Frac (CO) Comp Mole Frac (CO) Comp Mole Frac (CO) Comp Mole Frac (CO2) Operation Name	(kPa) (gmole/h) (kg/d) (m3/h) (kW) J/kgmole)	24.883 107.32 2.6049 1.1263 4.703e-005 -0.2065 -2.854e+005 8 @TPL2 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	24.883 104.32 3.9072 1.1263 1.118e-004 -1.726e-005 -15.90 Material Strean 9 @TPL2 0.00000 0.00000 0.00000 0.00000 0.00000 0.99996 0.00004 Unit Ops Feeds 8 @TPL2 Electrolysis Pwr @TPL2	24.883 101.32 2.6049 0.12614 7.517e-005 -1.361e-005 -1.881 10 @TPL2 0.00000 0.33331 0.00000 0.00000 0.00000 0.66666 0.00003 Products 17 @TPL2 10 @TPL2 Electrolysis Pwr @	-3.	24.981 101.32 1.3023 1.0002 663e-005 650e-006 -10.09 Dut @TPL2 0.00000 1.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	0.2065
37 38 39 40 41 42 43 44 45 46 47	Pressure Molar Flow Mass Flow Liquid Volume Flow Heat Flow Molar Enthalpy (ku Name Comp Mole Frac (Carbon) Comp Mole Frac (Oxygen) Comp Mole Frac (H2O) Comp Mole Frac (Methane) Comp Mole Frac (CO) Comp Mole Frac (CO) Comp Mole Frac (CO) Comp Mole Frac (CO2) Operation Name	(kPa) (gmole/h) (kg/d) (m3/h) (kW) J/kgmole) Ope	24.883 107.32 2.6049 1.1263 4.703e-005 -0.2065 -2.854e+005 8 @TPL2 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	24.883 104.32 3.9072 1.1263 1.118e-004 -1.726e-005 -15.90 Material Strean 9 @TPL2 0.00000 0.00000 0.00000 0.00000 0.00000 0.99996 0.00004 Unit Ops Feeds 8 @TPL2	24.883 101.32 2.6049 0.12614 7.517e-005 -1.361e-005 -18.81 10 @TPL2 0.00000 0.33331 0.00000 0.00000 0.00000 0.06666 0.00003 Products 17 @TPL2 10 @TPL2	-3. Oxygen C	24.981 101.32 1.3023 1.0002 663e-005 650e-006 -10.09 Dut @TPL2 0.00000 1.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	0.2065
37 38 39 40 41 42 43 44 45 46 47 48 49 50 51 52 53 54 55 56 57 58 69 60 61	Pressure Molar Flow Mass Flow Liquid Volume Flow Heat Flow Molar Enthalpy (Kd) Name Comp Mole Frac (Carbon) Comp Mole Frac (Oxygen) Comp Mole Frac (H2O) Comp Mole Frac (H2O) Comp Mole Frac (H2O) Comp Mole Frac (H2O) Comp Mole Frac (CO) Comp Mole Frac (CO) Comp Mole Frac (CO2) Operation Name Electrolysis @TPL2	(kPa) (gmole/h) (kg/d) (m3/h) (kW) J/kgmole) Ope	24.883 107.32 2.6049 1.1263 4.703e-005 -0.2065 -2.854e+006 8 @TPL2 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	24.883 104.32 3.9072 1.1263 1.118e-004 -1.726e-005 -15.90 Material Strean 9 @TPL2 0.00000 0.00000 0.00000 0.00000 0.00000 0.99996 0.00004 Unit Ops Feeds 8 @TPL2 Electrolysis Pwr @TPL2	24.883 101.32 2.6049 0.12614 7.517e-005 -1.361e-005 -1.881 10 @TPL2 0.00000 0.33331 0.00000 0.00000 0.00000 0.66666 0.00003 Products 17 @TPL2 10 @TPL2 Electrolysis Pwr @ 9 @TPL2	-3. Oxygen C	24.981 101.32 1.3023 1.0002 663e-005 650e-006 -10.09 Dut @TPL2 0.00000 1.00000 0.00000 0.00000 0.00000 0.00000 0.00000 Ignored No	0.2065 0.2065 Calc. Level
37 38 39 40 41 42 43 44 45 46 47 48 49 50 51 52 53 54 55 56 57 58 69 60 61 62	Pressure Molar Flow Mass Flow Liquid Volume Flow Heat Flow Molar Enthalpy (k. Name Comp Mole Frac (Carbon) Comp Mole Frac (Doygen) Comp Mole Frac (Methane) Comp Mole Frac (CO) Comp Mole Frac (Tydrogen) Comp Mole Frac (CO2) Operation Name Electrolysis @TPL2 H2/O2 Splitter @TPL2	(kPa) (gmole/h) (kg/d) (m3/h) (kW) //kgmole) Ope	24.883 107.32 2.6049 1.1263 4.703e-005 -0.2065 -2.854e+006 8 @TPL2 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	24.883 104.32 3.9072 1.1263 1.118e-004 -1.726e-005 -15.90 Material Strean 9 @TPL2 0.00000 0.00000 0.00000 0.00000 0.00000 0.99996 0.00004 Unit Ops Feeds 8 @TPL2 Electrolysis Pwr @TPL2	24.883 101.32 2.6049 0.12614 7.517e-005 -1.361e-005 -1.881 10 @TPL2 0.00000 0.33331 0.00000 0.00000 0.00000 0.66666 0.00003 Products 17 @TPL2 10 @TPL2 Electrolysis Pwr @ 9 @TPL2	-3. Oxygen C	24.981 101.32 1.3023 1.0002 663e-005 650e-006 -10.09 Dut @TPL2 0.00000 1.00000 0.00000 0.00000 0.00000 0.00000 0.00000 No	Calc. Level
37 38 39 40 41 42 43 44 45 46 47 48 49 50 51 52 53 54 55 66 57 68 69 60 61 62 63	Pressure Molar Flow Mass Flow Liquid Volume Flow Heat Flow Molar Enthalpy Name Comp Mole Frac (Carbon) Comp Mole Frac (H2O) Comp Mole Frac (H2O) Comp Mole Frac (H4D) Comp Mole Frac (H4D) Comp Mole Frac (H4D) Comp Mole Frac (CO) Comp Mole Frac (CO2) Operation Name Electrolysis @TPL2 H2/O2 Splitter @TPL2 SET-1 @TPL2 SET-2 @TPL2 SET-3 @TPL2	(kPa) (gmole/h) (kg/d) (m3/h) (kW) //kgmole) Ope Conversi Compone Set Set Set	24.883 107.32 2.6049 1.1263 4.703e-005 -0.2065 -2.854e+006 8 @TPL2 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	24.883 104.32 3.9072 1.1263 1.118e-004 -1.726e-005 -15.90 Material Strean 9 @TPL2 0.00000 0.00000 0.00000 0.00000 0.00000 0.99996 0.00004 Unit Ops Feeds 8 @TPL2 Electrolysis Pwr @TPL2	24.883 101.32 2.6049 0.12614 7.517e-005 -1.361e-005 -1.881 10 @TPL2 0.00000 0.33331 0.00000 0.00000 0.00000 0.66666 0.00003 Products 17 @TPL2 10 @TPL2 Electrolysis Pwr @ 9 @TPL2	-3. Oxygen C	24.981 101.32 1.3023 1.0002 663e-005 650e-006 -10.09 Dut @TPL2 0.00000 1.00000 0.00000 0.00000 0.00000 0.00000 Volume TPL2 Volume TPL2 No	Calc. Level 500.0 * 500.0 * 500.0 *
37 38 39 40 41 42 43 44 45 46 47 48 49 50 51 52 53 54 55 56 57 58 59 60 61 62 63 64	Pressure Molar Flow Mass Flow Liquid Volume Flow Heat Flow Molar Enthalpy (K. Name Comp Mole Frac (Carbon) Comp Mole Frac (Oxygen) Comp Mole Frac (H2O) Comp Mole Frac (H2O) Comp Mole Frac (H2O) Comp Mole Frac (Hydrogen) Comp Mole Frac (CO) Comp Mole Frac (CO2) Operation Name Electrolysis @TPL2 H2/O2 Splitter @TPL2 SET-1 @TPL2 SET-2 @TPL2	(kPa) (gmole/h) (kg/d) (m3/h) (kW) (J/kgmole) Ope Conversi Compone Set Set	24.883 107.32 2.6049 1.1263 4.703e-005 -0.2065 -2.854e+006 8 @TPL2 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	24.883 104.32 3.9072 1.1263 1.118e-004 -1.726e-005 -15.90 Material Strean 9 @TPL2 0.00000 0.00000 0.00000 0.00000 0.00000 0.99996 0.00004 Unit Ops Feeds 8 @TPL2 Electrolysis Pwr @TPL2	24.883 101.32 2.6049 0.12614 7.517e-005 -1.361e-005 -1.881 10 @TPL2 0.00000 0.33331 0.00000 0.00000 0.00000 0.66666 0.00003 Products 17 @TPL2 10 @TPL2 Electrolysis Pwr @ 9 @TPL2	-3. Oxygen C	24.981 101.32 1.3023 1.0002 663e-005 650e-006 -10.09 Dut @TPL2 0.00000 1.00000 0.00000 0.00000 0.00000 0.00000 No	Calc. Level 500.0 ° 500.0 °
37 38 39 40 41 42 43 44 45 46 47 48 49 50 51 52 53 54 55 56 57 58 69 60 61 62	Pressure Molar Flow Mass Flow Liquid Volume Flow Heat Flow Molar Enthalpy Name Comp Mole Frac (Carbon) Comp Mole Frac (H2O) Comp Mole Frac (H2O) Comp Mole Frac (H4D) Comp Mole Frac (H4D) Comp Mole Frac (H4D) Comp Mole Frac (CO) Comp Mole Frac (CO2) Operation Name Electrolysis @TPL2 H2/O2 Splitter @TPL2 SET-1 @TPL2 SET-2 @TPL2 SET-3 @TPL2	(kPa) (gmole/h) (kg/d) (m3/h) (kW) //kgmole) Ope Conversi Compone Set Set Set	24.883 107.32 2.6049 1.1263 4.703e-005 -0.2065 -2.854e+005 8 @TPL2 0.00000	24.883 104.32 3.9072 1.1263 1.118e-004 -1.726e-005 -15.90 Material Strean 9 @TPL2 0.00000 0.00000 0.00000 0.00000 0.00000 0.99996 0.00004 Unit Ops Feeds 8 @TPL2 Electrolysis Pwr @TPL2	24.883 101.32 2.6049 0.12614 7.517e-005 -1.361e-005 -1.881 10 @TPL2 0.00000 0.33331 0.00000 0.00000 0.00000 0.66666 0.00003 Products 17 @TPL2 10 @TPL2 Electrolysis Pwr @ 9 @TPL2 Oxygen Out @TPL	-3. Oxygen C	24.981 101.32 1.3023 1.0002 663e-005 650e-006 -10.09 Dut @TPL2 0.00000 1.00000 0.00000 0.00000 0.00000 0.00000 Volume TPL2 Volume TPL2 No	Calc. Level 500.0 * 500.0 * 500.0 *

1	Dec.			Case Na	ame: C:\NAS	A Final\Bo	sch 3-Comp su	ıb atm.hsc			
3		, Alberta		Unit Set	: NASA						
4	CANAD	A		Date/Tir	ne: Mon Au	ıa 23 10:24	1:41 2010				
5					Date/Time: Mon Aug 23 10:24:41 2010						
7	Equilibriu	ım: B	oudou	ıard							
9 10				STOICHI	OMETRY						
11	Component			Molecula	r Weight		S	toichiometric C			
12 13		CO2				28.01 44.01			-2 °		
14		Carbon				12.01			1.		
15 16	Balance Error :	0.0000				Pos	tion Heat : -9	6316+004 61	/kamole		
17	PASIS										
19	Basis	Phase		Appro		ı	Min. Temp		Max. Temp		
20 21	Activity	Vapo	ourPhase	(0			(C) -273	3.15	(C) 3000.0		
22	•	PARAM	FTFRS								
23 24				1 AlVAIII							
25			S	ource : K	Vs. T Table						
26	Coeff A			-21.68	R2				1.000000 *		
27 28	Coeff B Coeff C			2.078e+004 6.615 e- 002	T High T Low						
29	Coeff D			-3.643e-005	1 200						
30											
31 32	Temperature (C)	Keq			KCalc		Perce	entage Error			
33 34	25.000 *			1.039e+021 '			.039e+021 *		1.641e-002 *		
35	127.00 * 227.00 *			2.026e+013 * 6.330e+008 *			.026e+013 * .335e+008 *		-1.147e-002 * -7.829e-002 *		
36	327.00 °			6.290e+005 ¹			.287e+005 °		4.151e-002 °		
37 38	427.00 °			4500 *			4501 '		-2.620e-002 *		
39	527.00 * 627.00 *			111.0 ° 6.210 °			110.8 * 6.211 *		0.1924 * -1.484 e -002 *		
40	727.00 °			0.6190 *			0.6195 *		-8.445e-002 °		
41 42	827.00 °			9.390e-002 *			0.396e-002 *	-5.988e-002 -5.029e-002			
43	927.00 ° 1027.0 °			1.950e-002 * 5.160e-003 *			1.951e-002 * 5.159e-003 *		2.623e-002 *		
44	1127.0 *			1.650e-003 *		1	.649e-003 *	4.861e-002 °			
45 46	Conversi	on: E	lectrol	ysis							
47 48				STOICHI	OMETRY						
49	Component							Ctaiabiamatri	Cooff		
51	Component H2O			Mole V	veignt	18.015		Stoichiometric	: Coeп. -2 *		
52	Hydrogen					2.016			2.		
53 54	Oxygen					32.000			1 *		
55											
56	Balance Error:	0.0000				Rea	ction Heat: 2.	410e+005 kJ/l	rgmole		
57 58				BAS	SIS						
59	Base Component: H2O		Convers	ion Percent:	100.00	•	Reactio	n Phase: Liq	uidPhase		
60 61				PARAM	ETERS						
62											
63											
64 65											
66	Hyprotech Ltd.		HY	SYS.Plant v2.	2.2 (Build 3806	6)			Page 5 of 5		
_	Licensed to: INL								* Specified by user.		

A-16

A.3 Bosch Process with 1 Compressor C02 In Oxygen Out Hydrogen Electrolysis Ξ Carbon Out Electrolysis Pwr Recycle Stream Condenser/Water Separator Bosch Reactor **M**2 Bosch Heat RCY-3 Water Recuperating HX Ŋ TAMB ⊗ Compressor ⋛ ⋛ Water In Compressor Power 0.2439 10.00 2.100 14.75 -9.684e-002 Bosch Calcs **Bosch Calcs** Recycle to CO2 and H2 ratio % Pass Conversion H2 to CO2 Ratio **Total Power** Total Heat

Figure A - 5 Process flow diagram of Bosch process with 1 compressor

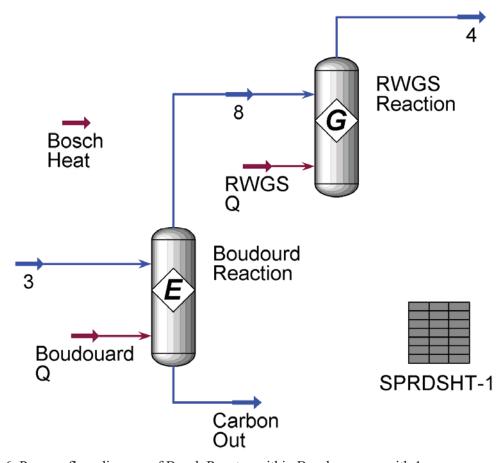


Figure A - 6 Process flow diagram of Bosch Reactor within Bosch process with 1 compressor

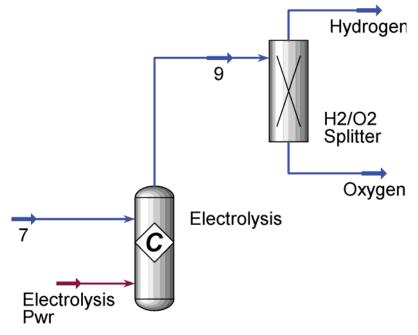


Figure A - 7 Process flow diagram of Electrolysis Module within Bosch process with 1 compressor

_										
1			Case Name:	C:\NASA Final\Bosch 1	Comp.hsc					
3	INL Calgary, A	Alberta	Unit Set:	NASA						
4 5	CANADA		Date/Time:	Date/Time: Mon Aug 23 10:28:41 2010						
6										
7	Workbook:	Case (Main	1)							
9			04							
10			Streams Compressor Rower 2							
11	Name	1	1r	Compressor Power	2	3				
12 13	Vapour Fraction Temperature (C)	1.0000 24.794	1.0000 24.792 *		1.0000 84.170	1.0000 623.87 *				
14	Pressure (kPa)	101.32	101.32 "		172.37 '	169.37				
15	Molar Flow (gmole/h)	71.552	71.525		71.525	71.525				
16	Mass Flow (kg/d)	22.610	22.613 *		22.613	22.613				
17	Liquid Volume Flow (m3/h)	2.718e-003	2.716e-003		2.716e-003	2.716e-003				
18	Heat Flow (kW)	-1.352	-1.353	3.742e-002	-1.316	-0.9141				
19	Molar Enthalpy (kJ/kgmole)	-6.804e+004	-6.810e+004		-6.622e+004	-4.601e+004				
20	Name	Bosch Heat	4	Carbon Out	5	AMB Q				
21	Vapour Fraction		1.0000	0.0000 *	1.0000					
22	Temperature (C)		650.00	650.00	109.17					
23	Pressure (kPa)		163.37	166.37	160.37					
24 25	Molar Flow (gmole/h)		70.221	1.2227	70.221					
	Mass Flow (kg/d)		22.261	0.35246	22.261					
26	Liquid Volume Flow (m3/h)		2.622e-003	8.944e-006	2.622e-003					
27	Heat Flow (kW)	-1.326e-002	-0.9308	3.477e-003	-1.332	-8.357e-002				
28	Molar Enthalpy (kJ/kgmole)		-4.772e+004	1.024e+004	-6.831e+004					
29	Name	Recycle Stream	Water	Water In	Water Pmp Pwr	6				
30	Vapour Fraction	1.0000	0.0000	0.0000		0.0000				
31	Temperature (C) Pressure (kPa)	25.000 *	25.000	21.111 * 101.32 *		21.116				
32	· · · - · · · · · · · · · · · · · · · ·	157.37 67.708	157.37 2.5129	9.1359e-002		157.37 9.1359e-002				
34	Molar Flow (gmole/h) Mass Flow (kg/d)	21.174	1.0865	3.9500e-002		3.9500e-002				
35	Liquid Volume Flow (m3/h)	2.576e-003	4.536e-005	1.649e-006		1.649e-006				
36	Heat Flow (kW)	-1.217	-0.1992	-7.251e-003	3.382e-008	-7.251e-003				
37	Molar Enthalpy (kJ/kgmole)	-6.469e+004	-2.854e+005	-2.857e+005		-2.857e+005				
38	Name	7	Electrolysis Pwr	Hydrogen	Oxygen Out	CO2 In				
39	Vapour Fraction	0.0000		1.0000	1.0000	1.0000				
40	Temperature (C)	24.864		24.864	25.014	21.111 *				
41	Pressure (kPa)	157.37		151.37	151.37	101.32 *				
42	Molar Flow (gmole/h)	2.6043		2.6043	1.3020	1.2401				
43	Mass Flow (kg/d)	1.1260		0.12609	0.99995	1.3098 *				
44	Liquid Volume Flow (m3/h)	4.701e-005		7.516e-005	3.662e-005	6.613e-005				
45	Heat Flow (kW)	-0.2065	0.2065	-1.250e-005	-5.004e-006	-0.1357				
46	Molar Enthalpy (kJ/kgmole)	-2.854e+005		-17.28	-13.84	-3.940e+005				
47 48			Composition							
48	Name	1	1r	2	3	Carbon Out				
50	Comp Mole Frac (Carbon)	0.00000	0.00000 *	0.00000	0.00000	1.00000				
51	Comp Mole Frac (Carbon)	0.00000	0.00000	0.00000	0.00000	0.00000				
52	Comp Mole Frac (H2O)	0.01891	0.01890 *	0.01890	0.01890	0.00000				
53	Comp Mole Frac (Methane)	0.27413	0.27366 *	0.27366	0.27366	0.00000				
54	Comp Mole Frac (CO)	0.17063	0.17088 *	0.17088	0.17088	0.00000				
55	Comp Mole Frac (Hydrogen)	0.47520	0.47526 *	0.47526	0.47526	0.00000				
56	Comp Mole Frac (CO2)	0.06113	0.06130 "	0.06130	0.06130	0.00000				
57	Name	4	5	Recycle Stream	Water	Water In				
58	Comp Mole Frac (Carbon)	0.00000	0.00000	0.00000	0.00000	0.00000 *				
59	Comp Mole Frac (Oxygen)	0.00000	0.00000	0.00000	0.00000	0.00000 *				
60	Comp Mole Frac (H2O)	0.05505	0.05505	0.01998	0.99996	1.00000 *				
61	Comp Mole Frac (Methane)	0.27933	0.27933	0.28970	0.00000	0.00000 *				
62	Comp Mole Frac (CO)	0.17386	0.17386	0.18032	0.00000	0.00000*				
63	Comp Mole Frac (Hydrogen)	0.44712	0.44712	0.46372	0.00000	0.00000 *				
64	Comp Mole Frac (CO2)	0.04463	0.04463	0.04628	0.00003	0.00000 *				
65 ee	Hyprotoch I td	1.07	eve Blant vo. 0.0.0 (Built	4 3806/		Dago 4 of 5				
66	Hyprotech Ltd.	HY	SYS.Plant v2.2.2 (Buil	u 3000)		Page 1 of 5				

Licensed to: INL Specified by user.

1											
2	INL				Case Name: C:\NASA Final\Bosch 1 Comp.hsc						
3	HYPROTECH	Calgary, A	Alberta		Unit Set:						
5		0,44,0,7			Date/Time: Mon Aug 23 10:28:41 2010						
6	\A(0 (84-			-1\					
8	Workb	ook:	Case (Ma	ain)	(continue	ed)					
9 10				Com	position (cont	inued)					
11	Name		6	7	7	Oxygen Out	Hydrogen	CO2 In			
12	Comp Mole Frac (Carbon)		0.000		0.00000	0.00000	0.00000	0.00000 *			
13	Comp Mole Frac (Oxygen)		0.000	_	0.00000	1.00000	0.00000	0.00000 *			
14 15	Comp Mole Frac (H2O)		1.000		0.99997	0.00000	0.00000	0.00000 *			
15	Comp Mole Frac (Methane) Comp Mole Frac (CO)		0.000		0.00000	0.00000	0.00000	0.00000 ° 0.00000 °			
17	Comp Mole Frac (Hydrogen)		0.000		0.00000	0.00000	0.99997	0.00000			
18	Comp Mole Frac (CO2)		0.000		0.00003	0.00000	0.00003	1.00000			
19						•	0.00000	1.00000			
20					leat Exchange	rs					
21	Name		Recuperating HX								
22	Duty	(kW)	0.40	15							
23	Tube Inlet Temperature	(C)	84.	17							
24	Tube Outlet Temperature	(C)	623	_							
25	Shell Inlet Temperature	(C)	650	0.0							
26	Shell Outlet Temperature	(C)	109								
27	UA	(kJ/C-h)	56.								
28	LMTD	(C)	25.	_							
29				00							
30 31					Compressors	;					
32	Name		Compressor		•						
33	Feed Pressure	(kPa)	101	3 *							
34	Product Pressure	(kPa)	172								
35		(gmole/h)	71.								
36	Energy	(kW)	3.742e-0								
37	Adiabatic Efficiency	(1117)		75 '							
38	Polytropic Efficiency			77							
39					Pumps						
40					rumps						
41	Name		Water Pump								
42	Delta P	(kPa)	56.	_							
43	Energy	(kW)	3.382e-0								
44 45	Feed Pressure Product Pressure	(kPa)	101								
45 46		(kPa) (gmole/h)	9.136e-0								
47	Adiabatic Efficiency	(gmole/n) (%)	9.136e-0	_							
48		(70)	, 75.				1				
49					Unit Ops						
50	Operation Name	Оре	eration Type		Feeds	Products	Ignored	Calc. Level			
51	Compressor	Compres	sor	1r		2	No	500.0 *			
52	Confibressor	Compres	301		oressor Power		140	300.0			
53					cle Stream	1					
54 55	M1	Mixer		CO2			No	500.0 *			
55				Hydro	ogen						
56 57	M2	Mixer		6	_	7	No	500.0 *			
57 58				Wate	er .	1					
59	Recuperating HX	Heat Exchanger		4		5	No	500.0 *			
60			5		Water						
61	Condenser/Water Separator	Separato	or.	AMB	0	Recycle Stream	No	500.0 *			
62		- speriore			-	AMB Q					
63	RCY-3	Recycle		1		1r	No	3500 °			
64	ADJ-1	Adjust		Ť.			No	3500 *			
65	Bosch Calcs	Spreadsh	neet				No	500.0 *			
66	Hyprotech Ltd.			HYSY	S.Plant v2.2.2 (Buil	d 3806)		Page 2 of 5			
_	Licensed to: INI							* Specified by user			

Licensed to: INL *Specified by user.

1	Do.	INL			Case Name: C:\NASA Final\Bosch 1 Comp.hsc					
3	HYPROTECH	Calgary, A	lberta		Unit Set: N	NASA				
3 4 5		CANADA			Date/Time: Mon Aug 23 10:28:41 2010					
6		_				•				
7	Workb	ook:	Case (Ma	ain)	(continue	d)				
9				Ur	nit Ops (continu	ed)				
11	Operation Name	Ope	ration Type		Feeds	Products		Ignored	Calc. Level	
12 13	Bosch Reactor	Standard	Sub-Flowsheet	3	sh Unat	4		No	2500 °	
14	4 7				ch Heat	Oxygen Out				
15	Electrolysis	Standard	Sub-Flowsheet	_	trolysis Pwr	Hydrogen		No	2500 *	
16 17	Water Pump	Pump		Wate	er In er Pmp Pwr	6		No	500.0 *	
18 19 20	Workbook: Bosch Reactor (BSHRCT)									
21 22					Streams					
23	Name		3 @BSHRCT	-	Boudouard Q @BSHI	8 @BSHRCT	Carbon	Out @BSHR	RWGS Q @BSHRCT	
24 25	Vapour Fraction Temperature	(C)	1.000 623.8			1.0000 650.00 *		0.0000 650.00		
26	Pressure	(kPa)	169.3			166.37		166.37		
27		(gmole/h)	71.5	-		70.303		1.2227		
28	Mass Flow	(kg/d)	22.6			22.260		0.35246		
29	Liquid Volume Flow	(m3/h)	2.716e-0	03		2.696e-003		3.944e-006		
30	Heat Flow	(kW)	-0.91	41	-3.616e-002	-0.9537	:	3.477e-003	2.290e-002	
31	Molar Enthalpy (k	J/kgmole)	-4.601e+0	04		-4.884e+004	1	.024e+004		
32	Name		4 @BSHRCT		Bosch Heat @BSHR					
33	Vapour Fraction		1.000	00						
34	Temperature	(C)	650.0	00 *						
35	Pressure	(kPa)	163.3	37						
36	Molar Flow	(gmole/h)	70.2	21						
37	Mass Flow	(kg/d)	22.20	61						
38	Liquid Volume Flow	(m3/h)	2.622e-0	03						
39	Heat Flow	(kW)	-0.930	80	-1.326e-002					
40	Molar Enthalpy (k	J/kgmole)	-4.772e+0	04						
41					Composition					
42 43 44 45	Name		3 @BSHRCT		8 @BSHRCT	Carbon Out @BSHR	4 @BSI	HRCT		
44						•				
45 46					Unit Ops					
47	Operation Name	Ope	ration Type		Feeds	Products		Ignored	Calc. Level	
48				8 @1	BSHRCT	10 @BSHRCT				
49	RWGS Reaction @BSHRCT	Gibbs Re	actor		SS Q @BSHRCT	4 @BSHRCT		No	500.0 *	
50 51						RWGS Q @BSHR	СТ			
51				3 @	BSHRCT	Carbon Out @BSI				
52 53	Boudourd Reaction @BSHR	Equilibriu	m Reactor	Boud	douard Q @BSHRCT	8 @BSHRCT		No	500.0 *	
53						Boudouard Q @BS	SHRCT			
54	SPRDSHT-1 @BSHRCT	Spreadsh	eet					No	500.0 *	
55										
55										
50										
50										
60										
54 55 56 57 58 59 60 61 62 63 64 65										
62										
63										
64										
65										
66	Hyprotech Ltd.			HYSY	S.Plant v2.2.2 (Build	13806)			Page 3 of 5	
_	Licensed to: INI								* Specified by user	

Licensed to: INL * Specified by user.

2	INL			(Case Name: C:\NASA Final\Bosch 1 Comp.hsc					
3	HYPROTECH	Calgary, All	berta	ι	Unit Set: NASA					
5		ONINDA		С	Date/Time: Mon Aug 23 10:28:41 2010					
6	1A/a wha	المامم		roio (E	LCT)					
8	VVOIKD	OOK.	Electroly	/515 (E	LCI					
9					Streams					
11	Name		7 @ELCT	Elect	trolysis Pwr @E	1 9@	ELCT	Oxygei	n @ELCT	Hydrogen @ELCT
12	Vapour Fraction		0.00				1.00		1.0000	1.0000
13	Temperature	(C)	24.8				24.8	-	25.014	24.864
14	Pressure	(kPa)	157			-	154		151.37	151.37
15 16		(gmole/h)	2.60				3.90		1.3020	2.6043
17	Mass Flow Liquid Volume Flow	(kg/d) (m3/h)	1.12 4.701e-0				1.12 1.118e-0		0.99995 3.662e-005	0.12609 7.516e-005
18	Heat Flow	(kW)	-0.20		0.2065		-1.750e-0		-5.004e-006	-1.250e-005
19		J/kgmole)	-2.854e+0		0.2003		-1.7506-0		-13.84	-17.28
20	mout annually (m	orngmoto,	2.00101		omposition				10.01	11120
21 22	Name		7 @ELCT		ELCT	_	frogen @EL0	CT Oxyge	n @ELCT	
23	Comp Mole Frac (Carbon)		0.000	_	0.00000	1190	0.000		0.00000	
24	Comp Mole Frac (Oxygen)		0.000		0.33331		0.000	_	1.00000	
25	Comp Mole Frac (H2O)		0.999		0.00000		0.000	000	0.00000	
26	Comp Mole Frac (Methane)		0.000	000	0.00000		0.000	000	0.00000	
27	Comp Mole Frac (CO)		0.000	000	0.00000		0.000	000	0.00000	
28	Comp Mole Frac (Hydrogen)		0.000	000	0.66666		0.999	997	0.00000	
29	Comp Mole Frac (CO2)			003	0.00002		0.000	003	0.00000	
30 31					Unit Ops					
32	Operation Name	Oper	ation Type		Feeds		Prod	lucts	Ignored	Calc. Level
33			,,,	7 @ELC				3		
34	Electrolysis @ELCT	Conversio	n Reactor	Electroly	olysis Pwr @ELCT 9 @ELCT				No	500.0 *
35					Electrolysis Pwr @			Pwr @ELCT		
36	H2/O2 Splitter @ELCT	Componer	nt Solitter	9 @ELC	9 @ELCT		Hydrogen @ELCT		No	500.0 *
37			п орине.				Oxygen @EL	.CT		
38 39	SET-1 @ELCT	Set Set				+			No No	500.0 * 500.0 *
40	SET-2 @ELCT SET-3 @ELCT	Set		+		+			No	500.0
41	SET-4 @ELCT	Set		_		+			No	500.0
42	3E1-4 @EE01	GEL							140	300.0
43	Equil	libriun	n: Boud	ouard						
44 45	•									
46				STC	DICHIOMET	RY				
47	Componer	nt		М	lolecular Weight			S	toichiometric C	
48			со		28.01					-2*
49			CO2							1*
50			Carbon		12.01					
51 52	Palanas	Error: 0.0	000				Paga	tion Heat · •	.631e+004 kJ/	kamole
53	Balance	Error: 0.0	000				Reac	uon neat: -8	.00 re+004 KJ/	Nymore
54					BASIS					
55 56	Basis		Phase		Approach		1	Vlin. Temp		Max. Temp (C)
57	Activity			е	(C) (C) -2			-273	3.15	3000.0
58 59				P/	RAMETER	S				
60				Source	e : K Vs. T	Γable				
61 62	Coeff A				20.52 R2					1.000000 *
63	Coeff B			-1.962e						
64	Coeff C			-4.644€						
65	Coeff D			2.437€						
66	Hyprotech Ltd.				lant v2.2.2 (Bui	ld 380	16)			Page 4 of 5
	Licensed to: INL Specified by user.									

1		Case Name	e: C:\NASA Final\Bo	sch 1 Comp.hsc							
3	INL Calgary, Alberta	Unit Set:	NASA								
4 5	CANADA	Date/Time:	Date/Time: Mon Aug 23 10:28:41 2010								
6											
7	Equilibrium: E	Boudouard (cor	ntinued)								
8		DADAME	EDC								
10 11											
12	Source : K VS. 1 Table										
13 14	Temperature	Vog	KCalc		Percentage Error						
15	(C)	Keq	KCaic		Percentage Error						
16 17	25.000 *	1.640e-020 *		1.640e-020 *	-2.452e-002 *						
18	127.00 °	3.140e-013 * 5.650e-009 *		3.139e-013 * 5.648e-009 *	3.731e-002 * 3.529e-002 *						
19	327.00 °	3.880e-006 *		3.879e-006 °	3.547e-002 °						
20	427.00 °	4.120e-004 *		1.120e-004 *	-1.092e-002 *						
21	527.00 °	1.360e-002 *		1.363e-002 *	-0.2546 °						
22	627.00 °	0.2075		0.2073 *	6.258e-002 °						
23	727.00 *	1.830 *		1.829 *	6.516e-002 *						
24	827.00 °	10.87 *		10.86 *	5.621e-002 *						
25	927.00 *	47.97 *		47.95 *	4.263e-002 *						
26	1027.0 °	168.5 *		168.4 *	1.777e-002 °						
27	1127.0 *	494.5 *		494.5 *	-1.079e-002 *						
28	1227.0 *	1257 '		1258 "	-5.204 e- 002 *						
29		.									
30 31	Conversion: E	Electrolysis									
32		a Tolollio	/ETD\/								
33		STOICHION									
34	Component	Mole Wei		Stoi	chiometric Coeff.						
35	H2O		18.015		-2*						
36 37	Hydrogen		2.016		2'						
38	Oxygen		32.000		1,						
39											
40	Balance Error: 0.0000		Rea	ction Heat: 2.410	+005 kJ/kgmole						
41		BASIS			<u></u>						
42 43	Base Component: H2O	Conversion Percent: 100		Reaction Ph	ase: LiquidPhase						
	base Component. H2O	•	,,,,,,	Reaction	ase. Liquiuriiase						
44 45		PARAMET	ERS								
46											
46 47 48											
48											
49											
50											
51											
52											
53											
54											
50											
57											
58											
59											
60											
61											
62											
63											
50 51 52 53 54 55 56 57 58 69 60 61 62 63 64 65											
66	Hyprotech Ltd.	HYSYS.Plant v2.2.2	? (Build 3806)		Page 5 of 5						
	Licensed to: INL				* Specified by user.						

66 Hyprotech Ltd.
Licensed to: INL Page 5 of 5
* Specified by user.

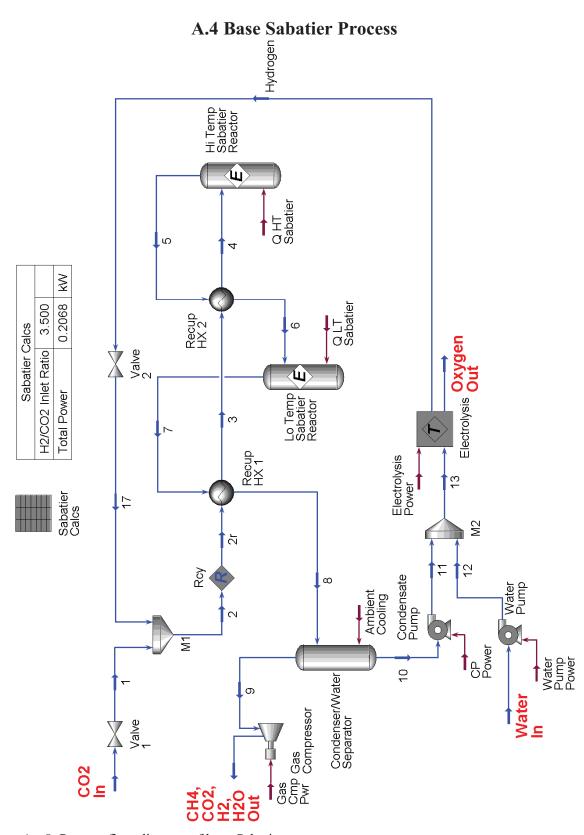


Figure A - 8 Process flow diagram of base Sabatier process

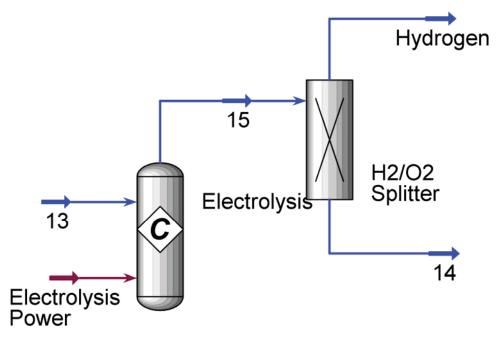


Figure A - 9 Process flow diagram of Electrolysis module within Sabatier process

_									
2	INL		Case Name:	C:\NASA Final\Sabatier	6.hsc				
3	HYPROTES H Calgary, A	Alberta	Unit Set:	NASA2	SA2				
5	CANADA		Date/Time:	Date/Time: Mon Aug 23 10:33:42 2010					
6									
7	Workbook:	Case (Main	1)						
9									
10			Material Stream						
11	Name	CO2 In	1	2	2r	3			
12 13	Vapour Fraction Temperature (C)	1.0000 21.111 *	1.0000 20.551	1.0000 22.152	1.0000 22.153 *	1.0000 178.37 *			
14	Pressure (kPa)	131.00 *	80.669	80.669 *	80.669 *	79.979			
15	Molar Flow (gmole/h)	0.74407	0.74407	3.3486	3.3486 '	3.3486			
16	Mass Flow (kg/d)	0.78591 *	0.78591	0.91199	0.91199	0.91199			
17	Liquid Volume Flow (m3/h)	3.968e-005	3.968e-005	1.148e-004	1.148e-004	1.148e-004			
18	Heat Flow (kW)	-8.143e-002	-8.143e-002	-8.148e-002	-8.148e-002	-7.694e-002			
19	Name	4 0000	5	6	7	8			
20 21	Vapour Fraction Temperature (C)	1.0000 510.61 *	1.0000 565.00 *	1.0000 198.37	1.0000 240.00 *	0.9550 79.175			
22	Pressure (kPa)	79.290	78.600	77.911	77.221	76.532			
23	Molar Flow (gmole/h)	3.3486	2.7897	2.7897	2.0702	2.0702			
24	Mass Flow (kg/d)	0.91199	0.91198	0.91198	0.91198	0.91198			
24 25	Liquid Volume Flow (m3/h)	1.148e-004	8.812e-005	8.812e-005	6.430e-005	6.430e-005			
26	Heat Flow (kW)	-6.668e-002	-7.757e-002	-8.782e-002	-0.1058	-0.1104			
27	Name	9	CH4, CO2, H2, H2O	10	11	Water In			
28	Vapour Fraction	1.0000	1.0000	0.0000	0.0000	0.0000			
29	Temperature (C)	25.000 *	52.367	25.000	25.003	21.111 '			
30	Pressure (kPa)	75.842	101.33 *	75.842	106.32	101.32 *			
31 32	Molar Flow (gmole/h) Mass Flow (kg/d)	0.82585 0.37392	0.82585 0.37392	1.2444 0.53806	1.2444 0.53806	1.3601 0.58807 *			
33	Mass Flow (kg/d) Liquid Volume Flow (m3/h)	4.184e-005	4.184e-005	2.246e-005	2.246e-005	2.455e-005			
34	Heat Flow (kW)	-2.705e-002							
			-2.683e-002	-9.866e-002	-9.866e-002	-0.1079			
35	Name	13	-2.683e-002 Oxygen Out	-9.866e-002 Hydrogen	-9.866e-002	-0.1079 12			
35 36	()		-2.683e-002 Oxygen Out 1.0000	-9.866e-002 Hydrogen 1.0000					
36 37	Name	13	Oxygen Out	Hydrogen	17	12			
36 37 38	Name Vapour Fraction Temperature (C) Pressure (kPa)	0.0000 22.971 106.32	0xygen Out 1.0000 23.071 101.32	1.0000 22.971 101.32	17 1.0000 22.970 80.669	0.0000 21.112 106.32*			
36 37 38 39	Various Column Temperature (C) Pressure (kPa) Molar Flow (gmole/h)	0.0000 22.971 106.32 2.6045	0xygen Out 1.0000 23.071 101.32 1.3022	Hydrogen 1.0000 22.971 101.32 2.6045	17 1.0000 22.970 80.669 2.6045	0.0000 21.112 106.32 1.3601			
36 37 38 39 40	Various Column Temperature (C) Pressure (kPa) Molar Flow (gmole/h) Mass Flow (kg/d)	0.0000 22.971 106.32 2.6045 1.1261	0xygen Out 1.0000 23.071 101.32 1.3022 1.0001	Hydrogen 1.0000 22.971 101.32 2.6045 0.12607	17 1.0000 22.970 80.669 2.6045 0.12607	0.0000 21.112 106.32 * 1.3601 0.58807			
36 37 38 39 40 41	Name Vapour Fraction (C) Temperature (kPa) Molar Flow (gmole/h) Mass Flow (kg/d) Liquid Volume Flow (m3/h)	0.0000 22.971 106.32 2.6045 1.1261 4.702e-005	0xygen Out 1.0000 23.071 101.32 1.3022 1.0001 3.663e-005	1.0000 22.971 101.32 2.6045 0.12607 7.516e-005	17 1.0000 22.970 80.669 2.6045 0.12607 7.516e-005	0.0000 21.112 106.32 * 1.3601 0.58807 2.455e-005			
36 37 38 39 40 41	Various (C) Pressure (kPa) Molar Flow (gmole/h) Mass Flow (kg/d)	0.0000 22.971 106.32 2.6045 1.1261	0xygen Out 1.0000 23.071 101.32 1.3022 1.0001 3.663e-005 -2.392e-005	Hydrogen 1.0000 22.971 101.32 2.6045 0.12607 7.516e-005 -4.808e-005	17 1.0000 22.970 80.669 2.6045 0.12607	0.0000 21.112 106.32 * 1.3601 0.58807			
36 37 38 39 40 41	Name Vapour Fraction (C) Temperature (kPa) Molar Flow (gmole/h) Mass Flow (kg/d) Liquid Volume Flow (m3/h)	0.0000 22.971 106.32 2.6045 1.1261 4.702e-005	0xygen Out 1.0000 23.071 101.32 1.3022 1.0001 3.663e-005	Hydrogen 1.0000 22.971 101.32 2.6045 0.12607 7.516e-005 -4.808e-005	17 1.0000 22.970 80.669 2.6045 0.12607 7.516e-005	0.0000 21.112 106.32 * 1.3601 0.58807 2.455e-005			
36 37 38 39 40 41 42 43 44 45	Name Vapour Fraction (C) Temperature (kPa) Molar Flow (gmole/h) Mass Flow (kg/d) Liquid Volume Flow (m3/h)	0.0000 22.971 106.32 2.6045 1.1261 4.702e-005	0xygen Out 1.0000 23.071 101.32 1.3022 1.0001 3.663e-005 -2.392e-005	Hydrogen 1.0000 22.971 101.32 2.6045 0.12607 7.516e-005 -4.808e-005	17 1.0000 22.970 80.669 2.6045 0.12607 7.516e-005	0.0000 21.112 106.32 * 1.3601 0.58807 2.455e-005			
36 37 38 39 40 41 42 43 44 45	Name Vapour Fraction Temperature (C) Pressure (kPa) Molar Flow (gmole/h) Mass Flow (kg/d) Liquid Volume Flow (m3/h) Heat Flow (kW) Name Comp Mole Frac (Oxygen)	13 0.0000 22.971 106.32 2.6045 1.1261 4.702e-005 -0.2066 CO2 In	0xygen Out 1.0000 23.071 101.32 1.3022 1.0001 3.663e-005 -2.392e-005 Compositions 1	Hydrogen 1.0000 22.971 101.32 2.6045 0.12607 7.516e-005 -4.808e-005	17 1.0000 22.970 80.669 2.6045 0.12607 7.516e-005 -4.808e-005	12 0.0000 21.112 106.32 * 1.3601 0.58807 2.455e-005 -0.1079			
36 37 38 39 40 41 42 43 44 45 46 47	Name	13 0.0000 22.971 106.32 2.6045 1.1261 4.702e-005 -0.2066 CO2 In 0.00000 *	0xygen Out 1.0000 23.071 101.32 1.3022 1.0001 3.663e-005 -2.392e-005 Compositions 1 0.00000 0.00000	Hydrogen 1.0000 22.971 101.32 2.6045 0.12607 7.516e-005 -4.808e-005 2 0.00000 0.00000	17 1.0000 22.970 80.669 2.6045 0.12607 7.516e-005 -4.808e-005 2r 0.00000 *	12 0.0000 21.112 106.32 * 1.3601 0.58807 2.455e-005 -0.1079 3 0.00000 0.00000			
36 37 38 39 40 41 42 43 44 45 46 47	Name	13	0xygen Out 1.0000 23.071 101.32 1.3022 1.0001 3.663e-005 -2.392e-005 Compositions 1 0.00000 0.00000 0.00000	Hydrogen 1.0000 22.971 101.32 2.6045 0.12607 7.516e-005 -4.808e-005 2 0.00000 0.00000 0.00000	17 1.0000 22.970 80.669 2.6045 0.12607 7.516e-005 -4.808e-005 2r 0.00000 ° 0.00000 °	12 0.0000 21.112 106.32 * 1.3601 0.58807 2.455e-005 -0.1079 3 0.00000 0.00000 0.00000			
36 37 38 39 40 41 42 43 44 45 46 47 48	Name	13	0xygen Out 1.0000 23.071 101.32 1.3022 1.0001 3.663e-005 -2.392e-005 Compositions 1 0.00000 0.000000 1.000000	Hydrogen 1.0000 22.971 101.32 2.6045 0.12607 7.516e-005 -4.808e-005 2 0.00000 0.00000 0.00000 0.22222	17 1.0000 22.970 80.669 2.6045 0.12607 7.516e-005 -4.808e-005 2r 0.00000 ° 0.00000 ° 0.00000 °	12 0.0000 21.112 106.32 1.3601 0.58807 2.455e-005 -0.1079 3 0.00000 0.00000 0.00000 0.22222			
36 37 38 39 40 41 42 43 44 45 46 47 48 49 50	Name	13	0xygen Out 1.0000 23.071 101.32 1.3022 1.3022 1.0001 3.663e-005 -2.392e-005 Compositions 1 0.00000 0.00000 1.00000 0.00000	Hydrogen 1.0000 22.971 101.32 2.6045 0.12607 7.516e-005 -4.808e-005 2 0.00000 0.00000 0.00000 0.22222 0.77778	17 1.0000 22.970 80.669 2.6045 0.12607 7.516e-005 -4.808e-005 2r 0.00000 * 0.00000 * 0.00000 * 0.22222 * 0.77778 *	3 0.0000 21.112 106.32 ° 1.3601 0.58807 2.455e-005 -0.1079 3 0.00000 0.00000 0.00000 0.22222 0.77778			
36 37 38 39 40 41 42 43 44 45 46 47 48	Name	13	0xygen Out 1.0000 23.071 101.32 1.3022 1.0001 3.663e-005 -2.392e-005 Compositions 1 0.00000 0.000000 1.000000	Hydrogen 1.0000 22.971 101.32 2.6045 0.12607 7.516e-005 -4.808e-005 2 0.00000 0.00000 0.00000 0.22222	17 1.0000 22.970 80.669 2.6045 0.12607 7.516e-005 -4.808e-005 2r 0.00000 ° 0.00000 ° 0.00000 °	12 0.0000 21.112 106.32 1.3601 0.58807 2.455e-005 -0.1079 3 0.00000 0.00000 0.00000 0.22222			
36 37 38 39 40 41 42 43 44 45 46 47 48 49 50 51	Name	13	0xygen Out 1.0000 23.071 101.32 1.3022 1.3022 1.0001 3.663e-005 -2.392e-005 Compositions 1 0.00000 0.00000 1.00000 0.00000 0.00000	Hydrogen 1.0000 22.971 101.32 2.6045 0.12607 7.516e-005 -4.808e-005 2 0.00000 0.00000 0.00000 0.22222 0.77778 0.00000	17 1.0000 22.970 80.669 2.6045 0.12607 7.516e-005 -4.808e-005 2r 0.00000 * 0.00000 * 0.22222 * 0.77778 * 0.00000 *	3 0.0000 21.112 106.32 1.3601 0.58807 2.455e-005 -0.1079 3 0.00000 0.00000 0.00000 0.22222 0.77778 0.00000			
36 37 38 39 40 41 42 43 44 45 46 47 48 49 50 51	Name	0.0000 22.971 106.32 2.6045 1.1261 4.702e-005 -0.2066 CO2 In 0.00000 * 0.00000 * 0.00000 * 0.00000 * 0.00000 * 0.00000 * 0.00000 *	0xygen Out 1.0000 23.071 101.32 1.3022 1.3022 1.0001 3.663e-005 -2.392e-005 Compositions 1 0.00000 0.00000 1.00000 0.00000 0.00000 0.00000 0.00000	Hydrogen 1.0000 22.971 101.32 2.6045 0.12607 7.516e-005 -4.808e-005 2 0.00000 0.00000 0.00000 0.22222 0.77778 0.00000 0.00000	17	3 0.0000 0.0000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000			
36 37 38 39 40 41 42 43 44 45 46 47 48 49 50 51 52 53 54 55	Name	13	0xygen Out 1.0000 23.071 101.32 1.3022 1.0001 3.663e-005 -2.392e-005 Compositions 1 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	Hydrogen 1.0000 22.971 101.32 2.6045 0.12607 7.516e-005 -4.808e-005 2 0.00000 0.00000 0.00000 0.22222 0.77778 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	17	3 0.0000 0.0000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000			
36 37 38 39 40 41 42 43 44 45 46 47 48 49 50 51 52 53 54 55 56	Name	13	0xygen Out 1.0000 23.071 101.32 1.3022 1.3002 1.0001 3.663e-005 -2.392e-005 Compositions 1 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 5 0.00000	Hydrogen 1.0000 22.971 101.32 2.6045 0.12607 7.516e-005 -4.808e-005 2 0.00000 0.00000 0.00000 0.22222 0.77778 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	17	3 0.0000 21.112 106.32 1.3601 0.58807 2.455e-005 -0.1079 3 0.00000 0.00000 0.00000 0.22222 0.77778 0.00000 0.00000 0.00000 0.00000 0.00000 8 0.00000			
36 37 38 39 40 41 42 43 44 45 46 47 48 49 50 51 52 53 54 55 56 57	Name	13	0xygen Out 1.0000 23.071 101.32 1.3022 1.3022 1.0001 3.663e-005 -2.392e-005 Compositions 1 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 5 0.00000 5 0.00000	Hydrogen	17	3 0.0000 21.112 106.32 * 1.3601 0.58807 2.455e-005 -0.1079 3 0.00000 0.00000 0.00000 0.22222 0.77778 0.00000 0.00000 0.00000 0.00000 8 0.00000 0.00000			
36 37 38 39 40 41 42 43 44 45 46 47 48 49 50 51 52 53 54 55 56 57 58	Name	13	0xygen Out 1.0000 23.071 101.32 1.3022 1.3022 1.0001 3.663e-005 -2.392e-005 Compositions 1 0.00000 0.00000 1.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	Hydrogen	17	3 0.0000 21.112 106.32 1.3601 0.58807 2.455e-005 -0.1079 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000			
36 37 38 39 40 41 42 43 44 45 46 47 48 49 50 51 52 53 54 55 56 57 58	Name	13	0xygen Out 1.0000 23.071 101.32 1.3022 1.3022 1.0001 3.663e-005 -2.392e-005 Compositions 1 0.00000 0.00000 1.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	Hydrogen	17	3 0.0000 21.112 106.32 1.3601 0.58807 2.455e-005 -0.1079 3 0.00000 0.00000 0.00000 0.22222 0.77778 0.00000 0.00000 0.00000 0.00000 8 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000			
36 37 38 39 40 41 42 43 44 45 46 47 48 49 50 51 52 53 54 55 56 57 58	Name	13	0xygen Out 1.0000 23.071 101.32 1.3022 1.3022 1.0001 3.663e-005 -2.392e-005 Compositions 1 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 5 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	Hydrogen 1.0000 22.971 101.32 2.6045 0.12607 7.516e-005 -4.808e-005 2 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 6 0.00000 0.00000 6 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	17	3 0.0000 21.112 106.32 * 1.3601 0.58807 2.455e-005 -0.1079 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 8 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000			
36 37 38 39 40 41 42 43 44 45 46 47 48 49 50 51 52 53 54 65 57 58 59 60	Name	13	0xygen Out 1.0000 23.071 101.32 1.3022 1.3022 1.0001 3.663e-005 -2.392e-005 Compositions 1 0.00000 0.00000 1.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	Hydrogen	17	3 0.0000 21.112 106.32 1.3601 0.58807 2.455e-005 -0.1079 3 0.00000 0.00000 0.00000 0.22222 0.77778 0.00000 0.00000 0.00000 0.00000 8 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000			
36 37 38 39 40 41 42 43 44 45 46 47 48 49 50 51 52 53 54 55 56 67 58 69 60 61	Name	13	0xygen Out 1.0000 23.071 101.32 1.3022 1.3022 1.0001 3.663e-005 -2.392e-005 Compositions 1 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 5 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	Hydrogen 1.0000 22.971 101.32 2.6045 0.12607 7.516e-005 -4.808e-005 2 0.00000 0.00000 0.00000 0.02222 0.77778 0.00000 0.00000 0.00000 0.00000 6 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000	17	3			
36 37 38 39 40 41 42 43 44 45 46 47 48 49 50 61 52 53 54 55 56 57 58 59 60 61 62	Name	13	0xygen Out 1.0000 23.071 101.32 1.3022 1.3002 1.0001 3.663e-005 -2.392e-005 Compositions 1 0.00000	Hydrogen 1.0000 22.971 101.32 2.6045 0.12607 7.516e-005 -4.808e-005 2 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.005699 0.10958 0.47591 0.25734 0.10017	17 1.0000 22.970 80.669 2.6045 0.12607 7.516e-005 -4.808e-005 2r 0.00000° 0.00000° 0.00000° 0.00000° 0.00000° 0.00000° 7 0.00000° 0.00000° 0.00000° 0.00000° 0.00000° 0.00000° 0.00000° 0.000000° 0.000000° 0.000000° 0.000000° 0.000000° 0.000000° 0.00000000	12			
36 37 38 39 40 41 42 43 44 45 46 47 48 49 50 51 52 53 54 55 56 57 58 59 60 61 62 63	Name	13	0xygen Out 1.0000 23.071 101.32 1.3022 1.3022 1.0001 3.663e-005 -2.392e-005 Compositions 1 0.00000	Hydrogen 1.0000 22.971 101.32 2.6045 0.12607 7.518e-005 -4.808e-005 2 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.05699 0.10958 0.47591 0.25734 0.10017 0.00000 0.00000 0.00000	17 1.0000 22.970 80.669 2.6045 0.12607 7.516e-005 -4.808e-005 2r 0.00000° 0.00000° 0.00000° 0.00000° 0.00000° 7 0.00000°	12 0.0000 21.112 106.32 * 1.3601 0.58807 2.455e-005 -0.1079 3 0.00000			

Licensed to: INL Specified by user.

_										
1			Case Name:	Case Name: C:\NASA Final\Sabatier 6.hsc						
3	INL Calgary,		Unit Set:	NASA2						
5	CANADA		Date/Time:	Date/Time: Mon Aug 23 10:33:42 2010						
6				•						
7	Workbook:	Case (Mair	ı) (continue	(continued)						
9 10		Cor	mpositions (cont	inued)						
11	Name	9	CH4, CO2, H2, H2O	10	11	Water In				
12	Comp Mole Frac (Oxygen)	0.00000	0.00000	0.00000	0.00000	0.00000 *				
13 14	Comp Mole Frac (Carbon)	0.00000	0.00000	0.00000	0.00000	0.00000*				
15	Comp Mole Frac (CO)	0.00002 0.12701	0.00002 0.12701	0.00000 0.00005	0.00000 0.00005	0.00000 *				
16	Comp Mole Frac (CO2) Comp Mole Frac (Hydrogen)	0.05783	0.05783	0.00000	0.00000	0.00000				
17	Comp Mole Frac (H2O)	0.04120	0.04120	0.99995	0.99995	1.00000				
18	Comp Mole Frac (Methane)	0.77394	0.77394	0.00000	0.00000	0.00000 *				
19	Comp Mole Frac (Argon)	0.00000	0.00000	0.00000	0.00000	0.00000 *				
20	Comp Mole Frac (Nitrogen)	0.00000	0.00000	0.00000	0.00000	0.00000 *				
21	Name	13	Oxygen Out	Hydrogen	17	12				
22	Comp Mole Frac (Oxygen)	0.00000	1.00000	0.00000	0.00000	0.00000				
23	Comp Mole Frac (Carbon)	0.00000	0.00000	0.00000	0.00000	0.00000				
24	Comp Mole Frac (CO)	0.00000	0.00000	0.00000	0.00000	0.00000				
25	Comp Mole Frac (CO2)	0.00002	0.00000	0.00002	0.00002	0.00000				
26	Comp Mole Frac (Hydrogen)	0.00000	0.00000	0.99998	0.99998	0.00000				
27	Comp Mole Frac (H2O)	0.99998	0.00000	0.00000	0.00000	1.00000				
28	Comp Mole Frac (Methane)	0.00000	0.00000	0.00000	0.00000	0.00000				
29 30	Comp Mole Frac (Argon)	0.00000	0.00000	0.00000	0.00000	0.00000				
31	Comp Mole Frac (Nitrogen)	0.00000	0.00000	0.00000	0.00000	0.00000				
32			Energy Stream							
33	Name	Q HT Sabatier	Q LT Sabatier	Ambient Cooling	Gas Cmp Pwr	CP Power				
34	Heat Flow (kW)	-1.088e-002	-1.801e-002	-1.534e-002	2.268e-004	2.513e-007				
35 36	Name Heat Flow (kW)	Electrolysis Power 0.2065	Water Pump Power 4.492e-008							
37	near riow (kvv)	0.2005	_							
38 39	Name	Gas Compressor	Compressors							
40	Feed Pressure (kPa)	75.84								
41	Product Pressure (kPa)	101.3 *								
42	Molar Flow (gmole/h)	0.8259								
43	Energy (kW)	2.268e-004								
44	Adiabatic Efficiency	75 °								
45	Polytropic Efficiency	76								
46 47			Pumps							
48	Name	Condensate Pump	Water Pump							
49	Delta P (kPa)	30.48	5.000							
50	Energy (kW)		4.492e-008							
51	Feed Pressure (kPa)		101.3*							
52	Product Pressure (kPa)	106.3	106.3 *							
53 54	Molar Flow (gmole/h)		1.360			<u> </u>				
54 55	Adiabatic Efficiency (%)	75.00 *	75.00 °							
56	Heat Exchangers									
57	Name	Recup HX 1	Recup HX 2							
58	Duty (kW)		1.025e-002							
59	Tube Inlet Temperature (C)	22.15 *	178.4 *							
60	Tube Outlet Temperature (C)		510.6 *							
61	Shell Inlet Temperature (C)		565.0 °							
62	Shell Outlet Temperature (C)		198.4							
63	UA (W/C)		0.2820							
64	LMTD (C)		36.36							
65	Minimum Approach (C)	20.00	20.00	4 3000)		De 0 6 -				
66	Hyprotech Ltd.	HY	SYS.Plant v2.2.2 (Buil	u 3606)		Page 2 of 5				

Licensed to: INL *Specified by user.

_												
1	Do.				Case Name:	Case Name: C:\NASA Final\Sabatier 6.hsc						
3	HYPROTECH	INL Calgary, A	lberta		Unit Set:	Unit Set: NASA2						
5	S. S	CANADA			Date/Time:	Date/Time: Mon Aug 23 10:33:42 2010						
6												
8	Workb	ook:	Case (Ma	lin) (continue	ed)						
9					Unit Ops							
11	Operation Name	Ope	ration Type		Feeds	Products		Ignored	Calc. Level			
12 13	Hi Temp Sabatier Reactor		m Reactor	4	HT Sabatier	16		No	500.0 *			
14	ri Tellip Sabatier Reactor	Equilibriu	III Reactor	Q I	TI Sabatier	Q HT Sabatier		1 140	300.0			
15						15						
16 17	Lo Temp Sabatier Reactor	Sabatler Reactor Equilibrium Reactor		QI	LT Sabatier	7 Q LT Sabatier		No	500.0 *			
18				8		10						
19	Condenser/Water Separator	Separato	r	Am	bient Cooling	9		No	500.0 *			
20 21	Rcy	Recycle		2		Ambient Cooling 2r		No	3500 *			
22	-			1		2						
23	M1	Mixer		17				No	500.0 *			
24 25	M2	Mixer		11 12		13		No	500.0 *			
26	Min App Adj	Adjust						No	3500 *			
27	ADJ-1	Adjust						No	3500 *			
28 29	ADJ-2 ADJ-3	Adjust Adjust						No No	3500 °			
30			Cat Flameters	13		Oxygen Out						
31	Electrolysis		Sub-Flowsheet	Ele	ectrolysis Power	Hydrogen		No	2500 *			
32 33	Sabatier Calcs	Spreadsh	eet	9		CH4, CO2, H2, H	20 Out	No	500.0 *			
34	Gas Compressor	Compres	sor		s Cmp Pwr	CH4, CO2, H2, H	20 Out	No	500.0			
35 36	Condensate Pump	Pump		10 CP Power		11		No	500.0 *			
37 38	Water Pump	Pump		Water In Water Pump Power		12		No	500.0 *			
39	D 1197.4			2r	ater Fullip Fower	3			500.0			
40	Recup HX 1	Heat Exc	nanger	7		8		No	500.0 *			
41 42	Recup HX 2	Heat Exc	hanger	5		6		No	500.0 *			
43	Valve 1	Val∨e)2 In	1		No	500.0 *			
44	Valve 2	Val∨e		Ну	drogen	17		No	500.0 *			
45 46	Workb	ook:	Electroly	sis	s (TPL1)							
47 48												
49					Streams							
50	Name		13 @TPL1		Electrolysis Power @		14 @TI		Hydrogen @TPL1			
51 52	Vapour Fraction	/C\	0.000	_		1.0000		1.0000 23.071	1.0000			
52 53	Temperature Pressure	(C) (kPa)	22.97 106.3			22.971 103.82		101.32	22.971 101.32			
54		(gmole/h)	2.604	$\overline{}$		3.9067		1.3022	2.6045			
55	Mass Flow	(kg/d)	1.126			1.1261		1.0001	0.12607			
56 57	Liquid Volume Flow Heat Flow	(m3/h)	4.702e-00 -0.200		0.2065	1.118e-004 -7.201e-005		3.663e-005 2.392e-005	7.516e-005 -4.808e-005			
58		(kW) J/kgmole)	-2.856e+0		0.2065	-7.201e-005 -66.36	_	-66.14	-4.808e-005 -66.46			
59												
60												
60 61												
63 64												
65 66	Hyprotech Ltd.			HVC	SYS.Plant v2.2.2 (Build	4 3806)			Page 3 of 5			
00	Licensed to: INL			1113	71-O.FIAITE VZ.Z.Z (DUIII	u 0000)			* Specified by user.			

2	No.	15.11		Case Name:	C:\NASA Final\Sal	oatier 6.hsc		
3	HYPROTECH	INL Calgary, Alberta CANADA		Unit Set:	NASA2			
5		CANADA		Date/Time:	Mon Aug 23 10:33	3:42 2010		
6								
7	Workb	ook: Ele	ectrolys	sis (TPL1) (c	ontinued	1)		
9				Composition				
11	Name	13 (2)TPL1	15 @TPL1	14 @TPL1	Hydroge	en @TPL1	
12	Comp Mole Frac (Oxygen)		0.00000		1.000		0.00000	
13 14	Comp Mole Frac (Carbon)		0.00000		0.000		0.00000	
15	Comp Mole Frac (CO) Comp Mole Frac (CO2)		0.00000		0.000		0.00000	
16	Comp Mole Frac (CO2) Comp Mole Frac (Hydrogen)		0.00000		0.000		0.99998	
17	Comp Mole Frac (H2O)		0.99998		0.000		0.00000	
18	18 Comp Mole Frac (Methane) 0.00000			0.00000	0.00	000	0.00000	
19				0.00000	0.00	000	0.00000	
20	Comp Mole Frac (Nitrogen)		0.00000	0.00000	0.000	000	0.00000	
21 22				Unit Ops				
23	Operation Name	Operation	Туре	Feeds	Proc	lucts	Ignored	Calc. Level
24				13 @TPL1	2 @TPL1			
25	Electrolysis @TPL1	Conversion Rea	actor	Electrolysis Power @TPL		07014	No	500.0 *
26 27				15 @TDI 1		Power @TPL1		
28	H2/O2 Splitter @TPL1	Component Spli	tter	15 @TPL1	Hydrogen @ 14 @TPL1	IPLI	No	500.0 *
29	SET-1 @TPL1	Set			11.6.1.21		No	500.0 *
30	SET-2 @TPL1	Set					No	500.0 *
31	SET-3 @TPL1	Set					No	500.0 *
32	SET-4 @TPL1	Set					No	500.0 *
33 34 35 36	Conv	ersion:	Electro					
37				STOICHIOMETR	ΚΥ			
38	Compone	nt		Mole Weight			Stoichiometric C	
39	H2O				18.015			-1*
40 41	Hydrogen Oxygen				2.016 32.000			1°
42	Охуден				32.000			
43								
44	Balance	e Error: 0.0000			Read	ction Heat: 2.4	10e+005 kJ/kgr	nole
45 46				BASIS				
47	Base Component: H2C)	Conve	ersion Percent: 100.00		Reaction	Phase: Liquid	lPhase
48				PARAMETERS	 S			
49 50								
51	Equi	librium:	Sabati	er				
52	_9			··				
53				STOICHIOMETE	24			
52 53 54	A	-t			<u></u>		olobiomet-l- C	efficient.
56	Compone	nt Metha	ne	Molecular Weight	16.04	Ste	oichiometric Coe	-1 *
56 57			18.02			-1 *		
58 59	H2O CO				28.01			1*
		Hydrog	en		2.016			3 *
60	_ :			1	_			
61 62	Balance	Error: 0.0000			Reac	tion Heat: 2.0)53e+005 kJ/kgr	noie
63								
63 64								
65								
66	Hyprotech Ltd.		H	HYSYS.Plant v2.2.2 (Buil	d 3806)			Page 4 of 5
	Licensed to: INI							* Specified by user

_							
2		INL		Case N	ame: C:\NAS	A Final\Sabatier 6.hsc	
3	HYPROTECH	Calgary, Alberta	a	Unit Set	: NASA2	2	
4 5		CANADA		Date/Tir	ne: Mon Au	ug 23 10:33:42 2010	
6	E	In	0-14				
7	Equili	prium:	Sapatie	er (cont	inuea)		
9 10				ВА	sis		
11 12	Basis	Ph	ase	Appro	oach C)	Min. Temp (C)	Max. Temp (C)
13	Activity		VapourPhase	,		-273.	
14 15				PARAM	ETERS		
16 17				Source : K	Vs. T Table		
18	Coeff A			-20.55	R2		0.999961 *
19	Coeff B			-2.292e+004	T High		
20	Coeff C			7.195	T Low		
21 22	Coeff D			-2.949e-003			
23	Temperature		Keq			KCalc	Percentage Error
24	(C)		· .				· ·
25	93	3.333 *		7.813e-019 °		7.774e-019 *	0.5048 *
26		48.89 *		6.839e-015 *		6.854e-015 *	-0.2150 °
27		D4.44 *		7.793e-012 *		7.849e-012 *	-0.7139 *
28 29		60.00 *		2.173e-009 '		2.184e-009 °	-0.5191 *
29 30		15.56 *		2.186e-007 '		2.187e-007 °	-3.464e-002 *
31		71.11 ° 26.67 °		1.024e-005 * 2.659e-004 *		1.020e-005 * 2.644e-004 *	0.4196 ° 0.5493 °
32		82.22 *		4.338e-004		4.325e-003 °	0.2956 *
33		37.78 *		4.900e-003		4.891e-002 °	0.1845 *
34		93.33 *		0.4098 *		0.4096 *	5.895e-002 *
35		48.89 °		2.679 *		2.676 *	0.1033 *
36	70	04.44 *		14.26 '		14.21 *	0.3276 *
37	76	60.00 *		63.43 *		63.35 *	0.1193 *
38		15.56 *		242.6 *		243.2 *	-0.2394 °
39		71.11 *		816.6 *		820.7 *	-0.5042 *
40 41		26.67 *		2464		2477 *	-0.5388 *
41		82.22 ° 037.8 °		6755 * 1.701e+004 *		6783 * 1.704e+004 *	-0.4088 ° -0.2007 °
43		093.3 *		3.967e+004		3.970e+004 *	-8.074e-002 *
44		148.9 *		8.664e+004 *		8.645e+004 °	0.2204 *
45		204.4 *		1.784e+005 *		1.772e+005 *	0.6564 *
46 47 48							
47							
48							
49 50							
51							
52							
53							
54							
55							
56							
57							
58							
59							
61							
62							
51 52 53 54 55 56 57 58 60 61 62 63 64 65							
64							
_							
66	Hyprotech Ltd.		Н	YSYS.Plant v2.	2.2 (Build 3806	3)	Page 5 of 5

A.5 Sabatier Process with Co-electrolysis and Heat Recuperation 3.608e-003 KW 0.1849 kW H2,CO,H2O Out 3.500 Electrolysis Power Co-Electrolysis Calcs Water Gas Shift Heat Remaining From Sabatier H2 to sum of CO & CO2 ratio (U) (0) 55 High Temp Sabatier Total Power (Ú) 12 Low Temp Sabatier ₽ P P P P 3 Circ. †8<u>°</u> =

Figure A - 10 Process flow diagram of Sabatier process with co-electrolysis and heat recuperation

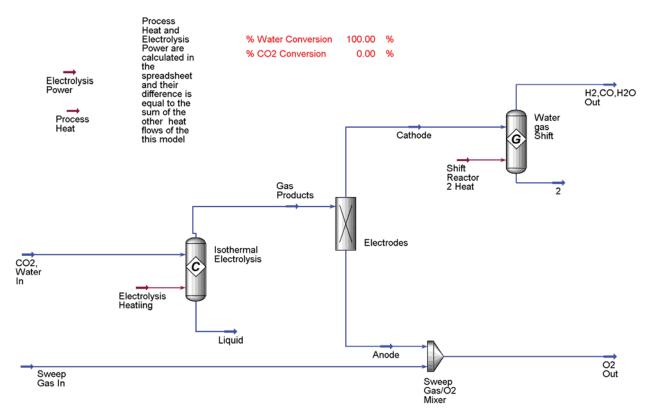


Figure A - 11 Process flow diagram of co-electrolysis module within Sabatier process with co-electrolysis and heat recuperation

_										
2	lin.	IN II		Case Name:	C:\NASA Final\NASA Co	o-Electrolysis 4.hsc				
3	HYPROTEC	INL Calgary, A	Mberta	Unit Set:	NASA					
5		CANADA		Date/Time:	Date/Time: Mon Aug 23 10:45:17 2010					
6										
7	Wor	kbook:	Case (Main	1)						
9				Streams						
11	Name		1	2	3	4	5			
12	Vapour Fraction		0.0000	0.0000	0.0000	1.0000	0.3357			
13	Temperature	(C)	15.556	19.698	93.868	20.781	58.858			
14	Pressure	(kPa)	102.70 *	102.70	101.33	101.33	101.33			
15	Molar Flow	(gmole/h)	1.4299	2.5468	2.5468	0.60435	3.5882			
16	Mass Flow	(kg/d)	0.61823	1.1011	1.1011	0.63833	1.8425			
17	Liquid Volume Flow	(m3/h)	2.581e-005	4.597e-005	4.597e-005	3.223e-005	9.097e-005			
18	Heat Flow	(kW)	-0.1137	-0.2022	-0.1981	-6.614e-002	-0.2718			
19	Molar Enthalpy	(kJ/kgmole)	-2.861e+005	-2.858e+005	-2.800e+005	-3.940e+005	-2.727e+005			
20	Name		5r	6	7	8 4 0000	9			
21	Vapour Fraction	201	0.3357	1.0000	1.0000	1.0000	1.0000			
22 23	Temperature	(C)	58.858 ⁻ 101.33 ⁻	91.597	103.98 110.98	775.00 *	800.00 *			
23	Pressure Molar Flow	(kPa)		99.946		109.60	108.22			
25	Mass Flow	(gmole/h)	3.5882 * 1.8425	3.5882 1.8425	3.5882 1.8425	3.5882 1.8425	3.5882 1.8425			
26	Liquid Volume Flow	(kg/d)	9.097e-005	9.097e-005	9.097e-005	9.097e-005	9.097e-005			
27	Heat Flow	(m3/h) (kW)	-0.2718	-0.2423	-0.2419	-0.2158	-0.2147			
28	Molar Enthalpy	(kJ/kgmole)	-2.727e+005	-2.431e+005	-2.427e+005	-2.165e+005	-2.154e+005			
29	Name	(KU/Kgillole)	10	11	12	13	14			
30	Vapour Fraction		1,0000	1.0000	1.0000	1.0000	1,0000			
31	Temperature	(C)	409.01	129.00 *	129.00	129.00	128.98			
32	Pressure	(kPa)	102.70	101.33	101.33	101.33	79.290 *			
33	Molar Flow	(gmole/h)	1.3021	3.5736	3,1365	0.43706	3.1365			
34	Mass Flow	(kg/d)	1,0000	0.84252	0.73948	0.10304	0.73948			
35	Liquid Volume Flow	(m3/h)	3.662e-005	1.044e-004	9.164e-005	1.277e-005	9.164e-005			
36	Heat Flow	(kW)	4.303e-003	-6.175e-002	-5.420e-002	-7.552e-003	-5.420e-002			
37	Molar Enthalpy	(kJ/kgmole)	1.190e+004	-6.220e+004	-6.220e+004	-6.220e+004	-6.220e+004			
38	Name		15	16	17	AmbCool	Circ Pwr			
39	Vapour Fraction		1.0000	1.0000	0.0000					
40	Temperature	(C)	565.00 *	150.00 *	25.000					
41	Pressure	(kPa)	77.911	76.532	75.153					
42	Molar Flow	(gmole/h)	2.5813	1.9425	1.1169					
43	Mass Flow	(kg/d)	0.73947	0.73947	0.48291					
44	Liquid Volume Flow	(m3/h)	8.033e-005	5.856e-005	2.016e-005					
45	Heat Flow	(kW)	-6.039e-002	-8.729e-002	-8.855e-002	-1.613e-002	4.246e-004			
46 47	Molar Enthalpy	(kJ/kgmole)	-8.422e+004	-1.618e+005	-2.854e+005	H0 00 H00 0:4	Heat Franc Och eff			
\vdash	Name Vanour Fraction		CO2 In	CO2, Water In	Electrolysis Power	H2,CO,H2O Out	Heat From Sabatier			
48 49	Vapour Fraction	(0)	1.0000 21.111 *	1.0000 799.25		1.0000				
50	Temperature Pressure	(C) (kPa)								
51	Pressure Molar Flow	(kPa) (gmole/h)	131.00 ° 0.60435	106.84 3.5903		102.70 3.5736				
52	Mass Flow	(gillole/ll) (kg/d)	0.63833 *	1.8425		0.84252				
53	Liquid Volume Flow	(m3/h)	3.223e-005	9.111e-005		1.044e-004				
54	Heat Flow	(kW)	-6.614e-002	-0.2147	0.1834	-4.050e-002	2.949e-002			
55	Molar Enthalpy	(kJ/kgmole)	-3.940e+005	-2.153e+005		-4.080e+004				
56	Name	(Hi Temp Pwr	Lo Tmp Sabtr Q	Methane, H2 Out	O2 Out	Oxygen Out			
57	Vapour Fraction				1.0000	1.0000	1.0000			
58	Temperature	(C)			25.000 °	800.00	44.698			
59	Pressure	(kPa)			75.153	104.08	101.33			
60	Molar Flow	(gmole/h)			0.82558	1.3021	1.3021			
61	Mass Flow	(kg/d)			0.25656	1.0000	1.0000			
62	Liquid Volume Flow	(m3/h)			3.840e-005	3.662e-005	3.662e-005			
63	Heat Flow	(kW)	1.074e-003	-2.690e-002	-1.487e-002	9.140e-003	2.061e-004			
64	Molar Enthalpy	(kJ/kgmole)			-6.484e+004	2.527e+004	569.7			
65										
66	Hyprotech Ltd.		HYS	SYS.Plant v2.2.2 (Buil	d 3806)		Page 1 of 8			

68 Hyprotech Ltd. HYSYS.Plant v2.2.2 (Build 3806) Page 1 of
Licensed to: INL * Specified by user.

_									
2	INL		Case Name:	C:\NASA Final\NASA Co	o-Electrolysis 4.hsc				
3	Calgary, A	Alberta	Unit Set:	NASA					
4 5	CANADA		Date/Time: Mon Aug 23 10:45:17 2010						
6	107 11 1								
7	Workbook:	Case (Main	ı) (continue	ed)					
9			Streams (continu	ued)					
10 11	Name	Rcycl Pmp Pwr	Recycle Water	Water In	Wtr Pmp Pwr				
12	Vapour Fraction		0.0000	0.0000					
13	Temperature (C)		25.003	15.556 *					
14	Pressure (kPa)		102.70	101.33 "					
15	Molar Flow (gmole/h)		1.1169	1.4299					
16	Mass Flow (kg/d)		0.48291	0.61823					
17	Liquid Volume Flow (m3/h)		2.016e-005	2.581e-005					
18	Heat Flow (kW)	2.038e-007	-8.855e-002	-0.1137	1.297e-008				
19	Molar Enthalpy (kJ/kgmole)		-2.854e+005	-2.861e+005					
20 21			Compressors	5					
22	Name	Circulator							
23	Feed Pressure (kPa)	99.95							
24	Product Pressure (kPa)	111.0							
25	Molar Flow (gmole/h)	3.588							
26	Energy (kW)	4.246e-004							
27	Adiabatic Efficiency	75 *							
28	Polytropic Efficiency	75							
29 30			Composition	1					
31	Name	1	2	3	4	5			
32	Comp Mole Frac (H2O)	1.00000	1.00000	1.00000	0.00000	0.72696			
33	Comp Mole Frac (Hydrogen)	0.00000	0.00000	0.00000	0.00000	0.08114			
34	Comp Mole Frac (Oxygen)	0.00000	0.00000	0.00000	0.00000	0.00000			
35	Comp Mole Frac (Argon)	0.00000	0.00000	0.00000	0.00000	0.00000			
36	Comp Mole Frac (Nitrogen)	0.00000	0.00000	0.00000	0.00000	0.00000			
37	Comp Mole Frac (CO2)	0.00000	0.00000	0.00000	1.00000	0.17275			
38	Comp Mole Frac (CO)	0.00000	0.00000	0.00000	0.00000	0.01886			
39	Comp Mole Frac (Methane)	0.00000	0.00000	0.00000	0.00000	0.00028			
40	Comp Mole Frac (Carbon)	0.00000	0.00000	0.00000	0.00000	0.00000			
41	Name	5r	6	7	8	9			
42	Comp Mole Frac (H2O)	0.72696 *	0.72696	0.72696	0.72696	0.72696			
43	Comp Mole Frac (Hydrogen)	0.08114 *	0.08114	0.08114	0.08114	0.08114			
44 45	Comp Mole Frac (Oxygen)	0.00000 *	0.00000	0.00000	0.00000	0.00000			
45 46	Comp Mole Frac (Argon)	0.00000 *	0.00000	0.00000	0.00000	0.00000			
46 47	Comp Mole Frac (CO2)	0.00000 ° 0.17275 °	0.00000 0.17275	0.00000 0.17275	0.00000 0.17275	0.00000 0.17275			
48	Comp Mole Frac (CO2) Comp Mole Frac (CO)	0.17275	0.17275	0.17275	0.17275	0.17275			
49	Comp Mole Frac (Methane)	0.00028 *	0.00028	0.00028	0.00028	0.00028			
50	Comp Mole Frac (Carbon)	0.00020	0.00000	0.00000	0.00000	0.00000			
51	Name	10	11	12	13	14			
52	Comp Mole Frac (H2O)	0.00000	0.14115	0.14115	0.14115	0.14115			
53	Comp Mole Frac (Hydrogen)	0.00000	0.66617	0.66617	0.66617	0.66617			
54	Comp Mole Frac (Oxygen)	1.00000	0.00000	0.00000	0.00000	0.00000			
55	Comp Mole Frac (Argon)	0.00000	0.00000	0.00000	0.00000	0.00000			
56	Comp Mole Frac (Nitrogen)	0.00000	0.00000	0.00000	0.00000	0.00000			
57	Comp Mole Frac (CO2)	0.00000	0.03553	0.03553	0.03553	0.03553			
58	Comp Mole Frac (CO)	0.00000	0.15482	0.15482	0.15482	0.15482			
59	Comp Mole Frac (Methane)	0.00000	0.00233	0.00233	0.00233	0.00233			
60 61	Comp Mole Frac (Carbon)	0.00000	0.00000	0.00000	0.00000	0.00000			
FC CO									
92 02									
61 62 63									
65									
36	Hyprotech Ltd.	LIV	SYS.Plant v2.2.2 (Bui	ld 3806)		Page 2 of 8			
~	rijprotoori Etd.	ПК	5 . 5.1 Idili 12.2.2 (Dul	u 0000)		1 490 2 01 0			

1 2 3 4 5 6 7 8	INL Calgary, A CANADA		Case Name:	C:\NASA Final\NASA Co	o-Electrolysis 4.hsc	
4 5 6 7	Calgary, A					
5 6 7	CANADA	Mberta	Unit Set:	NASA		
7			Date/Time:	Mon Aug 23 10:45:17 2	010	
_						
	Workbook:	Case (Main) (continue	ed)		
9		Co	mposition (conti	inued)		
10	Nama		<u> </u>		002 l-	000 14(-11-
12	Name Comp Mole Frac (H2O)	0.24483	0.59264	1.00000	0.00000 °	CO2, Water In 0.72538
13	Comp Mole Frac (Hydrogen)	0.52105	0.09624	0.00000	0.00000	0.08283
14	Comp Mole Frac (Oxygen)	0.00000	0.00000	0.00000	0.00000 *	0.00000
15	Comp Mole Frac (Argon)	0.00000	0.00000	0.00000	0.00000 *	0.00000
16	Comp Mole Frac (Nitrogen)	0.00000	0.00000	0.00000	0.00000 *	0.00000
17	Comp Mole Frac (CO2)	0.07740	0.00000	0.00000	1.00000 *	0.17354
18	Comp Mole Frac (CO)	0.04634	0.00000	0.00000	0.00000 *	0.01825
19	Comp Mole Frac (Methane)	0.11038	0.31112	0.00000	0.00000 *	0.00000
20	Comp Mole Frac (Carbon)	0.00000	0.00000	0.00000	0.00000 *	0.00000
21	Name	H2,CO,H2O Out	Methane, H2 Out	O2 Out	Oxygen Out	Recycle Water
22	Comp Mole Frac (H2O)	0.14115	0.04152	0.00000	0.00000	1.00000
23	Comp Mole Frac (Hydrogen)	0.66617	0.22645	0.00000	0.00000	0.00000
24 25	Comp Mole Frac (Oxygen)	0.00000	0.00000	1.00000	1.00000	0.00000
25	Comp Mole Frac (Argon)	0.00000	0.00000	0.00000	0.00000	0.00000
26 27	Comp Mole Frac (Nitrogen)	0.00000	0.00000	0.00000	0.00000	0.00000
	Comp Mole Frac (CO2)	0.03553	0.00000	0.00000	0.00000	0.00000
28 29	Comp Mole Frac (CO)	0.15482	0.00000	0.00000	0.00000	0.00000
30	Comp Mole Frac (Methane) Comp Mole Frac (Carbon)	0.00233 0.00000	0.73203 0.00000	0.00000	0.00000	0.00000
31	Name	Water In	0.00000	0.00000	0.00000	0.00000
32	Comp Mole Frac (H2O)	1.00000 *				
33	Comp Mole Frac (Hydrogen)	0.00000				
34	Comp Mole Frac (Oxygen)	0.00000				
35	Comp Mole Frac (Argon)	0.00000 *				
36	Comp Mole Frac (Nitrogen)	0.00000 *				
37	Comp Mole Frac (CO2)	0.00000 *				
38	Comp Mole Frac (CO)	0.00000 *				
39	Comp Mole Frac (Methane)	0.00000 *				
40	Comp Mole Frac (Carbon)	0.00000 -				
41 42			Heat Exchange	rs		
43	Name	Low Temp Recuperat				
44	Duty (kW)	-4.097e-003				
45	Tube Inlet Temperature (C)	409.0				
46	Tube Outlet Temperature (C)	44.70				
47	Shell Inlet Temperature (C)	19.70				
48	Shell Outlet Temperature (C)	93.87				
49	LMTD (C)	117.5				
50	UA (kJ/C-h)	0.1255				
51	Minimum Approach (C)	25.00				
52 53		Ot	ther Heat Exchar	ngers		
54	Name	High Temperature Re				
55	Number of Sides	3 '				
56	LMTD (C)	41.41 *				
57	UA (Calculated) (kJ/C-h)	2.268				
58	Hot Pinch Temperature (C)	800.0				
59	Cold Pinch Temperature (C)	775.0				
60	Minimum Approach (C)	25.00				
61	Exchanger Cold Duty (kW)	2.608e-002				
62						
63						
64						
65	Liverate of 1 td	1.02	OVE Diant to 0.0 (Dell	4 3006/		Do == 0 =6 0
66	Hyprotech Ltd. Licensed to: INL	HYS	SYS.Plant v2.2.2 (Buil	a 3806)		Page 3 of 8 * Specified by user.

_								
1	lbs.				Case Name:	C:\NASA Final\NASA C	o-Electrolysis 4.hsc	
3	HYPROTECH	INL Calgary, A	Alberta		Unit Set:	NASA		
4		CANADA			Date/Time:	Mon Aug 23 10:45:17 2	2010	
6						3		
1	Workb	ook:	Case (Ma	in)	(continue	ed)		
9					Pumps			
11	Name		Feedwater Pump		Recycle Pump			
12	Delta P	(kPa)	1.3	-	27.55			
13	Energy	(kW)	1.297e-0	80	2.038e-007			
14	Feed Pressure	(kPa)	101	_	75.15			
15	Product Pressure Molar Flow	(kPa)	102		102.7 1.117			
17	Adiabatic Efficiency	(gmole/h) (%)	75.		75.00 *			
18	,	(14)		-				
19		_			Unit Ops			
20	Operation Name	Ope	eration Type	8	Feeds	9 Products	Ignored	Calc. Level
27	Hi Temp Heater	Heater		_	emp Pwr	9	No	500.0 *
23				5r	emp r wi	6		
24	Sabatier Heater	Heater		_	t From Sabatier		No	500.0 *
25	T1	Tee		11		12	No	500.0
26	.,	100				13	140	300.0
27	Low Temp Recuperator	Heat Exc	hanger	10		Oxygen Out	No	500.0 *
29				4		5		
30	M2	Mixer		3			No	500.0 *
31				13				
32	M3	Mixer		1		2	No	500.0
33				Rec 6	ycle Water	7		
35	Circulator	Compres	sor	-	Pwr	1	No	500.0 *
36					CO,H2O Out	11		
37	High Temperature Recupera	LNG		7		8	No	500.0 *
38				02 (10		
40					ep Gas In 2, Water In	O2 Out H2,CO,H2O Out		
41	High Temperature Co-Electro	Standard	Sub-Flowsheet		ess Heat	112,00,1120 001	No	2500 *
42					trolysis Power			
43	Electrolysis Input and Output	Spreadsh	neet				No	500.0 *
44	Co-Electrolysis Calcs	Spreadsh	neet			000	No	500.0 *
45	High Temp Sabatier	Equilibriu	m Reactor	14 Hi T	mp Sabtr Q	300 15	No	500.0
47	riigii Tellip Sabatiei	Equilibria	III IXEACIOI		nip Sabii Q	Hi Tmp Sabtr Q	140	300.0
48				15		200		
49	Low Temp Sabatier	Equilibriu	m Reactor	Lo T	mp Sabtr Q	16	No	500.0 *
50						Lo Tmp Sabtr Q		
52	Feedwater Pump	Pump			er In Pmp Pwr	1	No	500.0 *
53	December December	D.		17		Recycle Water		500.5
54	Recycle Pump	Pump		Rcy	cl Pmp Pwr		No	500.0 *
55	RCY	Recycle		5		5r	No	3500 °
56	Condenser/Mater Conservator	Congrete		16	Cool	17	No.	500.01
58	Condenser/Water Separator	Separato	"	Amb	Cool	Methane, H2 Out AmbCool	No	500.0 *
59	Water Can Chin	Oibt - 5		9		400	.,	500.0
60	Water Gas Shift	Gibbs Re	eactor			CO2, Water In	No	500.0 *
61	SET-2	Set					No	500.0 *
62	VLV 1	Valve		12	? In	4	No.	500.0 *
64	VLV 2	Valve		12		14	No	500.0 *
65								
66	Hyprotech Ltd.			HYSY	'S.Plant v2.2.2 (Buil	d 3806)		Page 4 of 8

66 Hyprotech Ltd. HYSYS.Plant v2.2.2 (Build 3806) Page 4 of 8

Licensed to: INL *Specified by user.

1				0N	0.114.04.5	Electrologic Alban	
2		INL			C:\NASA Final\NASA Co	-Electrolysis 4.nsc	
3	HYPROTEC	Calgary, A CANADA	Alberta	Unit Set:	NASA		
5	pp.			Date/Time:	Mon Aug 23 10:45:17 2	010	
6 7 8	Worl	kbook:	High Temp	erature Co	-Electrolysi	is (TPL2)	
9 10				Streams			
11	Name		Sweep Gas In @TPL	O2 Out @TPL2	Gas Products @TPL:	Liquid @TPL2	Anode @TPL2
12	Vapour Fraction		1.0000	1.0000	1.0000	0.0000	1.0000
13	Temperature	(C)	799.25	800.00	* 00.00	800.00	800.00
14	Pressure	(kPa)	104.08	104.08	105.46	105.46	104.08
15	Molar Flow	(gmole/h)	3.4662e-009	1.3021	4.8923	0.00000	1.3021
16	Mass Flow	(kg/d)	2.4000e-009	1.0000	1.8425	0.00000	1.0000
10	Liquid Volume Flow	(m3/h)	1.156e-013	3.662e-005	1.559e-004	0.0000	3.662e-005
18 19	Heat Flow	(kW)	2.341e-011	9.140e-003	-3.574e-002	0.0000 -2.630e+004	9.140e-003
20	Molar Enthalpy Name	(kJ/kgmole)	2.432e+004 H2,CO,H2O Out @TF	2.527e+004 Cathode @TPL2	-2.630e+004 2 @TPL2	CO2, Water In @TPL	2.527e+004 Electrolysis Heatiing
21	Vapour Fraction		1.0000	1.0000	0.0000	1.0000	
22	Temperature	(C)	800.00	800.00	800.00	799.25	
23	Pressure	(kPa)	102.70	104.08	102.70	106.84	
24	Molar Flow	(gmole/h)	3.5736	3.5903	0.00000	3.5903	
25	Mass Flow	(kg/d)	0.84252	0.84252	0.00000	1.8425	
26	Liquid Volume Flow	(m3/h)	1.044e-004	1.193e-004	0.0000	9.111e-005	
27	Heat Flow	(kW)	-4.050e-002	-4.488e-002	0.0000	-0.2147	0.1790
28	Molar Enthalpy	(kJ/kgmole)	-4.080e+004	-4.500e+004	-4.080e+004	-2.153e+005	
29	Name		Process Heat @TPL:	Shift Reactor 2 Heat	Electrolysis Power @		
30	Vapour Fraction						
31	Temperature	(C)					
32	Pressure	(kPa)					
33	Molar Flow	(gmole/h)					
34	Mass Flow	(kg/d)					
35	Liquid Volume Flow	(m3/h)					
36	Heat Flow	(kW)	-1.453e-009	4.380e-003	0.1834		
37	Molar Enthalpy	(kJ/kgmole)					
38 39				Composition			
40	Name		Sweep Gas In @TPL	O2 Out @TPL2	Gas Products @TPL:	Liquid @TPL2	Anode @TPL2
41	Comp Mole Frac (H2O)		0.00000	0.00000	0.00000	0.00000	0.00000
42	Comp Mole Frac (Hydro	gen)	0.00000	0.00000	0.59311	0.59311	0.00000
43	Comp Mole Frac (Oxyge	en)	0.21000	1.00000	0.26615	0.26615	1.00000
44	Comp Mole Frac (Argon))	0.00000	0.00000	0.00000	0.00000	0.00000
45	Comp Mole Frac (Nitrog	en)	0.79000	0.00000	0.00000	0.00000	0.00000
46	Comp Mole Frac (CO2)		0.00000	0.00000	0.12735	0.12735	0.00000
47	Comp Mole Frac (CO)		0.00000	0.00000	0.01339	0.01339	0.00000
48	Comp Mole Frac (Metha		0.00000	0.00000	0.00000	0.00000	0.00000
49 50	Comp Mole Frac (Carbo	n)	0.00000	0.00000	0.00000	0.00000	0.00000
50 51	Name		H2,CO,H2O Out @TF		2 @TPL2	CO2, Water In @TPL	
52	Comp Mole Frac (H2O) Comp Mole Frac (Hydro	nen)	0.14115 0.66617	0.00000 0.80821	0.14115 0.66617	0.72538 0.08283	
53	Comp Mole Frac (Oxyge		0.00000	0.00000	0.00000	0.00000	
54	Comp Mole Frac (Oxyge		0.00000	0.00000	0.00000	0.00000	
55	Comp Mole Frac (Nitrog		0.00000	0.00000	0.00000	0.00000	
56	Comp Mole Frac (CO2)	,	0.03553	0.17354	0.03553	0.17354	
57	Comp Mole Frac (CO)		0.15482	0.01825	0.15482	0.01825	
58	Comp Mole Frac (Metha	ine)	0.00233	0.00000	0.00233	0.00000	
59	Comp Mole Frac (Carbo		0.00000	0.00000	0.00000	0.00000	
60 61 62 63 64							
	Hyprotoch I td		LDV	eve Blant vo a a (Built	4 3806/		Dago 5 of 0
66	Hyprotech Ltd.		HYS	SYS.Plant v2.2.2 (Build	J 38Ub)		Page 5 of 8

1	h.				Case Name: C	:\NASA Fir	nal\NASA Co-Electroly	sis 4.hsc	
2		INL	NII 4						
3	HYPROTECH	Calgary, A	Alberta			VASA			
5	Pr:				Date/Time: N	/lon Aug 23	10:45:17 2010		
7 8	Workb	ook:	High	Tem	perature Co-	-Elect	rolysis (T	PL2) (c	ontinued)
9 10					Equilibrium React	tors			
11	Name								
12	Separator Type								
13	Vessel Temperature	(C)							
14	Vessel Pressure	(kPa)							
15		(gmole/h)							
16		(gmole/h)							
17	Heat Flow	(kW)							
18 19					Gibbs Reactors	5			
20	Name		Water ga	s Shift @	TP				
21	Separator Type) *				
22	Vessel Temperature	(C)		800.00)				
23	Vessel Pressure	(kPa)		102.70)				
24	Vapour Molar Flow	(gmole/h)		3.574	1				
25	Liquid Molar Flow	(gmole/h)		0.0000)				
26	Heat Flow	(kW)	4.	380e-003	3				
27					Component Splitt	erc			
28									
29	Name		Electrode						
30	Overhead Stream Pressure	(kPa)		104.1					
31	Overhead Stream Vapour Fra			1.000					
32	Bottoms Stream Pressure	(kPa)		104.1					
33 34	Bottoms Stream Vapour Fraction(1)	tion		1.0000					
35	Overhead Fraction(2)			1.00000					
36	Overhead Fraction(3)			0.00000					
37	Overhead Fraction(4)			1.00000					
38	Overhead Fraction(5)			1.00000					
39	Overhead Fraction(6)			1.00000					
40	Overhead Fraction(7)			1.00000					
41	Overhead Fraction(8)			1.00000					
42	Overhead Fraction(9)			0.00000					
43	• • • • • • • • • • • • • • • • • • • •				Unit Ops		,		
44		_							1
45	Operation Name		eration Type	:	Feeds		Products	Ignored	Calc. Level
46 47	Temp Average ASR @TPL2 Electrolysis Spreadsheet @	Spreadsh Spreadsh		-				Yes No	500.0 °
48	Steam Electrolysis @TPL2	Spreadsh						No No	500.0
49	CO2 Electrolysis @TPL2	Spreadsh		\rightarrow				No	500.0
50					Anode @TPL2	Q2 Ou	@TPL2		
51	Sweep Gas/O2 Mixer @TPL	Mixer		F	Sweep Gas In @TPL2	1 32 34	J	No	500.0 *
					CO2, Water In @TPL2	Liquid	@TPL2		
52 53	Isothermal Electrolysis @TP	Conversi	on Reactor		Electrolysis Heatiing @TP		oducts @TPL2	No	500.0 *
54							lysis Heatiing @TPL:		
55	Floatradas @TDL0	00000	ont Calltter		Gas Products @TPL2		le @TPL2		500.01
56	Electrodes @TPL2		ent Splitter			Anode	@TPL2	No	500.0 *
57	ADJ-1 @TPL2	Adjust		-	A # 1 ATC: -			Yes	3500 *
58				 	Cathode @TPL2	2 @TP			
59	Water gas Shift @TPL2	Gibbs Re	actor	 	Shift Reactor 2 Heat @TP		,H2O Out @TPL2	No	500.0 *
60	CET 4 OTDLC	C-4		-		Shift R	eactor 2 Heat @TPL		
61	SET-1 @TPL2	Set						No	500.0 *
62	SET-3 @TPL2	Set						No	500.0 *
63 64	SET-2 @TPL2	Set						No	500.0 *
64 65									
66	Hyprotech Ltd.			L	IYSYS.Plant v2.2.2 (Build	13806)			Page 6 of 8
vo	Licensed to: INI				11010.1 Idili VZ.Z.Z (Dullu	, 5000)			1 Consider houses

_							
2	lbs.	NL		Case Name: C:\N	ASA Final\NA	SA Co-Electrolysis 4.	hsc
3	HYPROTECH	ol Calgary, Alberta CANADA		Unit Set: NAS	A		
5		CANADA		Date/Time: Mon	Aug 23 10:4	5:17 2010	
6	Ca	i 2 <i>C</i>	202-2	00.00			
8	Conve	ersion: 20	JUZ=2	CO+O2			
9 10				STOICHIOMETRY			
11	Component			Mole Weight		Stoich	niometric Coeff.
12 13	CO2				44.010 28.011		-2°
14	Oxygen				32.000		1'
15 16							
17	Balance I	Error: 0.0000			Rea	ction Heat: 2.832e+	005 kJ/kgmole
18 19				BASIS			
20	Base Component: CO2		Conversi	ion Percent: 100.00		Reaction Phas	se: Overall
21				PARAMETERS			
22 23							
24 25	Conve	ersion: 2H	120=2	H2+O2			
26 27				STOICHIOMETRY			
28	Component			Mole Weight		Stoich	niometric Coeff.
29 30	H2O				18.015		-2 '
31	Hydrogen Oxygen				2.016 32.000		2* 1*
32							
33 34	Palanas I				Boo	etion Host: 2 440a+	OOE k likemala
35	Dalance i	Error: 0.0000		BASIS	Rea	ction Heat: 2.410e+	005 kJ/kgmole
36 37	Base Component: H2O		Conversi	ion Percent: 90.00		Reaction Phas	se: Overall
38	Base Component. 1120		Conversi	PARAMETERS		reaction i has	Se. Overall
39 40				.,			
41	Equili	brium: Co	O2 Me	thanation			
43 44				STOICHIOMETRY			
45	Component			Molecular Weight		Stoichio	metric Coefficient
46 47		Methane H2O			16.04 18.02		-1 ° -2 °
48		CO2			44.01		1.
49		Hydrogen			2.016		4 *
50 51	Balance E	rror: 0.0000			Read	ction Heat : 1.631e+	005 kJ/kamole
52	Daniel 199 L			BASIS			
53 54	Basis	Phase		Approach		Min. Temp	Max. Temp
55 56	Acti∨ity		urPhase	(C)		(C) -273.15	(C) 3000.0
57	, was the	таро		PARAMETERS		2.00	5550.0
58 59			Sou	rce : Gibbs Free En	eray		
60 61							
62							
63 64							
65							
66	Hyprotech Ltd.		HY:	SYS.Plant v2.2.2 (Build 38	(06)		Page 7 of 8
	Licensed to: INL						 Specified by user.

A-39

1				Case N	ame: C:\NAS	A Final\NA	SA Co-Electrol	ysis 4.h	sc
2 3 4 5 6 7 8		algary, Alberta		Unit Set	: NASA				
4	CA	ANADA		Date/Ti	ne: Mon Au	ıg 23 10:48	5:17 2010		
6									
7	Equilib	orium:	Methar	nation					
9				STOICHI	OMETRY				
10 11	Component			Molecula			Si	toichiom	netric Coefficient
12		Metha			Ť	16.04			-1 *
13 14		H2	20			18.02 28.01			-1 °
15		Hydrog	en			2.016			3 "
16 17	Balance Err	or: 0.0000				Read	tion Heat: 2.	053e+0	05 kJ/kgmole
18 19				ВА	SIS				
20	Basis	Pha	••	Appr	oach		Min. Temp		Max. Temp
21 22				((C)		(C) -273	16	(C)
23	Activity	\	/apourPhase	PARAM	ETEDS		-2/3	o. 10	3000.0
23 24 25 26				PARAIN	ETERS				
26				Source : K	Vs. T Table				
27 28	Coeff A Coeff B			-20.55 -2.292e+004	R2 T High				0.999961 *
29	Coeff C			7.195	T Low				
30	Coeff D			-2.949e-003					
31 32	- .					160 1			
33	Temperature (C)		Keq			KCalc			Percentage Error
34		333 *		7.813e-019 *		7	7.774e-019 °		0.5048 *
34 35 36		3.89		6.839e-015 *			i.854e-015 *		-0.2150 *
36	204	.44 *		7.793e-012 ¹ 2.173e-009 ¹			'.849e-012 ° '.184e-009 °		-0.7139 ° -0.5191 °
37 38		5.56 *		2.175e-009 2.186e-007 *			1.184e-009		-3.464e-002 *
39		.11 *		1.024e-005 *			.020e-005 *		0.4196
40		5.67 ·		2.659e-004 °			.644e-004 *		0.5493 *
41		2.22 *		4.338e-003 *			.325e-003 *		0.2956 *
42		7.78 *		4.900e-002 *			.891e-002 *		0.1845 *
43	593	3.33 *		0.4098 *			0.4096 *		5.895e-002 *
44	648	3.89 *		2.679 *			2.676 *		0.1033 *
45	704	.44 *		14.26 *			14.21 *		0.3276*
46		0.00 *		63.43 '			63.35 *		0.1193 '
43 44 45 46 47 48		5.56 *		242.6 *			243.2 *		-0.2394 *
48		3.67 °		816.6 *			820.7 °		-0.5042 *
_		2.22 *		2464 ° 6755 °			6783 *		-0.5388 * -0.4088 *
51		7.8		1.701e+004 *		1	.704e+004 *		-0.2007 *
52		3.3 *		3.967e+004 *			.970e+004 *		-8.074e-002 *
53		8.9 *		8.664e+004 *			.645e+004 *		0.2204 *
54)4.4 °		1.784e+005 *			.772e+005 °		0.6564 *
50 51 52 53 54 55 56 57 58 59 60 61 62 63 64 65 66									
56									
57									
58									
59									
60									
61									
62									
63									
65									
66	Hyprotech Ltd.		н	YSYS Plant v2	2.2 (Build 3806	3)			Page 8 of 8
~~	rijprotoori Eta.			. J I J I I I I I V Z	(Dalla 0000	1			1 490 0 01 0

Sabt Sabt Sabt 0.2419 KW H2,CO,H2O Out 3.500 (W) Electrolysis Power Co-Electrolysis Calcs Co-Electrolysis Calcs H2 to sum of CO & CO2 ratio 9 **(O)** Ğ5 Total Power Sabtr O Sabtr ത Condenser/Water Separator 000 000 (U) Poic ¥ ω Circulator Pmp Pwr Pwr RCYΜ2 7

A.6 Sabatier Process with Co-electrolysis without Heat Recuperation

Figure A - 12 Process flow diagram of Sabatier process with co-electrolysis without heat recuperation

1				Case Name:	CUNIACA FIREBNIACA C	a Flactrohysia wa Basu	, has
2		INL	NII			o-Electrolysis wo Recup	o.nsc
4	HYPROTEC	Calgary, A	Alberta		NASA2		
5	F -			Date/Time:	Mon Aug 23 11:24:48 2	2010	
6 7 8	Worl	kbook:	Case (Main)			
9				Streams			
11	Name		1	2	3	3r	4
12	Vapour Fraction		0.0000	1.0000	0.3127	0.3127	1.0000 *
13	Temperature	(C)	19.698	20.781	50.841	50.876 *	90.860
14	Pressure	(kPa)	101.33	101.33	101.33	101.33 '	99.946
15 16	Molar Flow Mass Flow	(gmole/h)	2.5460	0.60416	3.5870	3.5879	3.5879
17	Liquid Volume Flow	(kg/d) (m3/h)	1.1008 4.596e-005	0.63813 3.222e-005	1.8419 9.094e-005	1.8423 9.095e-005	1.8423 9.095e-005
18	Heat Flow	(kW)	-0.2021	-6.612e-002	-0.2732	-0.2733	-0.2423
19	Molar Enthalpy	(kJ/kgmole)	-2.858e+005	-3.940e+005	-2.742e+005	-2.742e+005	-2.431e+005
20	Name	(/	5	6	7	8	9
21	Vapour Fraction		1.0000	1.0000	1.0000	1.0000	1.0000
22	Temperature	(C)	100.22	* 00.00	800.00	800.00	800.01
23	Pressure	(kPa)	108.22	106.84	101.33	101.33	79.290 *
24	Molar Flow	(gmole/h)	3.5879	3.5879	0.43686	3.1367	3.1367
25	Mass Flow	(kg/d)	1.8423	1.8423	0.10297	0.73934	0.73934
26	Liquid Volume Flow	(m3/h)	9.095e-005	9.095e-005	1.276e-005	9.164e-005	9.164e-005
27	Heat Flow	(kW)	-0.2420	-0.2147	-4.948e-003	-3.553e-002	-3.553e-002
28	Molar Enthalpy	(kJ/kgmole)	-2.428e+005	-2.154e+005	-4.077e+004	-4.077e+004	-4.077e+004
29 30	Name Vapour Fraction		1.0000	1.0000	0.0000	AmbCool	CH4, H2 1.0000
31	Temperature	(C)	565.00	150.00 *	25.000		25.000
32	Pressure	(kPa)	77.911	76.532	75.153		75.153
33	Molar Flow	(gmole/h)	2.5811	1.9426	1,1166		0.82596
34	Mass Flow	(kg/d)	0.73933	0.73933	0.48279		0.25653
35	Liquid Volume Flow	(m3/h)	8.033e-005	5.856e-005	2.016e-005		3.840e-005
36	Heat Flow	(kW)	-6.038e-002	-8.727e-002	-8.853e-002	-1.612e-002	-1.487e-002
37	Molar Enthalpy	(kJ/kgmole)	-8.421e+004	-1.617e+005	-2.854e+005		-6.481e+004
38	Name		Circ Pwr	CO2 In	CO2, Water In	Electrolysis Power	H2,CO,H2O Out
39	Vapour Fraction			1.0000	1.0000		1.0000
40 41	Temperature	(C)		21.111 *	799.34		800.00
42	Pressure Molar Flow	(kPa) (gmole/h)		131.00 ° 0.60416	105.46 3.5898		101.33 3.5736
43	Mass Flow	(kg/d)		0.63813 *	1.8423		0.84231
44	Liquid Volume Flow	(m3/h)		3.222e-005	9.109e-005		1.044e-004
45	Heat Flow	(kW)	3.209e-004	-6.612e-002	-0.2147	0.1834	-4.047e-002
46	Molar Enthalpy	(kJ/kgmole)		-3.940e+005	-2.153e+005		-4.077e+004
47	Name		Hi Temp Pwr	Hi Tmp Sabtr Q	Lo Temp Pwr	Lo Tmp Sabtr Q	O2 CLR Q
48	Vapour Fraction						
49	Temperature	(C)					
50	Pressure	(kPa)					
51	Molar Flow Mass Flow	(gmole/h)					
52 53	Mass Flow Liquid Volume Flow	(kg/d) (m3/h)					
54	Heat Flow	(kW)	2.728e-002	-2.485e-002	3.096e-002	-2.690e-002	9.143e-003
55	Molar Enthalpy	(kJ/kgmole)	2.7200-002	2.4000 002		2.5555 552	
56	Name	()	O2 Out	Oxygen Out	Reyel Pmp Pwr	Recycle Water	Water In
57	Vapour Fraction		1.0000	1.0000		0.0000	0.0000
58	Temperature	(C)	800.00	25.000 *		25.003	15.556 *
59	Pressure	(kPa)	102.70	101.33 *		101.33	101.33 *
60	Molar Flow	(gmole/h)	1.3021	1.3021		1.1166	1.4294
61	Mass Flow	(kg/d)	1.0000	1.0000		0.48279	0.61801
62	Liquid Volume Flow	(m3/h)	3.662e-005	3.662e-005		2.016e-005	2.580e-005
63	Heat Flow	(kW)	9.140e-003	-3.452e-006	1.936e-007	-8.853e-002	-0.1136
64 65	Molar Enthalpy	(kJ/kgmole)	2.527e+004	-9.543		-2.854e+005	-2.861e+005
66	Hyprotech Ltd.		LIVO	SYS.Plant v2.2.2 (Buil	d 3806)		Page 1 of 19
~~	Licensed to: INL		HIN	21 3.1 Idili 12.2.2 (Dull	u 0000j		* Specified by user.

66 Hyprotech Ltd.
Licensed to: INL Page 1 of 19
* Specified by user.

_						
2	INI		Case Name:	C:\NASA Final\NASA Co	o-Electrolysis wo Recup).hsc
3	INL Calgary, A	Alberta	Unit Set:	NASA2		
5	CANADA		Date/Time:	Mon Aug 23 11:24:48 2	010	
6						
7	Workbook:	Case (Main	ı) (continue	ed)		
9 10			Compressors	3		
11	Name	Circulator				
12	Feed Pressure (kPa)	99.95				
13 14	Product Pressure (kPa) Molar Flow (gmole/h)	108.2 3.588				
15	Energy (kW)	3.209e-004				
16	Adiabatic Efficiency	75 *				
17	Polytropic Efficiency	75				
18			Composition			
19			-			
20	Name	1	2	3	3r	4
21	Comp Mole Frac (H2O)	1.00000	0.00000	0.72696	0.72703 *	0.72703
22 23	Comp Mole Frac (Hydrogen)	0.00000	0.00000	0.08115 0.00000	0.08111 ° 0.00000 °	0.08111 0.00000
24	Comp Mole Frac (Oxygen) Comp Mole Frac (Argon)	0.00000	0.00000	0.00000	0.00000*	0.00000
24 25	Comp Mole Frac (Argon) Comp Mole Frac (Nitrogen)	0.00000	0.00000	0.00000	0.00000	0.00000
26	Comp Mole Frac (CO2)	0.00000	1.00000	0.17275	0.17271 *	0.17271
27	Comp Mole Frac (CO)	0.00000	0.00000	0.01886	0.01888 *	0.01888
28	Comp Mole Frac (Methane)	0.00000	0.00000	0.00028	0.00027 *	0.00027
29	Comp Mole Frac (Carbon)	0.00000	0.00000	0.00000	0.00000 *	0.00000
30	Name	5	6	7	8	9
31	Comp Mole Frac (H2O)	0.72703	0.72703	0.14106	0.14106	0.14106
32	Comp Mole Frac (Hydrogen)	0.08111	0.08111	0.66631	0.66631	0.66631
33 34	Comp Mole Frac (Oxygen)	0.00000	0.00000	0.00000	0.00000	0.00000
35	Comp Mole Frac (Argon)	0.00000	0.00000	0.00000	0.00000	0.00000
36	Comp Mole Frac (Nitrogen) Comp Mole Frac (CO2)	0.17271	0.17271	0.03551	0.03551	0.03551
37	Comp Mole Frac (CO)	0.01888	0.01888	0.05551	0.15484	0.15484
38	Comp Mole Frac (Methane)	0.00027	0.00027	0.00227	0.00227	0.00227
39	Comp Mole Frac (Carbon)	0.00000	0.00000	0.00000	0.00000	0.00000
40	Name	10	11	12	CH4, H2	CO2 In
41	Comp Mole Frac (H2O)	0.24483	0.59247	1.00000	0.04152	0.00000 °
42	Comp Mole Frac (Hydrogen)	0.52109	0.09650	0.00000	0.22696	0.00000 *
43	Comp Mole Frac (Oxygen)	0.00000	0.00000	0.00000	0.00000	0.00000 *
44	Comp Mole Frac (Argon)	0.00000	0.00000	0.00000	0.00000	0.00000 *
45 46	Comp Mole Frac (Nitrogen)	0.00000 0.07737	0.00000	0.00000	0.00000	0.00000 *
47	Comp Mole Frac (CO2) Comp Mole Frac (CO)	0.07737	0.00000	0.00000	0.00000	1.00000 ° 0.00000 °
48	Comp Mole Frac (Methane)	0.11038	0.31103	0.00000	0.73151	0.00000
49	Comp Mole Frac (Carbon)	0.00000	0.00000	0.00000	0.00000	0.00000 *
50	Name	CO2, Water In	H2,CO,H2O Out	O2 Out	Oxygen Out	Recycle Water
51	Comp Mole Frac (H2O)	0.72547	0.14106	0.00000	0.00000	1.00000
52	Comp Mole Frac (Hydrogen)	0.08278	0.66631	0.00000	0.00000	0.00000
53	Comp Mole Frac (Oxygen)	0.00000	0.00000	1.00000	1.00000	0.00000
54 55	Comp Mole Frac (Argon)	0.00000	0.00000	0.00000	0.00000	0.00000
55 56	Comp Mole Frac (Nitrogen) Comp Mole Frac (CO2)	0.00000 0.17351	0.00000 0.03551	0.00000 0.00000	0.00000	0.00000 0.00000
57	Comp Mole Frac (CO2)	0.17351	0.03551	0.00000	0.00000	0.00000
58	Comp Mole Frac (CO)	0.00000	0.00227	0.00000	0.00000	0.00000
59	Comp Mole Frac (Carbon)	0.00000	0.00000	0.00000	0.00000	0.00000
60 61 62 63 64 65						
66	Hyprotech Ltd.	HY	SYS.Plant v2.2.2 (Buil	d 3806)		Page 2 of 19
_	Licensed to: INL					* Specified by user.

1					Ozza Name	OUNIACA Final	NIACA O- FI	tbi D		
2		INL			Case Name:	C:\NASA Final	INASA Co-El	ectrolysis wo Recu	p.hsc	
3	HYPROTECH	Calgary,	Alberta		Unit Set:	NASA2				
5		CANADA			Date/Time:	Mon Aug 23 1	1:24:48 2010)		
6			_	<i>.</i>						
8	Workb	ook:	Case	(Main	ı) (continu	ed)				
9				Co	mposition (con	tinued)				
11	Name		Water In							
12	Comp Mole Frac (H2O)			1.00000 *						
13	Comp Mole Frac (Hydrogen)			0.00000 *						
14	Comp Mole Frac (Oxygen)			0.00000 *						
15	Comp Mole Frac (Argon)			0.00000 *						
16	Comp Mole Frac (Nitrogen)			0.00000 *						
17	Comp Mole Frac (CO2)			0.00000 *						
18	Comp Mole Frac (CO)			0.00000					-	
19	Comp Mole Frac (Methane)			0.00000						
20	Comp Mole Frac (Carbon)			0.00000 *						
21 22					Heat Exchange	ers				
23	Name									
24	Duty	(kW)								
25	Tube Inlet Temperature	(C)								
26	Tube Outlet Temperature	(C)								
27	Shell Inlet Temperature	(C)								
28	Shell Outlet Temperature	(C)								
29	LMTD	(C)								
30	UA	(W/C)								
31	Minimum Approach	(C)								
32	Ψ,	(-/		_						
33				0	ther Heat Excha	ingers				
34	Name									
35	Number of Sides									
36	LMTD	(C)								
37	UA (Calculated)	(W/C)								
38	Hot Pinch Temperature	(C)								
39	Cold Pinch Temperature	(C)								
40	Minimum Approach	(C)								
41	Exchanger Cold Duty	(kW)								
42					Pumps					
43			1		1 dilips	1				
44	Name		Recycle P							
45	Delta P	(kPa)		26.17						
46	Energy	(kW)	1.8	936e-007					-	
47	Feed Pressure	(kPa)		75.15		-				
48	Product Pressure	(kPa)		101.3						
49 50		(gmole/h)		1.117						
51	Adiabatic Efficiency	(%)		75.00 *						
					Unit Ops					
52 53	Operation Name	One	eration Type		Feeds		Products	Ignored		Calc. Level
54	·			5		6				
55	Hi Temp Heater	Heater			Temp Pwr	1		No		500.0 *
	La Tana Haster	Hact		3r		4				500.0-
56 57	Lo Temp Heater	Heater			Temp Pwr			No		500.0 *
58	T4	Tor			2,CO,H2O Out	7				500.0-
58 59	T1	Tee				8		No		500.0 *
60				1		3				
60 61	M2	Mixer		2				No		500.0 *
62				7						
63	140	N. Aliano			ecycle Water	1				500.0
64	M3	Mixer			ater In			No		500.0 *
65	Circulator	Compres	sor	4		5		No		500.0 *
66	Hyprotech Ltd.			HY	SYS.Plant v2.2.2 (Bu	ild 3806)				Page 3 of 19
_	Licensed to: INL									ecified by user.

2	Dr.		INL	Case Name:	C:\NASA Final\NASA	Co-Electrolysis wo Recu	ıp.hsc
3	HY	PROTECH	Calgary, Alberta	Unit Set:	NASA2		
5			CANADA	Date/Time:	Mon Aug 23 11:24:48	3 2010	
6 7		Workb	ook: Case (M	ain) (continu	ied)		
8							
10				Unit Ops (conti			
11 12	Ope	eration Name	Operation Type Compressor	Feeds Circ Pwr	Produc	ts Ignored No	Calc. Level 500.0 °
13			•	O2 Out	Oxygen Out		
14	Oxygen (Cooler	Cooler		O2 CLR Q	No	500.0 *
15 16				Sweep Gas In CO2, Water In	02 Out		
17	High Ten	nperature Co-Electro	Standard Sub-Flowsheet	Process Heat	H2,CO,H2O Ou	No	2500 *
18				Electrolysis Power			
19	Electroly	sis Input and Outpul	Spreadsheet			No	500.0 *
20	Co-Elect	rolysis Calcs	Spreadsheet			No	500.0 *
21				9	300		
22	High Ten	np Sabatier	Equilibrium Reactor	Hi Tmp Sabtr Q	10	No	500.0 *
23 24				10	Hi Tmp Sabtr Q 200		
25	I ow Tem	np Sabatier	Equilibrium Reactor	Lo Tmp Sabtr Q	11	No	500.0
26	LOW TON	ip Gabatter	Equilibrium recustor	Lo Trip Gaba G	Lo Tmp Sabtr C		500.0
27	Daniela	D	D	12	Recycle Water		500.01
28	Recycle	Pump	Pump	Roycl Pmp Pwr		No	500.0 *
29	RCY		Recycle	3	3r	No	3500 *
30				11	12		500.0
31 32	Condens	er/Water Separator	Separator	AmbCool	CH4, H2	No	500.0 *
33				6	AmbCool 400		
34	Water G	as Shift	Gibbs Reactor		CO2, Water In	No	500.0
35	SET-2		Set			No	500.0 *
36	VLV 2		Valve	CO2 In	2	No	500.0 *
37	VLV 1		Valve	8	9	No	500.0 *
38 39 40 41		Sprea	dsheet: Co-El	ectrolysis C	alcs	U	nits Set: NASA
42				CONNECTIO	NS		
43 44				Imported Varia	ibles		
45	Cell		Object		Variable Description		Value
46	B1	Material Strea		Comp Mole Frac (Hydro			0.66631
47	B2	Material Strea	m: 9	Comp Mole Frac (CO2)			0.03551
48	B3	Material Strea		Comp Mole Frac (CO)			0.15484
49	D1		m: Electrolysis Power	Power			0.1834 kW
50 51	D3 D4		m: Lo Temp Pwr	Power			3.096e-002 kW
52	D5		m: Hi Temp Pwr m: Circ Pwr	Power Power			2.728e-002 kW 3.209e-004 kW
53	D6		m: Roycl Pmp Pwr	Power			1.936e-007 kW
54				rted Variables' For	mula Paculto		
55 56	Cell		Object	nteu variables FOI	Variable Description		Value
57	Oeii		Objetit	PARAMETE			value
58 59				Exportable Vari			
60 61	Cell	\/i	sible Name	Variable De		Variable Type	Value
62	B4	B4: H2 to sum of 0		H2 to sum of CO & CO2			3.500
63	B6	B6: Comp Molar F		Comp Molar Flow (Hydro		Comp. Mole Flow	<empty></empty>
64	В7	B7: Comp Molar F		Comp Molar Flow (Hydro		Comp. Mole Flow	<empty></empty>
65	D2	D2:				Power	0.0000 kW
66	Hyprote	ch Ltd.		HYSYS.Plant v2.2.2 (B	uild 3806)		Page 4 of 19

2	Do-		INI	Case Name:	C:\NASA Final\NASA	Co-Electrolysis wo R	ecup.hsc
3			INL Calgary, Alberta	Unit Set:	NASA2		
4			CANADA	Date/Time:		9 2010	
5	F 1			Date/Time:	Mon Aug 23 11:24:4	8 2010	
6		Spread	dsheet: Co-El	actrolycie (Calce (conti	nued\	Units Set: NASA
8		Spicat	isileet. CO-Li	ectionysis (Jaics (Conti	iiueu)	Office Sec. NASA
9				PARAMETI	=De		
10				FARAIVIETI			
11 12				Exportable Va	riables		
13	Ce	ll Vis	ible Name	Variable [Description	Variable Type	Value
14	D7	D7: Total Power		Total Power	·	Power	0.2419 kW
15				User Varial	bles		
16 17							
18				FORMULA	AS		
19	Ce			Formula			Result
20	B4	,					3.500
21 22	D7	' =D1+D2+D3+D4+E	D5+D6				0.2419 kW
23				Spreadsh	eet		
24		Α	В	С	D		
25	1	H2 @ 14 °	0.66631	Electrolysis Power *	0.1834 kW		
26	2	CO2 @ 14 *	0.03551		0.0000 kW *		
27	3	CO @ 14 °	0.15484	Lo Temp Pwr *	3.096e-002 kW		
28		sum of CO & CO2 ratio *	3.500	Hi Temp Pwr *	2.728e-002 kW		
29	5		4t-> 1	Circ Pwr *	3.209e-004 kW		
30 31	6		<empty> '</empty>	Reyel Pmp Pwr *	1.936e-007 kW		
32	7		<empty> *</empty>	Total Power *	0.2419 kW		
33	9						
34	10						
35 36		Snrage	sheet: Elect	rolveie Innu	it and Outni	ıt	Units Set: Electrolysis
37		Opicac	asileet. Liecti	iorysis iripo	it and Outpi	и с	Cinta det. Lieutolysis,
38 39				CONNECTI	ONS		
40 41				Imported Var	iables		
42	Се	II .	Object	-	Variable Description		Value
43	B6		r: Isothermal Electrolysis @	Spec % Conversion (Spec % Conversion_1)		100.00
44	B7						0.0000
45	D1	Material Stream	1: 6	Comp Mole Frac (Hyd	rogen)		0.08111
46	D2	Material Stream	n: 6	Comp Mole Frac (CO)			0.01888
47 48			Expo	rted Variables' Fo	ormula Results		
48	Ce	II	Object		Variable Description		Value
50				DADAMET			1 20.00
51				PARAMETI	ERS		
52 53				Exportable Va	riables		
54	Ce	ll Vis	ible Name	Variable [Description	Variable Type	Value
55	B2			Number of Cells		"	2.444
56	В3			Cell Area		Small Area	64.00 cm2
57	B4			Current Density (Ampe		Vapour Fraction	<empty></empty>
58	B5			ASR @ 1100 K (ohm*			0.4000
59	B8			Comp Mole Frac (Hyd		Vapour Fraction	<empty></empty>
60	B9		ic (CO)	Comp Mole Frac (CO)		Vapour Fraction	<empty></empty>
61	D3					Vapour Fraction	0.1000
62	D4			Mass Flow		Mass Flow	<empty></empty>
63	DE						<empty></empty>
64 65	D7			Hoot Flour		Enormy	<empty></empty>
65	DS DS			Heat Flow	(Build 2006)	Energy	<empty></empty>
00		rotech Ltd. ed to: INL		HYSYS.Plant v2.2.2 (Duilu 3000)		Page 5 of 19 * Specified by user.
_							

A-46

2	Dr.		INL		Case Name	e: C:\l	NASA Final\NASA C	o-Electrolysis wo Recup	.hsc
3	-	HYPROTECH	Calgary, A	Alberta	Unit Set:	NA:	SA2		
4		HYPROTECH	CANADA		D-1- (Fi		- 4 22 44-24-40	2040	
5	P 1				Date/Time:	IVIO	n Aug 23 11:24:48 2	2010	
6		Spra	adebo	et: Electroly	reie Inn	ut ar	ad Output	Loontine us	to Set: Electrolysis
8		Shie	ausile	et. Election	ysis ilip	ut ai	iu Outpu	i (Contini on	ts Set: Electrolysis
9					DADAMET				
10					PARAMET	ERS			
11 12				E	xportable V	ariable	es		
13	Ce	II	Visible Name		Variable	Descript	tion	Variable Type	Value
14	D9	D9:							<empty></empty>
15					User Varia	ables			
16 17									
18					FORMUL	_AS			
19	Ce				Formula				Result
20 21	D3	3 =D1+D2							0.1000
22					Spreadsl	neet			
23		Α		В	С		D		
24	1	Inpu	t *	Input *	H2 @ 9 *		0.08111		
25	2	Number of Cell	s *	2.444 *	CO @ 9 ¹		0.01888		
26	3	Cell Are	a *	64.00 cm2 *			0.1000		
27	4			<empty> *</empty>			<empty> "</empty>		
28		1100 K (ohms * cm2	_	0.4000 '					
29 30	6	% Water Conversion		100.00 '			<empty> *</empty>		
31	7 8	% CO2 Conversion	n -	0.0000 <empty> *</empty>			<empty> *</empty>		
32	9			<empty> '</empty>			<empty> * <empty> *</empty></empty>		
33	10			-empty-			veriipty>		
34 35 36 37		Work	book:	High Tempe	erature Stream		Electrolys	is (TPL2)	
38 39	Nam	•		Sweep Gas In @TPL	O2 Out @TPL2		Gas Products @TPL	: Liquid @TPL2	Anode @TPL2
40		our Fraction		1.0000		000	1.0000	0.0000	1.0000
41		perature	(C)	799.34		0.00	800.00	800.00	800.00
42		sure	(kPa)	102.70		2.70	104.08	104.08	102.70
43	Mola	r Flow	(gmole/h)	3.4662e-009	1.3	021	4.8919	0.00000	1.3021
44	Mas	s Flow	(kg/d)	2.4000e-009	1.0	000	1.8423	0.00000	1.0000
45	Liqui	id Volume Flow	(m3/h)	1.156e-013	3.662e-	005	1.559e-004	0.0000	3.662e-005
46		Flow	(kW)	2.342e-011	9.140e-		-3.572e-002	0.0000	9.140e-003
47			(kJ/kgmole)	2.432e+004	2.527e+		-2.629e+004	-2.629e+004	2.527e+004
48	Nam			H2,CO,H2O Out @TF	Cathode @TPL		2 @TPL2	CO2, Water In @TPL	Electrolysis Heatiing
49 50		our Fraction	(C)	1.0000 800.00 °		000	0.0000	1.0000 799.34	
51		perature sure	(kPa)	101.33		2.70	101.33	105.46	
52		ar Flow	(gmole/h)	3.5736		898	0.00000	3.5898	
53		s Flow	(kg/d)	0.84231	0.84		0.00000	1.8423	
54	Liqui	id Volume Flow	(m3/h)	1.044e-004	1.192e-		0.0000	9.109e-005	
55	Heat	Flow	(kW)	-4.047e-002	-4.486e-	002	0.0000	-0.2147	0.1790
56	Mola	r Enthalpy	(kJ/kgmole)	-4.077e+004	-4.499e+	004	-4.077e+004	-2.153e+005	
57	Nam			Process Heat @TPL:	Shift Reactor 2	Heat E	Electrolysis Power (2	
58		our Fraction							
59		perature	(C)						
60		sure	(kPa)						
61 62		ar Flow s Flow	(gmole/h)						
63		s Flow id Volume Flow	(kg/d) (m3/h)						
64		Flow	(kW)	-3.162e-012	4.392e-	_	0.1834		
65			(kJ/kgmole)	-5.1026-012			3.1004		
66		rotech Ltd.	J714)		YS.Plant v2.2.2	(Build 3	3806)	•	Page 6 of 19
_		ed to: INI							* Specified by user

1									
2	Do.	INL			Case Name: 0	C:\NASA Final\NASA Co	o-Electroly	sis wo Recup	.hsc
3	HYPROTECH	Calgary, A	Alberta		Unit Set:	NASA2			
5		CANADA			Date/Time:	Mon Aug 23 11:24:48 2	010		
6									
7	Workb	ook:	High Ten	npe	rature Co	-Electrolys	is (TF	PL2) (c	ontinued)
9 10					Composition				
11	Name		Sweep Gas In @	TPL (O2 Out @TPL2	Gas Products @TPL:	Liquid @	TPL2	Anode @TPL2
12	Comp Mole Frac (H2O)		0.000	_	0.00000	0.00000		0.00000	0.00000
13	Comp Mole Frac (Hydrogen)		0.000	00	0.00000	0.59312		0.59312	0.00000
14	Comp Mole Frac (Oxygen)		0.210	00	1.00000	0.26617		0.26617	1.00000
15	Comp Mole Frac (Argon)		0.000	00	0.00000	0.00000		0.00000	0.00000
16	Comp Mole Frac (Nitrogen)		0.790	00	0.00000	0.00000		0.00000	0.00000
17	Comp Mole Frac (CO2)		0.000	00	0.00000	0.12733		0.12733	0.00000
18	Comp Mole Frac (CO)		0.000	_	0.00000	0.01338		0.01338	0.00000
19	Comp Mole Frac (Methane)		0.000	_	0.00000	0.00000		0.00000	0.00000
20	Comp Mole Frac (Carbon)		0.000		0.00000	0.00000		0.00000	0.00000
21	Name		H2,CO,H2O Out		Cathode @TPL2	2 @TPL2	CO2. W	ater In @TPL	
22	Comp Mole Frac (H2O)		0.141	$\overline{}$	0.00000	0.14106		0.72547	
23	Comp Mole Frac (Hydrogen)		0.666		0.80825	0.66631		0.08278	
24	Comp Mole Frac (Oxygen)		0.000	-	0.00000	0.00000		0.00000	
25	Comp Mole Frac (Argon)		0.000	_	0.00000	0.00000		0.00000	
26	Comp Mole Frac (Nitrogen)		0.000		0.00000	0.00000		0.00000	
27	Comp Mole Frac (CO2)		0.035		0.17351	0.03551		0.17351	
28	Comp Mole Frac (CO)		0.154		0.01824	0.15484		0.01824	
29	Comp Mole Frac (Methane)		0.002	_	0.00000	0.00227		0.00000	
30	Comp Mole Frac (Carbon)		0.000	_	0.00000	0.00000		0.00000	
31	Comp Mole Frac (Carbon)		0.000					0.00000	
32				Co	nversion React	tors			
33	Name		Isothermal Electr	olve					
34	Separator Type		150thermal Liecti	0.					
35	Vessel Temperature	(C)	800.	-					
36	Vessel Pressure	(kPa)	104.						
37		(gmole/h)	4.8						
38	•	(gmole/h)	0.00	_					
39	Heat Flow	(kW)	0.17	_					
40	ricat riow	(KVV)	0.17	00					
41					Gibbs Reactors	s			
42	Name		Water gas Shift	@ ТР					
43	Separator Type			0 -					
44	Vessel Temperature	(C)	800.						
45	Vessel Pressure	(kPa)	101.3	33					
46	Vapour Molar Flow	(gmole/h)	3.5	74					
47	Liquid Molar Flow	(gmole/h)	0.00	00					
48	Heat Flow	(kW)	4.392e-0	03					
49 50					Unit Ops				
51	Operation Name	One	eration Type		Feeds	Products		Ignored	Calc. Level
52	Temp Average ASR @TPL2	Spreadsh			1 0003	rioddols		Yes	500.0 *
53	Electrolysis Spreadsheet @							No	500.0
54	Steam Electrolysis @TPL2	Spreadsh						No	500.0
55	CO2 Electrolysis @TPL2	Spreadsh						No	500.0 *
56	Sweep Gas/O2 Mixer @TPL		, cut		le @TPL2	O2 Out @TPL2		No	500.0
57	OTTOOK ORGANIZ MINEL WILL	IAIIVEI			ep Gas In @TPL2			140	300.0
58				CO2	, Water In @TPL2	Liquid @TPL2			
59	Isothermal Electrolysis @TP	Conversi	on Reactor	Elect	trolysis Heatiing @TF	PL2 Gas Products @T	PL2	No	500.0 *
60						Electrolysis Heatii	ng @TPL2		
61	Electrodes @TPL2	Comme	ant Calittan	Gas	Products @TPL2	Cathode @TPL2		NI-	500.0
62	Electrodes @TPL2	Compone	ent Splitter			Anode @TPL2		No	500.0 *
63	ADJ-1 @TPL2	Adjust						Yes	3500 *
64	Motor and Chift GTDLC	Cibbs D	antor	Cath	ode @TPL2	2 @TPL2		NI.	500.01
65	Water gas Shift @TPL2	Gibbs Re	racior	Shift	Reactor 2 Heat @TF	PL2 H2,CO,H2O Out @	TPL2	No	500.0 *
66	Hyprotech Ltd.				S.Plant v2.2.2 (Build				Page 7 of 19
_	Licensed to: INI								* Specified by user

1	Day.			Case Name:	C:\NASA Final\NASA C	o-Electroly	sis wo Recu	ıp.hsc	
3	HY	PROTECH	INL Calgary, Alberta	Unit Set:	NASA2				
4 5			CANADA	Date/Time:	Mon Aug 23 11:24:48	2010			
6									
7		Workb	ook: High Ter	nperature Co	-Electrolys	is (TF	PL2) (contir	nued)
9 10				Unit Ops (contin	ued)				
11		eration Name	Operation Type	Feeds	Products		Ignored	Ca	lc. Level
12 13	SET-1@	as Shift @TPL2 TPL2	Gibbs Reactor Set		Shift Reactor 2 H	eat @TPL2	No No		500.0 * 500.0 *
14	SET-3@		Set				No		500.0 *
15 16	SET-2@	TPL2	Set				No		500.0 *
17 18		Sprea	dsheet: CO2 I	Electrolysis (@TPL2		Uı	nits Set:	NewUser1
19 20				CONNECTION	ıs				
21 22				Imported Varial	oles				
23	Cell		Object		/ariable Description				ılue
24 25 26	A8 D2		am: CO2, Water In @TPL2	Pressure				0.10546 I 1072.5 K	
26	D3		am: CO2, Water In @TPL2 am: H2,CO,H2O Out @TPL2	Temperature Temperature				1072.5 K	
27	E2	Material Strea		Comp Mole Frac (CO2)				0.17351	
28 29 30	F2	Material Strea		Comp Mole Frac (CO)				0.01824	
29	G2	Material Strea		Comp Mole Frac (Oxyger	1)			0.21000	
31	E3 F3	Material Strea Material Strea		Comp Mole Frac (CO2) Comp Mole Frac (CO)				0.03551 0.15484	
32	G3	Material Strea		Comp Mole Frac (Oxyger)			1.00000	
33	00	Wild Circle						1.00000	
34	0-11			rted Variables' For					
35 36	Cell		Object	PARAMETER	Variable Description			Va	lue
37 38 39				Exportable Varia					
40 41	Cell	V	isible Name	Variable Des	cription	Variable	Туре	Va	lue
41	A1	A1:						2.815e+0	05
42	A2	A2:						-37.53	
43	A3 A4	A3: A4:						8.724e-0	
45	A5	A5:						-8.139	107
46	A6	A6:						9.649e+0	04
42 43 44 45 46 47 48 49	A7	A7:						8.314	
48	A9	A9:				Pressure		0.101321	MPa
_	C1	C1:						<empty></empty>	
50 51	C7 D4	C7: D4:				 Temperatu		<empty> 0.66058</empty>	κ
52	D6	D6:				Temperatu		1072.8 K	
53	D8	D8:						4.613e-0	
51 52 53 54 55 56 57 58 60 61 62 63 64	D9	D9:						6.984e-0	05
55	E4	E4:				Vapour Fra		-0.1380	
56	E5 F4	E5: F4:				Vapour Fra		0.3234	
58	F5	F4: F5:				Vapour Fra Vapour Fra		-0.3524	
59	G4	G4:				Vapour Fra		0.7900	
60	G5	G5:				Vapour Fra		-0.4623	
61	H2	H2:						0.2186	
62	H3	H3:						1.041	
63	H4 H5	H4: H5:						0.8223 -0.4482	
65	12	I2:				Molar Enth	alpy		05 J/gmole
65 66	Hyprote			HYSYS.Plant v2.2.2 (Bu	ild 3806)	our EIRI			ge 8 of 19

Hyprotech Ltd. Hysys.Plant v2.2.2 (Build 3806) Page 8 of *

Licensed to: INL *Specified by user.

Da.			Case Nam	e: C:\NASA Final\NASA	Co-Electrolysis wo Rec	up.hsc
		INL Calgary, Alberta	Unit Set:	NASA2		
	ATPROTECH	CANADA	Date/Time	: Mon Aug 23 11:24:4	8 2010	
	Spread	Isheet: CO2				Inits Set: NewUser1
			PARAME			
			Exportable \	/ariables		
C	ell Visi	ible Name	Variable	e Description	Variable Type	Value
13					Molar Enthalpy	1.893e+005 J/gmol
16	16:				Molar Enthalpy	1.893e+005 J/gmol
J:	2 J2:					2.533e+008
J:	3 J3:					2.535e+008
K	2 K2:					0.8420
K	3 K3:					1.050
K	6 K6:					0.9587
K	7 K7:				Vapour Fraction	0.9587
			User Vari	ahles		
			Oser vari	ables		
			FORMU	LAS		
C			Formula			Result
D						0.66058 K
•	(1072.8 K
D						4.613e-005
D		ł)				6.984e-005
E						-0.1380
E	, ,	- (E2*@LN(E2)-E2)				0.3234
F						0.1366
F	(- 0 - 1, 1 - 7 - 7	- (F2*@LN(F2)-F2)				-0.3524
G						0.7900
	,) - (G2*@LN(G2)-G2)				-0.4623
H						0.2186
Н						1.041
Н		410101111101101				0.8223
H 12		- (H2*@LN(H2)-H2)	011/00			-0.4482
12		D2^2 + A4^D2^3 + A5^D2^	-			1.894e+005 J/gmol
		'D3^2 + A4*D3^3 + A5*D3*				1.893e+005 J/gmol
J:		*D6^2 + A4*D6^3 + A5*D6*		20, 0.5)		1.893e+005 J/gmol
J:		^2 + A3/3*D2^3 + A4/4*D2^				2.533e+008 2.535e+008
		^2 + A3/3*D3^3 + A4/4*D3^	+ + MO12"U3"2"(@LN(L	JJ-U.3)		
K		2*@LN(E2/(F2*H2^0.5))) 3*@LN(E3/(F3*H3^0.5)))				0.8420 1.050
K	(=, (=	3~@LN(E3/(F3~H3~U.5))) 7*D6*((E5+F5)*H4 + H5/2*I	E4\\			0.9587
ĸ		/ "D6"((E5+F5)"H4 + H5/2"F 2^2)*((E5+F5)*H4 + H5/2*F	,,			0.9587
	-50 (7112 (50 2-5	, ((20.10) 117 110/2 1	Spreads	heet		3.0001
	Α	В	C	D	E	F
1	2.815e+005 *	A1 ·	<empty> *</empty>	Temperature *	y CO2 *	y CC
2	-37.53 '	A2 *	in '	1072.5 K	0.17351	0.01824
3	8.724e-003 *	A3 *	out *	1073.2 K *	0.03551	0.15484
4	-8.470e-007 *	A4 (J/gmole-K^3) *	Delta "	0.66058 K	-0.1380	0.1366
5	-8.139 °	A5 *	Integration Coeff *		0.3234	-0.3524
6	9.649e+004 °	Fa (J/Volt-gmole) *	Average *	1072.8 K		
7	8.314 *	Ru *	<empty> "</empty>			
8	0.10546 MPa	Pressure '	C isothermal '	4.613e-005		
9	0.10132 MPa *	Standard Pressure *	C '	6.984e-005		
10						
	G	Н		J	K	
1	y O2 °	у А *	Delta G	Delta G dT (J-K/gmole)	Nernst Voltage *	
_	0.21000	0.2186	1.894e+005 J/gmole	2.533e+008	0.8420	
2	0.21000					

2	Dr.	INL	Case Name:	C:\NASA Final\NASA	Co-Electrolysis wo Rec	up.hsc
3		Calgary, Alberta CANADA	Unit Set:	NASA2		
5		CANADA	Date/Time:	Mon Aug 23 11:24:4	8 2010	
6						
7		Spreadsheet: CO2	Electrolysis	@TPL2 (co	ontinued) 🔍	Jnits Set: NewUser1
9			Spreadsh	not.		
10 11	3	1.00000 1.041	1.893e+005 J/gmole	2.535e+008	1.050	
12	4	0.7900 0.8223	1.083e+003 3/gillole	2.000e+000	1.030	
13	5	-0.4623 -0.4482				
14	6		1.893e+005 J/gmole	Isothermal *	0.9587	
15 16	7 8			Average *	0.9587	
17	9					
18	10					
19		On mandala and Elect	l : - O	- d-b4-0'	TDLA	
20 21		Spreadsheet: Elect	rolysis Spre	eadsneet @	IPL2	Jnits Set: Electrolysis
22						
23			CONNECTI	ONS		
24			Imported Var	iables		
25	0-"		Imported var			
26 27	Cell B8	Object SpreadSheetCell: Electrolysis Input and O	B2: Number of Cells	Variable Description		Value 2.444
28	B9	SpreadSheetCell: Electrolysis Input and Or				64.00 cm2
29	D5	Material Stream: CO2, Water In @TPL2	Comp Mole Frac (Hyd	rogen)		0.08278
30	D6	Material Stream: H2,CO,H2O Out @TPL2	Comp Mole Frac (Hyd	rogen)		0.66631
31	D9	Material Stream: CO2, Water In @TPL2	Pressure			0.10546 MPa
32 33	D1 D2	Material Stream: CO2, Water In @TPL2	Temperature			1072.5 K
34	D3	Material Stream: H2,CO,H2O Out @TPL2 Material Stream: CO2, Water In @TPL2	Temperature Comp Mole Frac (H2C))		1073.2 K 0.72547
35	D4	Material Stream: H2,CO,H2O Out @TPL2				0.14106
36	D7	Material Stream: Sweep Gas In @TPL2	Comp Mole Frac (Oxy	gen)		0.21000
37	D8	Material Stream: O2 Out @TPL2	Comp Mole Frac (Oxy	-		1.00000
38 39	B16 D14	SpreadSheetCell: Electrolysis Input and O Energy Stream: Electrolysis Heatiing @1		hm*cm2)		0.4000 0.1790 kW
40	D17	Energy Stream: Shift Reactor 2 Heat @1				4.392e-003 kW
41	B18	Material Stream: CO2, Water In @TPL2	Comp Molar Flow (H20	D)		0.0007 gmole/s
42	B20	Material Stream: CO2, Water In @TPL2	Comp Molar Flow (CO			0.0002 gmole/s
43	D19	Conversion Reactor: Isothermal Electrolysis (1			100.0
44 45	D20 B19	Material Stream: Anode @TPL2 Conversion Reactor: Isothermal Electrolysis @	Comp Molar Flow (Oxy Act. % Conversion (Ac			0.0004 gmole/s 0.0000
46	210	,				0000
47		Expo	orted Variables' Fo	ormula Results		
48	Cell	Object		Variable Description		Value
49 50	D13 D18	Electrolysis Power @TPL2	Power Heat Flow			0.1834 kW -3.162e-012 kW
51	D10	Process Heat @TPL2	•			-3. 102e-012 KVV
52			PARAMETE	RS		
53 54			Exportable Va	riables		
55	Cell	Visible Name		escription	Variable Type	Value
56	B1	B1: Faraday Constant	Faraday Constant	-computori		9.649e+004
57	B2	B2: Universal Constant	Universal Constant		Entropy	8.314 J/gmole-K
58	В3	B3: A1 (J/gmol)	A1 (J/gmol)			-2.382e+005
59 60	B4	B4: A2 (J/gmol-K)	A2 (J/gmol-K)			-39.95
60	B5 B6	B5: A3 (J/gmol-K^2) B6: A4 (J/gmol-K^3)	A3 (J/gmol-K^2) A4 (J/gmol-K^3)			-3.319e-003 3.532e-008
62	B7	B7: A5 (J/gmol-K)	A5 (J/gmol-K)			12.85
63	B10	B10: B4: Current Density (Amperes/cm2)	B4: Current Density (A	mperes/cm2)		0.8923
64	B11	B11: C (J-K/(volt-gmole))	C (J-K/(volt-gmole))			-1.702e-005
65	B13	B13: Current (amperes)	Current (amperes)	Drille 2000)		57.11
66	Hypro	tech Ltd.	HYSYS.Plant v2.2.2 (Build 3806)		Page 10 of 19

	Iku	Case Name: C	:\NASA Final\NASA Co-Electrolysis wo R	ecup.hsc
	INL Calgary, Alberta	Unit Set: N	ASA2	
No.	CANADA	Date/Time: M	lon Aug 23 11:24:48 2010	
	Spreadsheet: Ele	ctrolysis Spread	sheet @TPL2 (con	Units Set: Electrolysi
	·	PARAMETERS		
		Exportable Variab	les	
Cell	Visible Name	Variable Descri	ption Variable Type	Value
B14	B14:		Flow	3.6169e-004 gmole
B15	B15: Nernst Average Voltage	Nernst Average Voltage		0.9567
B17	B17: Operating Voltage (Volts)	Operating Voltage (Volts)		1.314
D10	D10: Ambient Pressure	Ambient Pressure	Pressure	0.10132 MPa
D11	D11: Pressure in Atm	Pressure in Atm		1.041
D12	D12:			<empty></empty>
D13	D13: Power	Power	Power	0.1834 kW
D15	D15:		Energy	0.0000 kW
D16	D16: Heat Flow	Heat Flow	Energy	0.0000 kW
D18	D18: Heat Flow	Heat Flow	Energy	-3.162e-012 kW
E13	E13:			0.0000
F1	F1:		Vapour Fraction	-0.5410
F2	F2:		Vapour Fraction	0.6361
F3	F3:		Vapour Fraction	0.4623
F4	F4:		Vapour Fraction	0.9567
F5	F5:		Vapour Fraction	0.9567
F7	F7:		Molar Enthalpy	-1.887e+005 J/gmo
F8	F8:		Molar Enthalpy	-1.887e+005 J/gmo
F9	F9:			0.8424
F10	F10:			1.050
F15	F15: Comp Mole Frac (CO)	Comp Mole Frac (CO)	Vapour Fraction	<empty></empty>
F16	F16: Comp Mole Frac (CO)	Comp Mole Frac (CO)	Vapour Fraction	<empty></empty>
Н3	H3:		Temperature	1072.8 K
H4	H4:		Molar Enthalpy	-1.887e+005 J/gmo
H5	H5:		Entropy	-5.746e+004 J/gmo
H13	H13:			<empty></empty>
H14	H14:			<empty></empty>
H15	H15:			<empty></empty>
H16	H16:			<empty></empty>
H17	H17:			<empty></empty>
H18	H18:		Entropy	<empty></empty>
H19	H19:			<empty></empty>
		User Variables		
		FORMULAS		
Cell B10		Formula		Result
B10	=D20*4*B1/(B9*B8)			0.8923
B11	=-1/(2*B1*(D2-D1)*(D6-D5)*(D8-D7))			-1.702e-005
B13	=B9*B10			57.11
B14	=B8*B13/(4*B1)			3.6169e-004 gmole
B15	@IF(@ABS(D2-D1)<.01,F4,F5)			0.9567
B17	=B15+B16*B10			1.314
D11	=D9/D10			1.041
D13	=(B8*B13*B17)/1000			0.1834 kW
D18	=D14+D15+D17-D13			-3.162e-012 kW
E13	=(B14-D20)*1000			0.0000
F1	=D3*@LN(D3)-D4*@LN(D4)+(D4-D3)			-0.5410
F2	=D5*@LN(D5)-D6*@LN(D6)+(D6-D5)*(1-0	.5*@LN(D11))		0.6361
F3	=D7*@LN(D7)-D8*@LN(D8)+(D8-D7)			0.4623
F4	=-(H4*(D6-D5)*(D8-D7)+B2*H3*(F1+F2)*(D			0.9567
F5	=(H5+B2/2*(D2^2-D1^2)*(F1+F2)*(D8-D7)+			0.9567
	ech Ltd.	HYSYS.Plant v2.2.2 (Build	2006)	Page 11 of 19

_							
2	Ìò.		INL	Case Name:	C:\NASA Final\NAS	A Co-Electrolysis wo Rec	up.hsc
3		HYPROTECH	Calgary, Alberta	Unit Set:	NASA2		
5	1		CANADA	Date/Time:	Mon Aug 23 11:24:	48 2010	
6		_					
7		Spread	dsneet: Elec	trolysis Spre	eadsneet @	TPL2 (con u	Inits Set: Electrolysis
9				FORMUL	AS		
11	Ce	ell .		Formula			Result
12	F7		5*D1^2 + B6*D1^3 + B7*D				-1.887e+005 J/gmole
13 14	F8		5*D2*2 + B6*D2*3 + B7*D				-1.887e+005 J/gmole
15	F9 F1			SQRT(D7))) + B2*D1/(4*B SQRT(D8))) + B2*D2/(4*B			0.8424 1.050
16	H	()	2/(2 B1) @LN(D4/(D0 @	(SQR1(D0))) + B2 D2/(4 B	I) (QLIN(DII)		1072.8 K
17	H		3^2+B6*H3 ^3+B7*H3*@L	N(H3)			-1.887e+005 J/gmole
18	H	5 =(D6-D5)*(D8-D7)*	(B3*(D2-D1)+B4/2*(D2^2	-D1^2)+B5/3*(D2^3-D1^3)+	B6/4*(D2^4-D1^4)+B7*	(D2^2/2*(@LN(D2)-0.5)-D	-5.746e+004 J/gmole-
19 20							
21		Α	В	С	D	E	F
22	1	Fa (J/volt_mol) *	9.649e+004 °	Reactant Temperature *	1072.5 K	water *	-0.5410
23	2	Iniversal Gas Constant *	8.314 J/gmole-K *	Product Temperature *	1073.2 K [*]	hydrogen '	0.6361
24 25	3	A1 (J/gmol) *	-2.382e+005 *	H2O In Mole Frac *	0.72547	oxygen *	0.4623
25	4	A2 (J/gmol-K) *	-39.95	H2O Out Mole Frac *	0.14106	Average Nernst Voltage *	0.9567
26 27	5 6	A3 (J/gmol-K^2) * A4 (J/gmol-K^3) *	-3.319e-003 ° 3.532e-008 °	H2 In Mole Frac * H2 Out Mole Frac *	0.08278 0.66631	Average Nernst Voltage *	0.9567
28	7	A5 (J/gmol-K*3)	12.85	O2 In Mole Frac *	0.21000	Delta G Reactant '	-1.887e+005 J/gmole
29	8	Number of Cells *	2.444 '	O2 Out Mole Frac '	1.00000	Delta G Product '	-1.887e+005 J/gmole
30	9	Cell Area *	64.00 cm2 *	Pressure *	0.10546 MPa	rnst Potential Reactant *	0.8424
31	10	ensity (Amperes/cm2) *	0.8923	Ambient Pressure *	0.10132 MPa *	ernst Potential Product *	1.050
32	11	C (J-K/(volt-gmole)) *	-1.702e-005	Pressure in Atm *	1.041		
33	12				<empty> *</empty>		
34	13	Current (amperes) *	57.11	Electrolysis Power *	0.1834 kW	0.0000	
35 36	14	Molar Flow of Oxygen	3.6169e-004 gmole/s	Electrolysis Heating *	0.1790 kW		
37	15 16	lernst Average Voltage * Resistance (ohm*cm2) *	0.9567 0.4000 *	Sweep Gas Heat * Shift Reactor 1 Heat *	0.0000 kW * 0.0000 kW *		<empty> * <empty> *</empty></empty>
38		perating Voltage (Volts) *	1.314	Shift Reactor 2 Heat *	4.392e-003 kW		\cinpty>
39		Water Into Electrolysis	0.0007 gmole/s	Process Heat *	-3.162e-012 kW		
40	19	% CO2 Converted *	0.0000	%Converted H2O *	100.0		
41	20	O2 @ Into Electtolysis *	0.0002 gmole/s	lolar Flow of O2 ANode *	0.0004 gmole/s		
42		G	Н				
43	1						
44 45	2	Ta 1	4070.0 K				
46	3	Tave *	1072.8 K -1.887e+005 J/gmole				
46 47	5	Intregral of Delta G dT *					
48	6						
49	7						
50	8						
51	9						
52	10						
53 54	11 12						
55	13		<empty> *</empty>				
56	14		<empty> '</empty>				
56 57	15		<empty> *</empty>				
58	16		<empty> "</empty>				
59	17		<empty> "</empty>				
60	18		<empty> "</empty>				
61	19		<empty> *</empty>				
62 63	20						
64							
65							
66	Hvr	rotech Ltd.		HYSYS.Plant v2.2.2	(Build 3806)		Page 12 of 19
		ad to the					* Consider the second

2	INL	Case Name: C:\NASA Final\NAS	A Co-Electrolysis wo R	tecup.hsc
3	Calgary, Alberta	Unit Set: NASA2		
5	CANADA	Date/Time: Mon Aug 23 11:24:	48 2010	
6 7 8	Spreadsheet: Steam	Electrolysis @TPL2		Units Set: NewUser1
9		CONNECTIONS		
12		Imported Variables		
3 Ce		Variable Description		Value
4 D2	, , , , ,	Temperature		1072.5 K
5 D3		Temperature		1073.2 K
17 E3		Comp Mole Frac (H2O) Comp Mole Frac (H2O)		0.72547 0.14106
8 F2	, , ,	Comp Mole Frac (Hydrogen)		0.08278
9 F3		Comp Mole Frac (Hydrogen)		0.66631
60 G2		Comp Mole Frac (Oxygen)		0.21000
1 G3		Comp Mole Frac (Oxygen)		1.00000
22 A8		Pressure		0.10546 MPa
23		rted Variables' Formula Results		,
24 25 Ce		Variable Description		Value
26	·	PARAMETERS		Value
?7 ?8		.,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,		
19 30 Ce	II Neithe Neith	Exportable Variables	Madable Tona	Makin
0 Ce		Variable Description A1 for Gibbs Formation Energy	Variable Type Molar Enthalpy	Value 2.382e+005 J/gmole
32 A2	95	A2 for Gibbs Formation Energy	Entropy	39.95 J/gmole-K
3 A3		A3 for Gibbs Formation Energy	Gibbs, Coeff, CC	3.319e-003 kJ/kgmol
4 A4	-	A4 for Gibbs Formation Energy		-3.532e-008
4 A4		A5 for Gibbs Formation Energy	Entropy	-12.85 J/gmole-K
36 A6		Fa (J/Volt-gmole)		9.649e+004
37 A7	, , , , , , , , , , , , , , , , , , ,	Universal Gas Contant	Entropy	8.314 J/gmole-K
8 A9	A9: Standard Pressure	Standard Pressure	Pressure	0.10132 MPa
9 D4	D4:		Temperature	0.66058 K
10 DE	D6:		Temperature	1072.8 K
1 D8	B D8:			1.080e-005
2 D9				1.635e-005
13 E4			Vapour Fraction	-0.5844
4 E5			Vapour Fraction	0.5410
5 F4	1 11		Vapour Fraction	0.5835
6 F5	1 - 1		Vapour Fraction	-0.6478
7 G4 8 G5			Vapour Fraction	0.7900
8 GS			Vapour Fraction	-0.4623 0.2186
iii H3				1.041
1 H4				0.8223
				-0.4482
52 H5 53 I2 54 I3			Molar Enthalpy	1.887e+005 J/gmole
i4 I3			Molar Enthalpy	1.887e+005 J/gmole
5 16	16:		Molar Enthalpy	1.887e+005 J/gmole
55 I6 56 J2 57 J3 58 K2 59 K3				2.320e+008
7 J3				2.321e+008
8 K2				0.8424
9 K3				1.050
10 K6			Vapour Fraction	0.9567
51 K7	′ K7:			0.9567
52 53		User Variables		
34				
55				

No. Callagry, Alberta Callagry, Alberta	200			Case Nam	e: C:\NASA Final\NASA C	o-Electrolysis wo Rec	up.hsc
Date/Time: Mon Aug 23 11:24:48 2010	186			Unit Sat:			******
Spreadsheet: Steam Electrolysis @TPL2 (continued Units Set: NewUo Spreadsheet: Steam Spreadsheet: Steam Electrolysis @TPL2 (continued Units Set: NewUo Spreadsheet: Steam Electrolysis @TPL2 (continued Un	100						
Spreadsheet: Steam Electrolysis @TPL2 (continued Units Set: NewUR FORMULAS	F			Date/Time	: Mon Aug 23 11:24:48 2	2010	
	3	Spread	lsheet: Stea	am Electroly	sis @TPL2 (c	ontinued u	nits Set: NewUser1
12	0			FORMU	LAS		
10				Formula			
D8							
1.635e-005	4 D						
E4							
E.S.			,				
F4) - (E2*@LN(E2)-E2)				
G4	8 F4						0.5835
G.5	9 F8	5 = (F3*@LN(F3)-F3)	- (F2*@LN(F2)-F2)				-0.6478
2 H2 = G2*A8IA9	o G∙	4 =G3-G2					0.7900
a H4 =H3-H2 0.8223 b H5 = (H6*)*@LNH*(3)-H3*) - (H2*@LNH2)-H2*) -0.4482 c 12 = A1 + A2*D2 + A3*D2*2 + A4*D2*3 + A5*D2*@LN(D2) 1.887e+005 Jgn c 13 = A1 + A2*D3 + A3*D2*2 + A4*D2*3 + A5*D3*@LN(D2) 1.887e+005 Jgn c 16 = A1 + A2*D3 + A3*D2*2 + A3*D2*3 + A5*D3*@LN(D2) 1.887e+005 Jgn d 16 = A1 + A2*D3 + A2*D2*D2*4 + A3*D2*3*A5*D2*3 + A5*D2*@LN(D2)-0.5) 2.320e+0008 d 17 2.321 + A1*D3 + A2*D2*D2*2 + A33*D2*3 + A44*D3*4 + A5*D2*D3*2*(@LN(D3)-0.5) 2.321e+0008 d 18 K2 = 1/(2*A6)*(12-A7*D2*@LN(E2/(F2*H2*0.5))) 0.8424 d K3 = 1/(2*A6)*(12-A7*D2*@LN(E2/(F2*H2*0.5))) 0.8424 d K6 = D6*(16*F4*H4 + A7*D6*((E5*F5*H4 + H5/2*F4)) 0.9557 d K7 = D9*(A7/Z*(D3*2-D2*2)*((E5*F5)*H4 + H5/2*F4)) 0.9557 d 7 = 2 38.9 £ Jgmole* K A2* in ** 107*2.5 K 0.72547 0.08 d 7 2 38.9 £ Jgmole* K A2* in ** 107*2.5 K 0.72547 0.08 d 8 4 2 ** 1 ** 1 ** 10** 10** 10** 10** 10**	1 G		3) - (G2*@LN(G2)-G2)				
a H4 =H3-H2 0.8223 b H5 = (H6*)*@LNH*(3)-H3*) - (H2*@LNH2)-H2*) -0.4482 c 12 = A1 + A2*D2 + A3*D2*2 + A4*D2*3 + A5*D2*@LN(D2) 1.887e+005 Jgn c 13 = A1 + A2*D3 + A3*D2*2 + A4*D2*3 + A5*D3*@LN(D2) 1.887e+005 Jgn c 16 = A1 + A2*D3 + A3*D2*2 + A3*D2*3 + A5*D3*@LN(D2) 1.887e+005 Jgn d 16 = A1 + A2*D3 + A2*D2*D2*4 + A3*D2*3*A5*D2*3 + A5*D2*@LN(D2)-0.5) 2.320e+0008 d 17 2.321 + A1*D3 + A2*D2*D2*2 + A33*D2*3 + A44*D3*4 + A5*D2*D3*2*(@LN(D3)-0.5) 2.321e+0008 d 18 K2 = 1/(2*A6)*(12-A7*D2*@LN(E2/(F2*H2*0.5))) 0.8424 d K3 = 1/(2*A6)*(12-A7*D2*@LN(E2/(F2*H2*0.5))) 0.8424 d K6 = D6*(16*F4*H4 + A7*D6*((E5*F5*H4 + H5/2*F4)) 0.9557 d K7 = D9*(A7/Z*(D3*2-D2*2)*((E5*F5)*H4 + H5/2*F4)) 0.9557 d 7 = 2 38.9 £ Jgmole* K A2* in ** 107*2.5 K 0.72547 0.08 d 7 2 38.9 £ Jgmole* K A2* in ** 107*2.5 K 0.72547 0.08 d 8 4 2 ** 1 ** 1 ** 10** 10** 10** 10** 10**	2 H:						
S H6	3 H						
S 2	4 H						
1	5 H			24-01-1/00			
	6 12						•
2 J 2 = A1*D2 + A2/2*D2*2 + A3/3*D2*3 + A4/4*D2*4 + A5/2*D3*2*(@LN(D2)-0.5) 2.320e+008 J 3 = A1*D3 + A2/2*D3*2 + A3/3*D2*3 + A4/4*D3*4 + A5/2*D3*2*(@LN(D3)-0.5) 2.321e+008 J 62 = 11/(2*A6)*(12-A7*D2*@LN(E2/(F2*H2*0.5))) 1.050 J 7 = D2*(16*F4*H4 + A7*D3*(@E+5*F5*H4 + H5/2*F4)) 0.9567 J 8	0 16						
3 J3 = A1*D3 + A2/2*D3*2 + A3/3*D3*2* + A4/4*D3*4 + A5/2*D3*2*(@LN(D3)-0.5) L(Z) = 11/(2*A6)*(12-A7*D2*@LN(E2)/(F2*H2*0.5))) L(D50	0 10				12\-0.5\		
K2	0 .13						
1,050	1 K			0 1 - 7 10/2 50 2 (@211/2	,0,0.0,		
Second Color		- ' ' '	0				
Spreadsheet	3 K (2*F4))			0.9567
Spreadsheet		7 =D9*(A7/2*(D3^2-D	2^2)*((E5+F5)*H4 + H5/2	?*F4) + F4*H4*(J3-J2))			0.9567
1				Spreads	heet		
2 39.95 J/gmole-K A2 in 1072.5 K 0.72547 0.08 3 319e-003 kJ/kgmol-K*2 A3 out 1073.2 K 0.14106 0.66 4 -3.532e-008 A4 (J/gmole-K*3) Delta 0.66058 K -0.5844 0.5 4 -3.632e-008 A4 (J/gmole-K*3) Delta 0.66058 K -0.5844 0.5 5 -12.85 J/gmole-K A5 Integration Coeff 0.5410 -0.6 6 9.649e+004 Fa (J/Volt-gmole) Average 1072.8 K 7 8.314 J/gmole-K Ru	7	Α	В	С	D	E	F
3 319e-003 kJ/kgmol-K*2	_	2.382e+005 J/gmole *	A1 '		Temperature *	y H2O *	y H2
4				in *			0.08278
2 5 -12.85 J/gmole-K ' A5 ' Integration Coeff' 0.5410 -0.6 3 6 9.649e+004 ' Fa (J/Volt-gmole) ' Average ' 1072.8 K 4 7 8.314 J/gmole-K ' Ru ' 5 8 0.10546 MPa Pressure ' C isothermal ' 1.080e-005 6 9 0.10132 MPa ' Standard Pressure ' C isothermal ' 1.080e-005 7 10		_					0.66631
\$ 6					0.66058 K		0.5835
4 7 8.314 J/gmole-K ' Ru ' 5 8 0.10546 MPa Pressure ' C isothermal ' 1.080e-005 6 9 0.10132 MPa ' Standard Pressure ' C ' 1.635e-005 7 10 8 G H I J K 9 1	2 5			_	4070.01/	0.5410	-0.6478
Sample Pressure Cisothermal 1.080e-005	4 7			Average '	1072.8 K		
6 9 0.10132 MPa * Standard Pressure * C * 1.635e-005	5 6			C icothormal *	1.0900.006		
7 10	6 9						
G	7 10			_			
2 0.21000 0.2186 1.887e+005 J/gmole 2.320e+008 0.8424 1 3 1.00000 1.041 1.087e+005 J/gmole 2.321e+008 1.050 2 4 0.7900 0.8223 3 5 -0.4623 -0.4482 4 6 1.887e+005 J/gmole Isothermal* 0.9567 5 7 Average* 0.9567 8 8 0 0.9567	8	G	Н		J	K	
1 3 1.0000 1.041 1.087e+005 J/gmole 2.321e+008 1.050 2 4 0.7900 0.8223	_	y O2 *	y A *	Delta G *	Delta G dT (J-K/gmole) *	Nernst Voltage *	
4 6 1.887e+005 J/gmole Isothermal * 0.9567 5 7	0 2						
4 6 1.887e+005 J/gmole Isothermal * 0.9567 5 7	1 3			1.887e+005 J/gmole	2.321e+008	1.050	
4 6 1.887e+005 J/gmole Isothermal * 0.9567 5 7	2 4						
7 9 0 0.9567 8 10 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	3 5	-0.4623	-0.4482	4.007-1005-1/	1,	2 222-	
8	5 2			1.88/e+uU5 J/gmole			
7 9 10 10 10 10 10 10 10 10 10 10 10 10 10	6 P				Average '	0.9367	
8 10	- 6						
0 0 1 2 2 3 4 4	/ 1 94						
	8 10						
	8 10						
	8 10						
	8 10						
	8 10						
	8 10						
VE ETITO FOUND TELEVI. TELEVISION TO THE TELEVISION TO THE TABLE 14 DE	8 10						
Licensed to: INL * Specified by use	8 10 9 0 1 2 3 4 5	protech Ltd.		HYSYS.Plant v2.2.2	2 (Build 3806)		Page 14 of 19

Collary, Alberta Collary, Alberta Collary, Alberta Collary Collary	_											
Collary, Aberta CANADA	2	bo	INI	Case Name: C:\NASA Final\N/	ASA Co-Electrolysis wo Re	cup.hsc						
Date/Time: Mon Aug 23 11.24.45 2010	3	HY	Calgary, Alberta	Unit Set: NASA2								
Spreadsheet: Temp Average ASR @TPL2 (Ignored)	4 5		CANADA	Date/Time: Mon Aug 23 11:2	4:48 2010							
Consideration Consideratio	6		Careadahaati Tama	Average ACD @TDL	0							
Cell	8		Spreadsneet: Temp	Average ASR @ IPL	(Ignored)	Units Set: Electrolys						
Cell	9 10			CONNECTIONS								
Bil SpreadSheetCell Electroysis Input and File ASR 0 100 K Semply	11 12			Imported Variables								
E15	13			<u>'</u>	n							
Cell	14 15											
Cel	16											
PARAMETERS	17 18											
Cell Visible Name	19	OCII	Object	·		Value						
Cell	20 21											
A A A A A A A A A A	22			Exportable Variables								
Second S	23			Variable Description								
Sempty S	24 25				· ·							
	26											
3	27											
20 A8 A8 A8	28					1.0						
A	29	A8	A8:									
2	30	A9	A9:									
A12 A12 A13 A13 A13 A14 A14 A15 A15 A16 A16 A16 A16 A16 A16 A17 A17 A18 A19 A19 A19 A19 A20 A20	31	A10	A10:			<empty></empty>						
A 13 A13 A13 A14 A14 A14 A14 A14 A15 A15 A16 A16 A16 A16 A16 A17 A17 A17 A17 A19 A19	32	A11	A11:			<empty></empty>						
A14	33					<empty></empty>						
A15	34											
A16	35											
A17												
A18												
A19												
A20						1						
B2	41											
B3 B3 B3 B4 B4 B4 B4 B4	42			Temp Aver ASR		· · ·						
	43		-	Tomp / Wol / Wit								
Section Sect	44					1						
B6 B6 B6 B6 B7 B7 B7 B7	45											
B9 B9 B9 B9 B10 B10 B10 B11 B11 B11 B11 B12 Sempty Sempt	46	В6				1						
B9 B9 B9 B9 B10 B10 B10 B11 B11 B11 B11 B12 Sempty Sempt	47	В7	B7:									
B10 B10 B10 B10 B11 B11 B11 B11 B11 B12 Sempty Semp			B8:			<empty></empty>						
B11 B11 B11 B11 B11	49											
Second Part	50											
B13 B13 B14 B14 B14 B14 B15	51											
84 B14 B14: <empty> 85 B15 B15: <empty> 86 B16: <empty> 87 B17 B17: <empty> 88 B18: <empty> 89 B19 B19: <empty> 80 B20: <empty> 81 C1: <empty> 82 C2: <empty> 83 C3 C3: <empty> 84 C4 C4: <empty> 85 C5: C5: <empty> 86 Hyprotech Ltd. HYSYS.Plant v2.2.2 (Build 3806) Page 15 of 19</empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty>	52											
85 B15 B15: <empty> 86 B16 B16: <empty> 87 B17 B17: <empty> 88 B18 B18: <empty> 89 B19 B19: <empty> 80 B20 B20: <empty> 81 C1 C1: <empty> 82 C2 C2: <empty> 83 C3 C3: <empty> 84 C4 C4: <empty> 85 C5 C5: <empty> 86 Hyprotech Ltd. HYSYS.Plant v2.2.2 (Build 3806) Page 15 of 19</empty></empty></empty></empty></empty></empty></empty></empty></empty></empty></empty>	53 54											
Section Sect	54 55											
67 B17 B17: <empty> 88 B18 B18: <empty> 99 B19 B19: <empty> 90 B20 B20: <empty> 91 C1 C1: <empty> 92 C2 C2: <empty> 33 C3 C3 <empty> 44 C4 C4: <empty> 95 C5 C5: <empty> 96 Hyprotech Ltd. HYSYS.Plant v2.2.2 (Build 3806) Page 15 of 19</empty></empty></empty></empty></empty></empty></empty></empty></empty>	56											
Section Sect	57					1 1						
B19 B19 B19 B19 B20 B20	58											
B20 B20	59											
C1 C1:	60											
52 C2 C2: <empty> 53 C3 C3: <empty> 54 C4 C4: <empty> 55 C5 C5: <empty> 66 Hyprotech Ltd. HYSYS.Plant v2.2.2 (Build 3806) Page 15 of 19</empty></empty></empty></empty>	61											
C3 C3 C3 <empty> </empty>	62											
64 C4 C4: <empty> 55 C5 C5: <empty> 66 Hyprotech Ltd. HYSYS.Plant v2.2.2 (Build 3806) Page 15 of 19</empty></empty>	63											
Hysrotech Ltd. Hysrotech Ltd. Hysrotech Ltd. Hysrotech Ltd. Page 15 of 19	64					<empty></empty>						
	65											
	66			HYSYS.Plant v2.2.2 (Build 3806)								

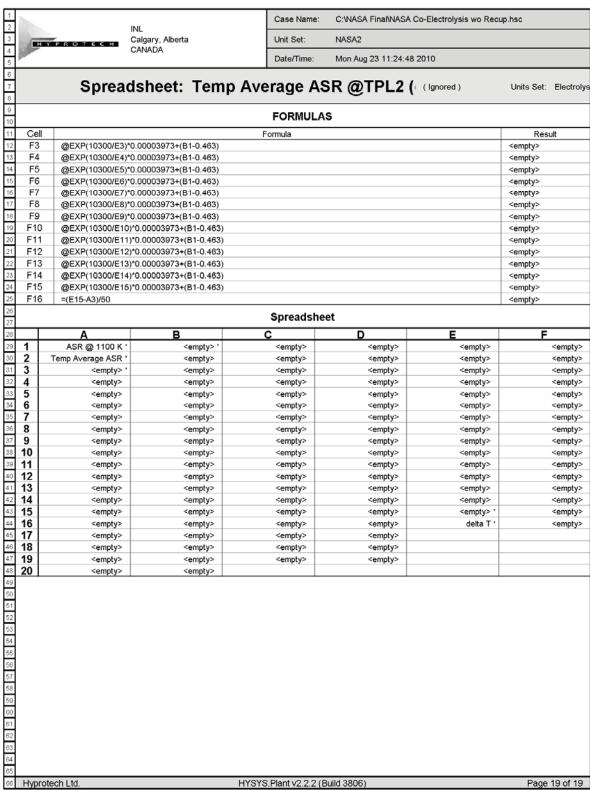
1	Do.		Case Name: C:\NASA Final\NASA Co	-Electrolysis wo Recup.hsc	
3		INL Calgary, Alberta	Unit Set: NASA2		
5		CANADA	Date/Time: Mon Aug 23 11:24:48 20	010	
6					
7		Spreadsheet: Temp A	Average ASR @TPL2 ((Ignored) Units Set: Elect	trolys
9			PARAMETERS		
11 12			Exportable Variables		
13	Cell	Visible Name	Variable Description	Variable Type Value	
14	C6	C6:		<empty></empty>	
15	C7	C7:	-		
16	C8	C8:		<empty></empty>	
17	C9	C9:	-	<empty></empty>	
18	C10	C10:		<empty></empty>	
19	C11	C11:	-	<empty></empty>	
20	C12	C12:		<empty></empty>	
21	C13	C13:	-	<empty></empty>	
22	C14	C14:	-	<empty></empty>	
23	C15	C15:		<empty></empty>	
24	C16	C16:	-	<empty></empty>	
25	C17	C17:		<empty></empty>	
26	C18	C18:		<empty></empty>	
27	C19	C19:		<empty></empty>	
28	D1	D1:	-	<empty></empty>	
29	D2	D2:	-	<empty></empty>	
30	D3	D3:		<empty></empty>	
31	D4	D4:		-cripty-	
32	D5	D5:	-	-cinpty-	
33	D6	D6:	-	-Gillpry-	
34	D7	D7:	-		
35	D8	D8:			
36 37	D9	D9:	-	- unique	
38	D10	D10:	-		
39	D11 D12	D11: D12:		- Ciripty	
40	D12	D12:	-		
41	D13	D13.			
42	D15	D15:		-c.iipty-	
43	D16	D16:		-ompry-	
44	D17	D17:			
45	D18	D18:			
46	D19	D19:			
47	E1	E1:			
48	E2	E2:			
49	E3	E3:	-		
50	E4	E4:		<empty></empty>	
51	E5	E5:	-		
52	E6	E6:			
53	E7	E7:			
54	E8	E8:			
55	E9	E9:			
56	E10	E10:	-		
57	E11	E11:			
58	E12	E12:		<empty></empty>	
59	E13	E13:		<empty></empty>	
60	E14	E14:	-	<empty></empty>	
61	F1	F1:		<empty></empty>	
62	F2	F2:		<empty></empty>	
63	F3	F3:		<empty></empty>	
64	F4	F4:	-	<empty></empty>	
65	F5	F5:		- unipry	
66	Hyprote	ch Ltd. H'	YSYS.Plant v2.2.2 (Build 3806)	Page 16 of	19

_										
2	Dr.	INL	Case Name:	C:\NASA Final\NASA	Co-Electrolysis wo Recu	p.hsc				
3	HY	Calgary, Alberta	Unit Set:	NASA2						
5		CANADA	Date/Time:	Mon Aug 23 11:24:48	3 2010					
6										
7		Spreadsheet: Temp Ave	erage AS	R @TPL2 ((Ignored)	Units Set: Electrolys				
9			PARAMETER	ns						
11 12		Ex	portable Vari	ables						
13	Cell	Visible Name	Variable Des	scription	Variable Type	Value				
14	F6	F6:				<empty></empty>				
15	F7	F7:				<empty></empty>				
16	F8	F8:				<empty></empty>				
17	F9	F9:				<empty></empty>				
18	F10	F10:				<empty></empty>				
19	F11	F11:				<empty></empty>				
20	F12	F12:				<empty></empty>				
21	F13	F13:				<empty></empty>				
22	F14	F14:				<empty></empty>				
23	F15	F15:				<empty></empty>				
24	F16	F16:				<empty></empty>				
25 26			User Variable	es						
27 28	EODMIII AC									
29	Cell	-	Formula			Result				
30	A4	=A3+F16				<empty></empty>				
31	A 5	=A4+F16				<empty></empty>				
32	A6	=A5+F16				<empty></empty>				
33	A7	=A6+F16				<empty></empty>				
34	A8	=A7+F16				<empty></empty>				
35	A9	=A8+F16				<empty></empty>				
36	A10	=A9+F16				<empty></empty>				
37	A11	=A10+F16				<empty></empty>				
38	A12	=A11+F16				<empty></empty>				
39	A13	=A12+F16				<empty></empty>				
40	A14	=A13+F16				<empty></empty>				
41	A15	=A14+F16				<empty></empty>				
42	A16	=A15+F16				<empty></empty>				
43	A17	=A16+F16				<empty></empty>				
44	A18	=A17+F16				<empty></empty>				
45	A19	=A18+F16				<empty></empty>				
46	A20	=4*(B4+B6+B8+B10+B12+B14+B16+B18+D1+D3+D5+	D7+D9+D11+D13	+D15+D17+D19+F2+F	4+F6+F8+F10+F12+F1	<empty></empty>				
47	B2	@if(E15==A3,F15,(1/3*F16*(B3+A20+B20+F15))/(E15-	A3))			<empty></empty>				
48	В3	@EXP(10300/A3)*0.00003973+(B1-0.463)				<empty></empty>				
49	B4	@EXP(10300/A4)*0.00003973+(B1-0.463)				<empty></empty>				
50	B5	@EXP(10300/A5)*0.00003973+(B1-0.463)				<empty></empty>				
51	B6	@EXP(10300/A6)*0.00003973+(B1-0.463)				<empty></empty>				
52	B7	@EXP(10300/A7)*0.00003973+(B1-0.463)				<empty></empty>				
53	B8	@EXP(10300/A8)*0.00003973+(B1-0.463)				<empty></empty>				
54	B9	@EXP(10300/A9)*0.00003973+(B1-0.463)				<empty></empty>				
55	B10	@EXP(10300/A10)*0.00003973+(B1-0.463)				<empty></empty>				
56	B11	@EXP(10300/A11)*0.00003973+(B1-0.463)				<empty></empty>				
57	B12	@EXP(10300/A12)*0.00003973+(B1-0.463)				<empty></empty>				
58 59	B13	@EXP(10300/A13)*0.00003973+(B1-0.463)				<empty></empty>				
59	B14	@EXP(10300/A14)*0.00003973+(B1-0.463)				<empty></empty>				
60	B15	@EXP(10300/A15)*0.00003973+(B1-0.463)				<empty></empty>				
61	B16	@EXP(10300/A16)*0.00003973+(B1-0.463)				<empty></empty>				
62	B17	@EXP(10300/A17)*0.00003973+(B1-0.463)				<empty></empty>				
63	B18	@EXP(10300/A18)*0.00003973+(B1-0.463)				<empty></empty>				
64	B19	@EXP(10300/A19)*0.00003973+(B1-0.463)				<empty></empty>				
65	B20	=2*(B5+B7+B9+B11+B13+B15+B17+B19+D2+D4+D6+			5+F7+F9+F11+F13)	<empty></empty>				
66	Hyprote	ch Ltd. HYSYS	S.Plant v2.2.2 (Bi	uild 3806)		Page 17 of 19				

Hyprotech Ltd. HYSYS.Plant v2.2.2 (Build 3806) Page 17 of 19

Licensed to: INL *Specified by user.

1	Do.		Case Name: C:\NASA Final\NASA Co-Electrolysis wo R	ecup.hsc
3	H Y	INL Calgary, Alberta	Unit Set: NASA2	
4 5		CANADA	Date/Time: Mon Aug 23 11:24:48 2010	
6				
7 8		Spreadsheet: Temp Av	verage ASR @TPL2 (((Ignored)	Units Set: Electrolys
9 10			FORMULAS	
11	Cell		Formula	Result
12	C1	=A19+F16		<empty></empty>
13	C2	=C1+F16		<empty></empty>
14	C3	=C2+F16		<empty></empty>
15	C4	=C3+F16		<empty></empty>
16 17	C5 C6	=C4+F16 =C5+F16		<empty></empty>
18	C7	=C6+F16		<empty></empty>
19	C8	=C7+F16		<empty></empty>
20	C9	=C8+F16		<empty></empty>
21	C10	=C9+F16		<empty></empty>
22	C11	=C10+F16		<empty></empty>
23	C12	=C11+F16		<empty></empty>
24	C13	=C12+F16		<empty></empty>
25	C14	=C13+F16		<empty></empty>
26	C15	=C14+F16		<empty></empty>
27	C16	=C15+F16		<empty></empty>
28	C17	=C16+F16		<empty></empty>
29	C18	=C17+F16		<empty></empty>
30	C19	=C18+F16		<empty></empty>
31	D1	@EXP(10300/C1)*0.00003973+(B1-0.463)		<empty></empty>
32	D2	@EXP(10300/C2)*0.00003973+(B1-0.463)		<empty></empty>
33	D3	@EXP(10300/C3)*0.00003973+(B1-0.463)		<empty></empty>
34 35	D4	@EXP(10300/C4)*0.00003973+(B1-0.463)		<empty></empty>
36	D5 D6	@EXP(10300/C5)*0.00003973+(B1-0.463)		<empty></empty>
37	D7	@EXP(10300/C6)*0.00003973+(B1-0.463)		<empty></empty>
38	D8	@EXP(10300/C7)*0.00003973+(B1-0.463) @EXP(10300/C8)*0.00003973+(B1-0.463)		<empty></empty>
39	D9	@EXP(10300/C9)*0.00003973+(B1-0.463)		<empty></empty>
40	D10	@EXP(10300/C10)*0.00003973+(B1-0.463)		<empty></empty>
41	D11	@EXP(10300/C11)*0.00003973+(B1-0.463)		<empty></empty>
42	D12	@EXP(10300/C12)*0.00003973+(B1-0.463)		<empty></empty>
43	D13	@EXP(10300/C13)*0.00003973+(B1-0.463)		<empty></empty>
44	D14	@EXP(10300/C14)*0.00003973+(B1-0.463)		<empty></empty>
45	D15	@EXP(10300/C15)*0.00003973+(B1-0.463)		<empty></empty>
46 47	D16	@EXP(10300/C16)*0.00003973+(B1-0.463)		<empty></empty>
	D17	@EXP(10300/C17)*0.00003973+(B1-0.463)		<empty></empty>
48	D18	@EXP(10300/C18)*0.00003973+(B1-0.463)		<empty></empty>
49	D19	@EXP(10300/C19)*0.00003973+(B1-0.463)		<empty></empty>
50	E1	=C19+F16		<empty></empty>
51	E2	=E1+F16		<empty></empty>
52 53	E3 E4	=E2+F16 -F3+F16		<empty></empty>
54	E5	=E3+F16 =E4+F16		<empty></empty>
55	E6	=E5+F16		<empty></empty>
56	E7	=E6+F16		<empty></empty>
57	E8	=E7+F16		<empty></empty>
58	E9	=E8+F16		<empty></empty>
59	E10	=E9+F16		<empty></empty>
60	E11	=E10+F16		<empty></empty>
61	E12	=E11+F16		<empty></empty>
62	E13	=E12+F16		<empty></empty>
63	E14	=E13+F16		<empty></empty>
64	F1	@EXP(10300/E1)*0.00003973+(B1-0.463)		<empty></empty>
65	F2	@EXP(10300/E2)*0.00003973+(B1-0.463)		<empty></empty>
66	Hyprote	ch Ltd. HYS	YS.Plant v2.2.2 (Build 3806)	Page 18 of 19



* Specified by use

A.7 Boudouard Process with Co-electrolysis

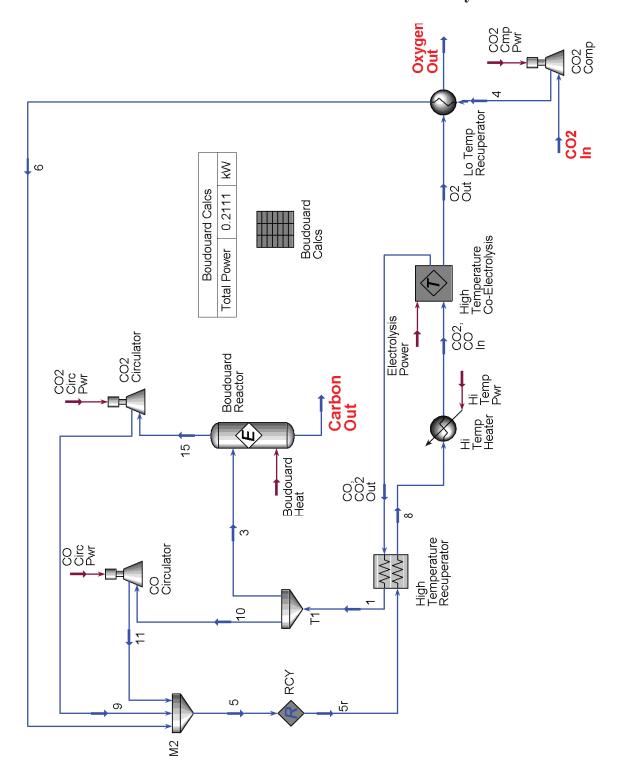


Figure A - 13 Process flow diagram of Boudouard process with co-electrolysis

_							
2	lbo	INL		Case Name:	C:\NASA Final\NASA C	o-Electrolysis w Boudou	uard.hsc
3	HYPROTEC	Calgary, A	Mberta	Unit Set:	NASA		
5		CANADA		Date/Time:	Mon Aug 23 11:47:57 2010		
6							
7	Wor	kbook:	Case (Main	1)			
9							
10				Streams			
11	Name Vancus Frantiscs		5	Sweep Gas In	CO, CO2 Out 1,0000	5r	CO2, CO In 1.0000
12 13	Vapour Fraction Temperature	(C)	1.0000 461.72	1.0000 800.00	800.00	1.0000 461.71 *	800.00
14	Pressure	(kPa)	185.75	175.37	175.37	185.75 '	179.75
15	Molar Flow	(gmole/h)	3.2553	3.4662e-009 °	3.2552	3.2553 *	3,2553
16	Mass Flow	(kg/d)	3.3134	2.4000e-009	2.3133	3.3133	3.3133
17	Liquid Volume Flow	(m3/h)	1.676e-004	1.156e-013	1.200e-004	1.676e-004	1.676e-004
18	Heat Flow	(kW)	-0.3136	2.344e-011	-0.1026	-0.3136	-0.2982
19	Molar Enthalpy	(kJ/kgmole)	-3.468e+005	2.434e+004	-1.135e+005	-3.468e+005	-3.297e+005
20	Name		CO2 Circ Pwr	CO2 Cmp Pwr	Electrolysis Power	CO Circ Pwr	Hi Temp Pwr
21	Vapour Fraction						
22	Temperature	(C)					
23	Pressure	(kPa)					
24 25	Molar Flow Mass Flow	(gmole/h)					
26	Liquid Volume Flow	(kg/d) (m3/h)					
27	Heat Flow	(HS/H)	2.847e-004	4.450e-004	0.2047	6.332e-005	5.595e-003
28	Molar Enthalpy	(kJ/kgmole)	2.047.0-004	4.4000-004	0.2047	0.5522-555	
29	Name	(noniginolo)	O2 Out	Boudouard Heat	8	4	6
30	Vapour Fraction		1.0000		1.0000	1.0000	1.0000
31	Temperature	(C)	800.00		680.97	53.253	568.99
32	Pressure	(kPa)	175.37		182.75	188.75 '	185.75
33	Molar Flow	(gmole/h)	1.3021		3.2553	1.3022	1.3022
34	Mass Flow	(kg/d)	1.0000		3.3133	1.3754	1.3754
35	Liquid Volume Flow	(m3/h)	3.662e-005		1.676e-004	6.944e-005	6.944e-005
36	Heat Flow	(kW)	9.140e-003	-6.638e-002	-0.3037	-0.1421	-0.1335
37 38	Molar Enthalpy Name	(kJ/kgmole)	2.527e+004	15	-3.359e+005	-3.928e+005	-3.690e+005
39	Vapour Fraction		Carbon Out 0.0000	1.0000	1.0000	Oxygen Out 1.0000	1.0000
40	Temperature	(C)	350.00	350.00 °	486.71	78.253	363.64
41	Pressure	(kPa)	169.37	169.37	172.37	172.37	185.75
42	Molar Flow	(gmole/h)	1.3021	1.5947	3.2552	1.3021	1.5947
43	Mass Flow	(kg/d)	0.37534	1.6832	2.3133	1.0000	1.6832
44	Liquid Volume Flow	(m3/h)	9.524e-006	8.498e-005	1.200e-004	3.662e-005	8.498e-005
45	Heat Flow	(kW)	1.609e-003	-0.1680	-0.1124	5.633e-004	-0.1678
46	Molar Enthalpy	(kJ/kgmole)	4450	-3.793e+005	-1.243e+005	1557	-3.787e+005
47	Name		3	10	11		
48	Vapour Fraction		1.0000	1.0000	1.0000		
49 50	Temperature	(C)	486.71	486.71	505.70		
51	Pressure Molar Flow	(kPa) (gmole/h)	172.37 2.8968	172.37 0.35844	185.75 0.35844		
52	Mass Flow	(gmole/n) (kg/d)	2.0586	0.35844	0.25473		
53	Liquid Volume Flow	(m3/h)	1.068e-004	1.322e-005	1.322e-005		
54	Heat Flow	(kW)	-0.1001	-1.238e-002	-1.232e-002		
55	Molar Enthalpy	(kJ/kgmole)	-1.243e+005	-1.243e+005	-1.237e+005		
56 57				Compressors			
57 58	Name		CO2 Circulator	CO2 Comp	CO Circulator		
59	Feed Pressure	(kPa)	169.4	131.0 *	172.4		
60	Product Pressure	(kPa)	185.7	188.7 *	185.7		
61	Molar Flow	(gmole/h)	1.595	1.302	0.3584		
62	Energy	(kW)	2.847e-004	4.450e-004	6.332e-005		
63	Adiabatic Efficiency		75 *	75 °	75 *		
64	Polytropic Efficiency		75	76	75		
65	I b manda ab 111			WO DI	14 2000)		D
66	Hyprotech Ltd.		HYS	SYS.Plant v2.2.2 (Buil	a 3806)		Page 1 of 6

1			Case Name:	C:\NASA Final\NASA Co	-Electrolysis w Boudou	uard.hsc
3	INL Calgary, A	Alberta	Unit Set:	NASA		
4 5	CANADA		Date/Time:	Mon Aug 23 11:47:57 2	010	
6						
7	Workbook:	Case (Main	ı) (continue	ed)		
9						
10			Composition			
11	Name	4	5	5r	6	8
12 13	Comp Mole Frac (H2O)	0.00000	0.00000	0.00000 *	0.00000	0.00000
14	Comp Mole Frac (Hydrogen)	0.00000		0.00000 *	0.00000	0.00000
15	Comp Mole Frac (Oxygen)	0.00000	0.00000	0.00000 *	0.00000	0.00000
16	Comp Mole Frac (Argon)	0.00000	0.00000	0.00000 * 0.00000 *	0.00000	0.00000
17	Comp Mole Frac (Nitrogen) Comp Mole Frac (CO2)	1.00000	0.90000	0.90000	1.00000	0.90000
18	Comp Mole Frac (CO2)					
19		0.00000	0.10000	0.10000 *	0.00000	0.10000
20	Comp Mole Frac (Methane) Comp Mole Frac (Carbon)	0.00000	0.00000 0.00000	0.00000 °	0.00000	0.00000
21	Name	CO2 In	CO2, CO In	CO, CO2 Out	O2 Out	Carbon Out
22	Comp Mole Frac (H2O)	0.00000 °	0.00000	0.00000	0.00000	0.00000
23	Comp Mole Frac (H2O) Comp Mole Frac (Hydrogen)	0.00000 *	0.00000	0.00000	0.00000	0.00000
24	Comp Mole Frac (Oxygen)	0.00000 *	0.00000	0.00000	1.00000	0.00000
25	Comp Mole Frac (Oxygen)	0.00000	0.00000	0.00000	0.00000	0.00000
26	Comp Mole Frac (Argon)	0.00000	0.00000	0.00000	0.00000	0.00000
27	Comp Mole Frac (CO2)	1.00000	0.90000	0.10000	0.00000	0.00000
28	Comp Mole Frac (CO2)	0.00000	0.10000	0.90000	0.00000	0.00000
29	Comp Mole Frac (Methane)	0.00000	0.00000	0.00000	0.00000	0.00000
30	Comp Mole Frac (Carbon)	0.00000	0.00000	0.00000	0.00000	1.00000
31	Name	15	1	Oxygen Out	9	3
32	Comp Mole Frac (H2O)	0.00000	0.00000	0.00000	0.00000	0.00000
33	Comp Mole Frac (Hydrogen)	0.00000	0.00000	0.00000	0.00000	0.00000
34	Comp Mole Frac (Oxygen)	0.00000	0.00000	1.00000	0.00000	0.00000
35	Comp Mole Frac (Argon)	0.00000	0.00000	0.00000	0.00000	0.00000
36	Comp Mole Frac (Nitrogen)	0.00000	0.00000	0.00000	0.00000	0.00000
37	Comp Mole Frac (CO2)	0.99816	0.10000	0.00000	0.99816	0.10000
38	Comp Mole Frac (CO)	0.00184	0.90000	0.00000	0.00184	0.90000
39	Comp Mole Frac (Methane)	0.00000	0.00000	0.00000	0.00000	0.00000
40	Comp Mole Frac (Carbon)	0.00000	0.00000	0.00000	0.00000	0.00000
41	Name	10	11	0.00000	0.00000	0.00000
42	Comp Mole Frac (H2O)	0.00000	0.00000			
43	Comp Mole Frac (Hydrogen)	0.00000	0.00000			
44	Comp Mole Frac (Oxygen)	0.00000	0.00000			
45	Comp Mole Frac (Argon)	0.00000	0.00000			
46	Comp Mole Frac (Nitrogen)	0.00000	0.00000			
47	Comp Mole Frac (CO2)	0.10000	0.10000			
48	Comp Mole Frac (CO)	0.90000	0.90000			
49	Comp Mole Frac (Methane)	0.00000	0.00000			
50	Comp Mole Frac (Carbon)	0.00000	0.00000			
51						
52			Heat Exchange	15		
53	Name	Lo Temp Recuperato				
54	Duty (kW)	8.578e-003				
55	Tube Inlet Temperature (C)	53.25				
56	Tube Outlet Temperature (C)	569.0				
57	Shell Inlet Temperature (C)	800.0				
58	Shell Outlet Temperature (C)	78.25				
59	LMTD (C)	92.06				
60	UA (kJ/C-h)	0.3354				
61	Minimum Approach (C)	25.00				
62						
63						
64						
65	I be marke als 16.		2VO PI	14 2000)		
66	Hyprotech Ltd.	HYS	SYS.Plant v2.2.2 (Buil	a 3806)		Page 2 of 6

_									
2	line.	INL			Case Name:	C:\NASA Final\NASA	Co-Electroly	sis w Boudouar	d.hsc
3	HYPROTECH	Calgary, /	Alberta		Unit Set:	NASA			
5		CANADA			Date/Time:	Mon Aug 23 11:47:5	7 2010		
6									
7	Workb	ook:	Case (N	lain)	(continu	ed)			
2 3 4 5 6 7 8 9				Oth	ner Heat Excha	ingers			
11	Name		High Tempera	ture Re					
12	Number of Sides			2 '					
13	LMTD	(C)		80.71 *					
14 15	UA (Calculated)	(kJ/C-h)		5819					
16	Hot Pinch Temperature Cold Pinch Temperature	(C)		86.7 61.7					
17	Minimum Approach	(C)		25.00					
18	Exchanger Cold Duty	(kW)	9.813€	-003					
19 20					Pumps				
21	Name								
22	Delta P	(kPa)							
23	Energy	(kW)							
24 25	Feed Pressure Product Pressure	(kPa)		-					
26		(kPa) (gmole/h)							
27	Adiabatic Efficiency	(%)							
27 28	•				Unit Ops		•		
29		_							
30 31	Operation Name	Ope	eration Type	8	Feeds	CO2, CO In	ts	Ignored	Calc. Level
32	Hi Temp Heater	Heater			emp Pwr	CO2, CO III		No	500.0 *
33	T4	T		1		3		N.	500.01
34	T1	Tee				10		No	500.0
35 36	Lo Temp Recuperator	Heat Exc	hanger	4		6		No	500.0 *
37				9	Out	Oxygen Out 5			
37 38 39	M2	Mixer		6				No	500.0
39				11					
40	CO2 Circulator	Compres	sor	15		9		No	500.0 *
41				CO	2 Circ Pwr	4			
43	CO2 Comp	Compres	sor		2 Cmp Pwr			No	500.0 *
44	00.0			10		11			500.0
45	CO Circulator	Compres	sor	co	Circ Pwr			No	500.0 *
46	High Temperature Recupera	LNG		5r		8		No	500.0 *
47	-			_	CO2 Out eep Gas In	1 02 Out			
42 43 44 45 46 47 48 49					2, CO In	CO, CO2 Out		i	
	High Temperature Co-Electro	Standard	Sub-Flowsheet		cess Heat	,		No	2500 °
51				Elec	trolysis Power				
52	Electrolysis Input and Output Boudouard Calcs	Spreadsl Spreadsl		_				No No	500.0 * 500.0 *
54	Boudouard Calcs	opreads	icel	3		Carbon Out		140	500.0
55	Boudouard Reactor	Equilibriu	m Reactor		idouard Heat	15		No	500.0 *
56		_				Boudouard Hea	t		
57	RCY	Recycle		5		5r		No	3500 *
53 54 55 56 57 58 60 61 62 63 64 65									
66	Hyprotech Ltd.			HYS	YS.Plant v2.2.2 (Bu	uild 3806)			Page 3 of 6

<u> </u>									
2		INL		Case Name:	C:\NASA	Final\NASA Co	-Electroly	sis w Boudou	ard.hsc
3	HYPROTECH	Calgary, A	Alberta	Unit Set:	NASA				
5		ONIMUM		Date/Time:	Mon Aug 2	23 11:47:57 2	010		
6	Ma ulch	l-:	Himb Tom		Flac	44010	- /TI) ()\	
7	VVOTKD	оок:	High Ten	perature Co	-Elec	trolys	IS (I I	² L2)	
9 10				Streams					
11	Name		Sweep Gas In @	TPL O2 Out @TPL2	Gas Pr	oducts @TPL:	Liquid @	TPL2	Anode @TPL2
12	Vapour Fraction		1.000			1.0000		0.0000	1.0000
13	Temperature	(C)	800.0			* 00.008		800.00	800.00
14 15	Pressure	(kPa)	175.3			176.75		176.75	175.37
16	Molar Flow Mass Flow	(gmole/h)	3.4662e-00			4.5573 3.3133		0.00000	1.3021
17	Liquid Volume Flow	(kg/d) (m3/h)	2.4000e-00 1.156e-01			1.566e-004		0.0000	3.662e-005
18	Heat Flow	(kW)	2.344e-01			9.348e-002		0.0000	9.140e-003
19		J/kgmole)	2.434e+00			7.384e+004	-7	.384e+004	2.527e+004
20	Name		CO, CO2 Out @T			lysis Heatiing		Heat @TPL:	Electrolysis Power @
21	Vapour Fraction		1.000						
22	Temperature	(C)	800.0	0 * 800.00					
23	Pressure	(kPa)	175.3	7 179.75					
24	Molar Flow	(gmole/h)	3.255	2 3.2553					
25	Mass Flow	(kg/d)	2.313	3 3.3133					
26	Liquid Volume Flow	(m3/h)	1.200e-00	4 1.676e-004					
27	Heat Flow	(kW)	-0.102	6 -0.2982		0.2047	8	3.050e-009	0.2047
28	Molar Enthalpy (k.	J/kgmole)	-1.135e+00	5 -3.297e+005					
29				Material Stream	ns				
30									
31	Name		Sweep Gas In @		Gas Pr	oducts @TPL:	Liquid @		Anode @TPL2
32	Comp Mole Frac (H2O)		0.0000			0.00000		0.00000	0.00000
33 34	Comp Mole Frac (Hydrogen)		0.0000			0.00000		0.00000	0.00000
35	Comp Mole Frac (Oxygen)		0.2100			0.28571		0.28571	1.00000
36	Comp Mole Frac (Argon)		0.0000			0.00000		0.00000	0.00000
37	Comp Mole Frac (Nitrogen) Comp Mole Frac (CO2)		0.7900			0.07143		0.00000	0.00000
38	Comp Mole Frac (CO2)		0.0000					0.64286	0.00000
39	Comp Mole Frac (Methane)		0.0000					0.00000	0.00000
40	Comp Mole Frac (Carbon)		0.0000					0.00000	0.00000
41	Name		CO, CO2 Out @T		1	0.0000		0.0000	0.0000
42	Comp Mole Frac (H2O)		0.0000						
43	Comp Mole Frac (Hydrogen)		0.0000						
44	Comp Mole Frac (Oxygen)		0.0000						
45	Comp Mole Frac (Argon)		0.0000						
46 47	Comp Mole Frac (Nitrogen)		0.0000	0.00000					
47	Comp Mole Frac (CO2)		0.1000	0.90000					
48	Comp Mole Frac (CO)		0.9000	0.10000					
49	Comp Mole Frac (Methane)		0.0000						
50	Comp Mole Frac (Carbon)		0.0000	0.00000					
51 52				Unit Ops					
53	Operation Name	One	eration Type	Feeds		Products		Ignored	Calc. Level
54	Temp Average ASR @TPL2	Spreadsh						Yes	500.0 *
55	Electrolysis Spreadsheet @	Spreadsh						No	500.0 *
56	Steam Electrolysis @TPL2	Spreadsh						No	500.0 *
57	CO2 Electrolysis @TPL2	Spreadsh						No	500.0 *
58				Anode @TPL2	02 (Out @TPL2		No	500.0 *
59	59		Sweep Gas In @TPL2				140	500.0	
60				CO2, Water In @TPL2		id @TPL2			1
61			on Reactor	Electrolysis Heatiing @T		Gas Products @TPL2		No	500.0 *
62						trolysis Heatii			
63	Electrodes @TPL2	@TPL2 Component Splitter Gas Products @TPL2 CO, CO2 Out @TPL2			No	500.0 *			
64				Anode @TPL2					
65							3500 °		
66	Hyprotech Ltd. Licensed to: INL			HYSYS.Plant v2.2.2 (Bui	id 3806)				Page 4 of 6 * Specified by user.
	Elderfised to: INE								opecified by USEr.

1										
2		INL		Case Name: C:\N	ASA Final\NA	SA Co-Electrolysi	is w Boudouard	i.hsc		
3	HYPROTECH	Calgary, Alberta CANADA		Unit Set: NAS	Α					
5		SARADA		Date/Time: Mon	Aug 23 11:47	7:57 2010				
6 7 8	Workb	ook: High	Temp	erature Co-E	lectrol	lysis (TP	L2) (co	ntinued)		
9 10			U	nit Ops (continued)					
11	Operation Name	Operation Type	•	Feeds	Pro	ducts	Ignored	Calc. Level		
12 13	SET-1 @TPL2 SET-3 @TPL2	Set Set					No No	500.0 °		
14	SET-2 @TPL2	Set					No	500.0 *		
15 16 17		ersion: 20	02=20	CO+O2						
18 19				STOICHIOMETRY						
20	Compone	ent		Mole Weight		SI	toichiometric C			
21	CO2				44.010			-2*		
22 23	CO Oxygen				28.011 32.000			2 · 1 ·		
24										
25							0005	-1-		
26 27	Balance Error: 0.0000 Reaction Heat: 2.832e+005 kJ/kgmole									
28	BASIS									
29	Base Component: CO2 Conversion Percent: 100.00 ' Reaction Phase: Overall									
30 31				PARAMETERS						
32 33 34	Conv	ersion: 2H	120=21	H2+O2						
35 36				STOICHIOMETRY						
37	Compone	nt		Mole Weight		SI	toichiometric C			
38 39	H2O Hydrogen				18.015 2.016			-2 *		
40	Oxygen				32.000			1.		
41	.,									
42 43	Ralance	e Error: 0.0000			Rea	ction Heat: 2.41	0e+005 k.l/kam	nole		
44	Dalance	e Liioi. 0.0000		BASIS	itea	ction rieat. 2.41	OE+OOS KS/Kgii	iole		
45	Dana Carrier and Area		0			B	Dhara Car			
46 47	Base Component: H20	,	Conversio	on Percent: 90.00		Reaction	Phase: Overa	II		
48				PARAMETERS						
49 50 51	Equi	librium: Bo	oudou	ard						
52 53				STOICHIOMETRY						
54 55	Compone			Molecular Weight		Stoi	chiometric Coe			
55 50		co			28.01			-2 *		
57		CO2 Carbon			44.01 12.01			1'		
58										
56 57 58 59	Balance	Error: 0.0000			Read	ction Heat: -8.63	31e+004 kJ/kgr	mole		
61 62				BASIS						
62 63	Basis	Phase		Approach (C)		Min. Temp (C)	N	Max. Temp (C)		
64	Activity	Vapo	urPhase	(C)		-273.1	5	3000.0		
65										
66	Hyprotech Ltd. Licensed to: INL		HYS	YS.Plant v2.2.2 (Build 38	306)			Page 5 of 6 * Specified by user.		
	Electrised to, INE							opeomed by dser.		

2		Case Na	ame: C:\NASA Final\NASA Co-Electroly	sis w Boudouard.hsc		
3	INL Calgary, Albe	rta Unit Set	: NASA			
5	CANADA	Date/Tir	Date/Time: Mon Aug 23 11:47:57 2010			
6						
7	Equilibrium	: Boudouard (co	ontinued)			
9		PARAM	ETERS			
11 12		Source : K	Vs. T Table			
13	Coeff A	-21.64	R2	1.000000 *		
14	Coeff B	2.078e+004	T High			
15 16	Coeff C	5.932e-002 -3.081e-005	T Low			
17	00011 5	0.0010-000				
18 19	Temperature (C)	Keq	KCalc	Percentage Error		
20	25.000 °	1.040e+021 *	1.040e+021 *	-9.850e-003 *		
21	127.00 *	2.030e+013 *	2.028e+013 *	7.997e-002 *		
22 23	227.00 *	6.330e+008 *	6.339e+008 *	-0.1356 * 1.221e-002 *		
24	327.00 ° 427.00 °	6.290e+005 * 4500 *	6.289e+005 ° 4502 °	-3.523e-002 *		
24 25	527.00 *	111.0 *	110.8 *	0.1967 *		
26	627.00 °	6.210 °	6.210 *	-3.002e-003 °		
27	727.00 *	0.6190 *	0.6194 *	-7.027e-002 *		
28	827.00 *	9.390e-002 '	9.394e-002 *	-4.777e-002 *		
29 30	927.00 *	1.950e-002 *	1.951e-002 *	-4.409e-002 *		
31	1027.0 ° 1127.0 °	5.160e-003 * 1.650e-003 *	5.159e-003 * 1.649e-003 *	2.318e-002 * 3.338e-002 *		
33 34 35 36 37 38 40 41 42 43 44 45 46 47 48 49 50 51 52 53 54 55 56 57 58 59 60 61 62 63 64 65 64 65						
65 66	Hyprotech Ltd.	HYSYS.Plant v2.	2.2 (Build 3806)	Page 6 of 6		

66 Hyprotech Ltd. HYSYS.Plant v2.2.2 (Build 3806) Page 6 of Licensed to: INL * Specified by user.

A.8 Hydrogenation Process with Co-electrolysis Electrolysis Power H2,CO,H2O Out Hydrogenation (0) (W) Hydrogenation Q 00 t Co-Electrolysis Calcs Recuperator 2 5 Total Power | 0.1985 kW 9 Co-Electrolysis Calcs Recuperator

Figure A - 14 Process flow diagram of hydrogenation process with co-electrolysis

2		INL		Case Name:	C:\NASA Final\Hydroger	nation w Co-Electrolysis	s.hsc		
3	HYPROTEC	Calgary, A	Alberta	Unit Set:	NASA				
5		CANADA		Date/Time:	Date/Time: Mon Aug 23 11:58:19 2010				
6	\A/	l-l l	0 (14-:	`					
7	vvor	кроок:	Case (Main	1)					
9				Streams					
10 11	Name		H2.CO.H2O Out		Oire Dire	9	00-t		
12	Name Vapour Fraction		1.0000	Sweep Gas In 1.0000	Circ Pwr	1.0000	OxygenOut 1.0000		
13	Temperature	(C)	800.00	705.29		800.00*	48.627		
14	Pressure	(kPa)	122.00	123.38		127.52	120.38		
15	Molar Flow	(gmole/h)	6.4603	3.4662e-009 °		6.4603	1.3021		
16	Mass Flow	(kg/d)	1.7029	2.4000e-009		2.7029	1.0000		
17	Liquid Volume Flow	(m3/h)	1.933e-004	1.156e-013		2.031e-004	3.662e-005		
18 19	Heat Flow	(kW)	-7.783e-002	2.041e-011	1.291e-003	-0.2605	2.474e-004		
20	Molar Enthalpy Name	(kJ/kgmole)	-4.337e+004 5r	2.120e+004 CO2 Cmp Pwr	CO2 In	-1.452e+005 Electrolysis Power	684.0 CO2, Water In		
21	Vapour Fraction		1.0000	CO2 Cmp Pwr	1.0000	Electrolysis Power	1.0000		
22	Temperature	(C)	427.79 *		21.111 *		705.29		
23	Pressure	(kPa)	131.90 '		131.00 *		126.14		
24 25	Molar Flow	(gmole/h)	6.4603 *		1.3022		6.5011		
25	Mass Flow	(kg/d)	2.7029		1.3754 *		2.7029		
26	Liquid Volume Flow	(m3/h)	2.031e-004		6.944e-005		1.882e-004		
27	Heat Flow	(kW)	-0.2864	3.442e-005	-0.1425	0.1918	-0.2605		
28	Molar Enthalpy	(kJ/kgmole)	-1.596e+005		-3.940e+005		-1.443e+005		
29	Name		Hi Temp Pwr	8	Hydrogenation Q	4	15		
30 31	Vapour Fraction	(0)		1.0000 725.07		1.0000 23.627	1.0000 350.00 *		
32	Temperature Pressure	(C) (kPa)		128.90		23.627 134.90 °	116.00		
33	Molar Flow	(gmole/h)		6.4603		1,3022	5.1581		
34	Mass Flow	(kg/d)		2.7029		1.3754	1.3275		
35	Liquid Volume Flow	(m3/h)		2.031e-004		6.944e-005	1.336e-004		
36	Heat Flow	(kW)	5.395e-003	-0.2659	-5.417e-002	-0.1425	-0.1541		
37	Molar Enthalpy	(kJ/kgmole)		-1.482e+005		-3.939e+005	-1.076e+005		
38	Name		Carbon Out	6	2	1	5		
39	Vapour Fraction		0.0000	1.0000	1.0000	1.0000	1.0000		
40	Temperature	(C)	350.00	452.79	376.94	563.79	427.79		
41 42	Pressure Molar Flow	(kPa)	116.00 1.3023	119.00 6.4603	131.90 5.1581	131.90 1.3022	131.90 6.4603		
43	Mass Flow	(gmole/h) (kg/d)	0.37540	1.7029	1.3275	1.3754	2.7029		
44	Liquid Volume Flow	(m3/h)	9.526e-006	1.933e-004	1.336e-004	6.944e-005	2.031e-004		
45	Heat Flow	(kW)	1.610e-003	-9.834e-002	-0.1528	-0.1336	-0.2864		
46	Molar Enthalpy	(kJ/kgmole)	4450	-5.480e+004	-1.067e+005	-3.693e+005	-1.596e+005		
47	Name		O2 Out						
48	Vapour Fraction		1.0000						
49	Temperature	(C)	800.00						
50	Pressure	(kPa)	123.38						
51 52	Molar Flow Mass Flow	(gmole/h) (kg/d)	1.3021 1.0000						
53	Liquid Volume Flow	(m3/h)	3.662e-005						
54	Heat Flow	(kW)	9.140e-003						
55	Molar Enthalpy	(kJ/kgmole)	2.527e+004						
56	,,			Compressors					
57				•	1				
58 59	Name Feed Pressure	(I-D-)	CO2 Comp 131.0 *	Circulator 116.0					
60	Product Pressure	(kPa) (kPa)	131.0	116.0 131.9					
61	Molar Flow	(gmole/h)	1.302	5.158					
62	Energy	(kW)	3.442e-005	1.291e-003					
63	Adiabatic Efficiency	()	75 *	75 *					
64	Polytropic Efficiency		75	75					
65									
66	Hyprotech Ltd.		HY	SYS.Plant v2.2.2 (Buil	d 3806)		Page 1 of 6		
	Licensed to: INL						* Specified by user.		

66 Hyprotech Ltd.
Licensed to: INL Page 1 of 6
* Specified by user.

2	INL		Case Name:	C:\NASA Final\Hydroger	nation w Co-Electrolysi	s.hsc
3	HYPROTECH CANADA	Alberta	Unit Set:	NASA		
5	CANADA		Date/Time:	Mon Aug 23 11:58:19 2	010	
6	Morlehoole	Coop (Main) (oontinus	رم. دها/		
7	Workbook:	Case (Main) (continue	ea)		
9			Composition			
10 11	Name	4	5	5r	8	9
12	Comp Mole Frac (H2O)	0.00000	0.32176	0.32175 *	0.32175	0.32175
13	Comp Mole Frac (Hydrogen)	0.00000	0.43082	0.43082 *	0.43082	0.43082
14	Comp Mole Frac (Oxygen)	0.00000	0.00000	0.00000 *	0.00000	0.00000
15	Comp Mole Frac (Argon)	0.00000	0.00000	0.00000 *	0.00000	0.00000
16	Comp Mole Frac (Nitrogen)	0.00000	0.00000	0.00000 *	0.00000	0.00000
17	Comp Mole Frac (CO2)	1.00000	0.24307	0.24307 *	0.24307	0.24307
18 19	Comp Mole Frac (CO)	0.00000	0.00005	0.00005	0.00005	0.00005
20	Comp Mole Frac (Methane)	0.00000	0.00430	0.00430 ° 0.00000 °	0.00430	0.00430
21	Comp Mole Frac (Carbon) Name	0.00000 CO2 In	0.00000 CO2, Water In	H2,CO,H2O Out	0.00000 O2 Out	0.00000 OxygenOut
22	Comp Mole Frac (H2O)	0.00000	0.40060	0.12019	0.00000	0.00000
23	Comp Mole Frac (H2O) Comp Mole Frac (Hydrogen)	0.00000 *	0.40060	0.12019	0.00000	0.00000
24	Comp Mole Frac (Oxygen)	0.00000	0.00000	0.00000	1.00000	1.00000
24 25	Comp Mole Frac (Argon)	0.00000	0.00000	0.00000	0.00000	0.00000
26	Comp Mole Frac (Nitrogen)	0.00000 *	0.00000	0.00000	0.00000	0.00000
27	Comp Mole Frac (CO2)	1.00000 *	0.15754	0.04151	0.00000	0.00000
28	Comp Mole Frac (CO)	0.00000 *	0.08719	0.20162	0.00000	0.00000
29	Comp Mole Frac (Methane)	0.00000 *	0.00114	0.00430	0.00000	0.00000
30	Comp Mole Frac (Carbon)	0.00000 *	0.00000	0.00000	0.00000	0.00000
31	Name	15	Carbon Out	6	2	1
32	Comp Mole Frac (H2O)	0.40299	0.00000	0.12019	0.40299	0.00000
33	Comp Mole Frac (Hydrogen)	0.53958	0.00000	0.63239	0.53958	0.00000
34	Comp Mole Frac (Oxygen)	0.00000	0.00000	0.00000	0.00000	0.00000
35	Comp Mole Frac (Argon)	0.00000	0.00000	0.00000	0.00000	0.00000
36	Comp Mole Frac (Nitrogen)	0.00000	0.00000	0.00000	0.00000	0.00000
37 38	Comp Mole Frac (CO2)	0.05198 0.00006	0.00000	0.04151	0.05198 0.00006	1.00000
39	Comp Mole Frac (CO) Comp Mole Frac (Methane)	0.0008	0.00000	0.20162 0.00430	0.00006	0.00000
40	Comp Mole Frac (Carbon)	0.00000	1.00000	0.00000	0.00000	0.00000
41	Comp woie Frac (Carbon)	0.00000			0.00000	0.00000
42			Heat Exchange	rs		
43	Name	Recuperator 1	Recuperator 2			
44	Duty (kW)	-8.893e-003	2.051e-002			
45	Tube Inlet Temperature (C)	800.0	427.8*			
46	Tube Outlet Temperature (C)	48.63	725.1			
47 48	Shell Inlet Temperature (C)	23.63	800.0			
48	Shell Outlet Temperature (C) LMTD (C)	563.8 92.86	452.8 45.38			
50	LMTD (C) UA (kJ/C-h)	0.3448	1.627			
51	Minimum Approach (C)	25.00	25.00			
52	(0)		ther Heat Exchar	agore		1
53		U	uiei neat Exchar	igers		
54	Name					
55	Number of Sides					
56 57	LMTD (C)					
57 58	UA (Calculated) (kJ/C-h)					
59	Hot Pinch Temperature (C) Cold Pinch Temperature (C)					
60	Minimum Approach (C)					
61	Exchanger Cold Duty (kW)					
62	(100)					
63						
64						
65						
66	Hyprotech Ltd.	HYS	SYS.Plant v2.2.2 (Buil	d 3806)		Page 2 of 6
	Licensed to: INL					 Specified by user.

_											
1	line.				Case Name:	C:\NASA Final\Hydroge	nation w C	o-Electrolysis	s.hsc		
3	INL Calgary, Alberta				Unit Set:	Unit Set: NASA					
5	CANADA				Date/Time:	Date/Time: Mon Aug 23 11:58:19 2010					
6											
7	Workbook: Case (Main) (continued)										
9 10	→ Pumpe										
11	Name										
12	Delta P	(kPa)									
13 14	Energy Feed Pressure	(kW)		\rightarrow							
15	Product Pressure	(kPa) (kPa)		\rightarrow							
16		(gmole/h)									
17	Adiabatic Efficiency	(%)									
18 19					Unit Ops						
20	Operation Name	Ope	ration Type	^	Feeds	Products		Ignored	Calc. Level		
21 22	Hi Temp Heater	Heater		8 Hi T	Temp Pwr	9		No	500.0 *		
23					Out	OxygenOut					
24	Recuperator 1	Heat Exc	hanger	4		1		No	500.0 *		
25	Recuperator 2	Heat Exc	hanner	5r		8		No	500.0 *		
26	recuperator 2	TIER LAC	nanger	_	CO,H2O Out		6		300.0		
27 28	M2	Mixer		1		5		No	500.0 °		
29				2	2 In	4					
30	CO2 Comp	Compressor		CO2 In CO2 Cmp Pwr				No	500.0 *		
31	Circulator	Compressor		15		2		No	500.0 *		
32	Circulator	Compres	501	Circ Pwr					300.0		
33					ep Gas In O2 Out						
34 35	High Temperature Co-Electro	Standard	Sub-Flowsheet	CO2, Water In Process Heat		H2,CO,H2O Out	No		2500 °		
36					ctrolysis Power						
37	Electrolysis Input and Output	Spreadsheet			,				500.0 *		
38	Co-Electrolysis Calcs	Spreadsh	Spreadsheet					No	500.0 *		
39						Carbon Out					
40 41	Hydrogenation	Equilibriu	m Reactor	Hyd	frogenation Q	15		No	500.0 *		
42	RCY	Recycle		5		Hydrogenation Q 5r		No	3500 *		
43				9		400					
44	Water Gas Shift	Gibbs Re	actor			CO2, Water In		No	500.0 *		
45								·			
46 47	Workb	ook:	High Ten	npe	erature Co	-Electrolys	IS (TE	² L2)			
48 49					Streams						
50	Name		Sweep Gas In @			Gas Products @TPL	Liquid @		Anode @TPL2		
51	Vapour Fraction	(2)	1.00		1.0000	1.0000		0.0000	1.0000		
52 53	Temperature Pressure	(C) (kPa)	705. 123.		800.00 123.38	800.00 ° 124.76		800.00 124.76	800.00 123.38		
54		(gmole/h)	3.4662e-0		1.3021	7.8032		0.00000	1.3021		
55	Mass Flow	(kg/d)	2.4000e-0		1.0000	2.7029		0.00000	1.0000		
56	Liquid Volume Flow	(m3/h)	1.156e-0		3.662e-005	2.530e-004		0.0000	3.662e-005		
57	Heat Flow	(kW)	2.041e-0		9.140e-003	-7.488e-002		0.0000	9.140e-003		
58	Molar Enthalpy (k.	J/kgmole)	2.120e+0	04	2.527e+004	-3.455e+004	-3	.455e+004	2.527e+004		
59 eo											
61											
60 61 62 63 64											
63											
65	11			1 13	VO DI	10000			B		
66	Hyprotech Ltd.			HYS	YS.Plant v2.2.2 (Build	a 3806)			Page 3 of 6		

1					Casa Name (CANACA Eigent Lide		a Flastraturi			
2	Calgary, Alberta				Case Name: C:\NASA Final\Hydrogenation w Co-Electrolysis.hsc						
3					Unit Set: NASA						
5	pr.		Date/Time: Mon Aug 23 11:58:19 2010								
6 7 8	Workb	ook:	High Tem	per	ature Co	-Electrolys	is (TI	PL2) (c	ontinued)		
9 10	Streams (continued)										
11	Name		H2,CO,H2O Out @	20TF Cat	thode @TPL2	2 @TPL2	CO2, W	ater In @TPL	Electrolysis Heatiing		
12	Vapour Fraction		1.000	0	1.0000	0.0000		1.0000			
13	Temperature	(C)	800.0		* 00.008	800.00		705.29			
14	Pressure	(kPa)	122.0		123.38	122.00		126.14			
15		(gmole/h)	6.460		6.5011	0.00000		6.5011			
16 17	Mass Flow	(kg/d)	1.702		1.7029	0.00000	ļ .	2.7029			
18	Liquid Volume Flow	(m3/h)	1.933e-00		2.164e-004	0.0000					
19	Heat Flow	(kW)	-7.783e-00	_	-8.402e-002 0.0000		1	-0.2605	0.1856		
20	Molar Enthalpy (k. Name	J/kgmole)	-4.337e+00 Process Heat @T		ft Reactor 2 Heat	653e+004 -4.337e+004 actor 2 Heat Electrolysis Power @		.443e+005			
21	Vapour Fraction		Process neat @1	PLI SIII	it Reactor 2 neat	Electrolysis Power @	4				
22	Temperature	(C)									
23	Pressure	(kPa)									
24		(gmole/h)									
25	Mass Flow	(kg/d)	_	_							
26	Liquid Volume Flow	(m3/h)		_							
27	Heat Flow	(kW)	-2.272e-00	_	6.193e-003	0.1918					
28		J/kgmole)		_							
29	,	g,			· · · · · · · · · · · · · · · · · · ·						
30 31	Name		Sweep Gas In @T		Composition 2 Out @TPL2 Gas Products @TPL Liquid @TI			ATDL 2	Anode @TPL2		
32	Comp Mole Frac (H2O)		0.0000		0.00000	0.00000	, Liquiu @	0.00000	0.00000		
33	Comp Mole Frac (Hydrogen)		0.0000	_	0.00000	0.62829		0.62829	0.00000		
34	Comp Mole Frac (Oxygen)		0.21000		1.00000	0.16687		0.16687	1.00000		
35	Comp Mole Frac (Oxygen)		0.00000		0.00000	0.00000		0.00000	0.00000		
36	Comp Mole Frac (Nitrogen)		0.7900	_	0.00000	0.00000		0.00000	0.00000		
37	Comp Mole Frac (CO2)		0.0000		0.00000	0.13125		0.13126	0.00000		
38	Comp Mole Frac (CO)		0.0000		0.00000	0.07264		0.07264	0.00000		
39	Comp Mole Frac (Methane)		0.0000	0	0.00000	0.00095		0.00095	0.00000		
40	Comp Mole Frac (Carbon)		0.0000	0	0.00000	0.00000		0.00000	0.00000		
41	Name		H2,CO,H2O Out @	TF Ca	hode @TPL2	2 @TPL2	CO2, W	ater In @TPL			
42	Comp Mole Frac (H2O)		0.1201	9	0.00000	0.12019		0.40060			
43	Comp Mole Frac (Hydrogen)		0.6323	9	0.75413	0.63239		0.35353			
44	Comp Mole Frac (Oxygen)		0.0000		0.00000	0.00000	0.00000				
45	Comp Mole Frac (Argon)		0.0000	0	0.00000	0.00000	0.00000				
46	Comp Mole Frac (Nitrogen)		0.0000	0	0.00000	0.00000	0.0000				
47	Comp Mole Frac (CO2)		0.0415	1	0.15754	0.04151	0.15754				
48	Comp Mole Frac (CO)		0.2016	2	0.08719	0.20162		0.08719			
49	Comp Mole Frac (Methane)		0.0043	0	0.00114	0.00430	0.00114				
50	Comp Mole Frac (Carbon)		0.0000	0	0.00000	0.00000		0.00000			
51 52					Unit Ops						
53	Operation Name	Öne	eration Type		Feeds	Products		Ignored	Calc. Level		
54	Temp Average ASR @TPL2	Spreadsh			, 5545	1,1000010		Yes	500.0		
55	Electrolysis Spreadsheet @							No	500.0		
56	Steam Electrolysis @TPL2	Spreadsh						No	500.0		
57	CO2 Electrolysis @TPL2	Spreadsh						No	500.0		
58 59	Sweep Gas/O2 Mixer @TPL	Mixer		Anode (_	O2 Out @TPL2		No	500.0		
60				Sweep Gas In @TPL2 CO2, Water In @TPL2		Liquid @TPL2					
61 62	Isothermal Electrolysis @TP	TP Conversion Reactor		Electrol	ysis Heatiing @TP	L2 Gas Products @TPL2 Electrolysis Heatiing @TPL2		No	500.0		
63	Electrodes @TPL2	Compone	Gas Gas		oducts @TPL2	Cathode @TPL2		No	500.0		
			Ориссі			Anode @TPL2					
$\overline{}$	AD L1 @TDL2	Adimet	1					Voc	2500		
64 65	ADJ-1 @TPL2 Hyprotech Ltd.	Adjust		HVSVS	Plant v2.2.2 (Build	1 3806)		Yes	9500 Page 4 of 6		

1	<u></u>		Case Name: C:V	NASA Finally	drogenation w.C.	o-Flectrolysis b	ac.					
2	INL											
4	HYPROTECH	Calgary, Alberta CANADA		Unit Set: NASA								
5 6	r:		Date/Time: Mo	n Aug 23 11:5	B:19 2010							
7	Workb	ook: High T	emperature Co-E	Electro	lysis (TF	PL2) (co	ntinued)					
9 10			Unit Ops (continue	d)								
11	Operation Name	Operation Type	Feeds		ducts	Ignored	Calc. Level					
12 13 14	Water gas Shift @TPL2	Gibbs Reactor	Cathode @TPL2 Shift Reactor 2 Heat @TPL2		Out @TPL2 or 2 Heat @TPL2	No	500.0 *					
15	SET-1 @TPL2	Set				No	500.0 *					
16 17	SET-3 @TPL2 SET-2 @TPL2	Set Set				No No	500.0 °					
18 19 20 21	Conversion: 2CO2=2CO+O2											
22			STOICHIOMETRY									
23 24	CO2 Compone	nt	Mole Weight	44.010		Stoichiometric C	oett. -2 *					
25	CO			28.011			2*					
26 27	Oxygen			32.000			1*					
27 28												
29	Balance	e Error: 0.0000		Rea	ction Heat: 2.8	32e+005 kJ/kgn	nole					
30 31			BASIS									
32	Base Component: CO2	2	Conversion Percent: 100.00		Reaction	Phase: Overa	ill					
33 34			PARAMETERS									
35 36 37	Conv	ersion: 2H2	O=2H2+O2									
38 39			STOICHIOMETRY									
40	Compone	nt	Mole Weight			Stoichiometric C	oeff.					
41	H2O			18.015			-2 *					
42 43	Hydrogen Oxygen			2.016 32.000			2°					
44												
45 46	Palana	- E 0.0000		Page	ction Heat: 2.4	10 a + 00 E 4 11 4 mm	and a					
47	Dalance	e Error: 0.0000	BASIS	Rea	ction neat: 2.4	TUE+UUS KJ/Kgri	lole					
48 49	Base Component: H2C		Conversion Percent: 90.00		Penation	Phase: Overa	.u					
50	Base Component. H2C	,	PARAMETERS		Reaction	Filase. Overa						
51 52			FARAMETERS									
51 52 53 54 55	Equi	librium: Hyd	Irogenation									
56			STOICHIOMETRY									
57	Compone		Molecular Weight		Sto	ichiometric Coe						
58 59		CO Hydrogen		28.01 2.016			-1 °					
60		H2O		18.02			1.					
61		Carbon		12.01			1*					
62 63	Balance	Error: 0.0000		Pos	ction Heat : -1.3	104e+005 b 10	mole					
64	Daidnce	EITOI , 0.0000		Real	mon neat1.3	rogerous kurkgi	IIME					
65 66	Hyprotech Ltd.		HYSYS.Plant v2.2.2 (Build 3	806)			Page 5 of 6					
ت	Licensed to: INL		, , , o , o , , o , o , o , o , o , o ,	,			* Specified by user.					

1				Case Nr	- C:\NAC	A Finall-Lydrogonation w	Co. Electrolys	ic hee		
2	INL Calgary, Alberta				Case Name: C:\NASA Final\Hydrogenation w Co-Electrolysis.hsc Unit Set: NASA					
4		Calgary, Alberta CANADA	ı							
5	r:			Date/Tir	ne: Ivion Au	ug 23 11:58:19 2010				
7	Equilibrium: Hydrogenation (continued)									
9	BASIS									
11 12	Racis Phase Approach Min. Temp Max. Temp							Max. Temp (C)		
13	Activity		VapourPhase	1			3.15			
14 15				PARAM	ETERS					
16 17			;	Source : K	Vs. T Table					
18	Coeff A			-16.53	R2			1.000000 *		
19	Coeff B			1.582e+004	T High					
20 21	Coeff C Coeff D			6.290e-002 -3.147e-005	T Low					
22	COGII D			-J. 1476-003						
23	Temperature		Keq			KCalc	Pero	centage Error		
24	(C)									
25		5.000 *		1.050e+016 *		1.050e+016 *		-1.546e-003 *		
26		27.00 *		1.420e+010 *		1.420e+010 *		1.873e-002 *		
27 28		27.00 ° 27.00 °		5.280e+006 * 2.740e+004 *		5.285e+006 ° 2.736e+004 °		-8.965e-002 * 0.1553 *		
29		27.00 *		637.0 '		637.4 *		-5.515e-002 *		
30		27.00 *		38.00 *		38.01 *		-3.314e-002 *		
31		27.00 *		4.240 *		4.242 *		-5.571e-002 *		
32	7	27.00 *		0.7340 *		0.7341 "		-1.337e-002 °		
33		27.00 *		0.1750 *				0.1466 *		
34		27.00 *		5.280e-002 *				-6.267e-002 *		
35 36		027.0 *		1.920e-002 *		1.920e-002 *		2.720e-003 *		
37		127.0 ° 227.0 °		8.060e-003 * 3.800e-003 *		8.062e-003 * 3.800e-003 *		-2.036e-002 * 7.913e-003 *		
38	'	227.0		3.0000-003		5.0000-005		7.0100-000		
39										
40										
41										
42										
43										
45										
46										
47										
48										
39 40 41 42 43 44 45 46 47 48 49 50										
52										
53										
54										
55										
56										
57										
59										
60										
61										
62										
63										
51 52 53 54 55 56 57 58 60 61 62 63 64 65										
65 66	Hyprotech Ltd.		Ln	YSYS.Plant v2.	2.2 (Brilly 2000	3)		Page 6 of 6		
00	riyprotecti Ltd.		Н	1010.Flami VZ.	4.4 (Dullu 3600	7)		rage o oi o		

66 Hyprotech Ltd. HYSYS.Plant v2.2.2 (Build 3806) Page 6 of
Licensed to: INL * Specified by user.