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

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March 2010

Idaho National Laboratory

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High Temperature Electrolysis

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March 2010

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SUMMARY

NASA has been evaluating two closed-loop atmosphere revitalization architectures based on Sabatier and Bosch carbon dioxide, CO_2, reduction technologies. The CO_2 and steam, H_2O, 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 CO_2 and H_2O co-electrolysis process to produce oxygen and syngas (carbon monoxide, CO and hydrogen, H_2 mixture) for terrestrial (energy production) application. The technology is a combined process that involves steam electrolysis, CO_2 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, O_2, 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 CO_2 supply and constant O_2 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.

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Mathematical Analysis of High-Temperature Co-electrolysis 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 CO_2 reduction technologies. Schematics of the Sabatier and Bosch concepts are shown in Figures 1 and 2 respectively.

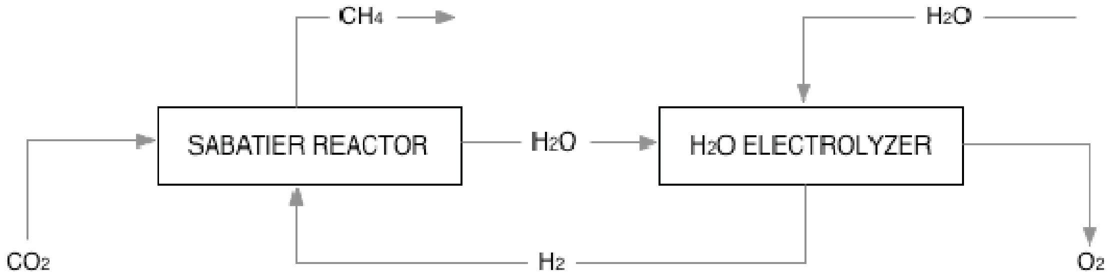


Figure 1 Sabatier process for atmosphere revitalization

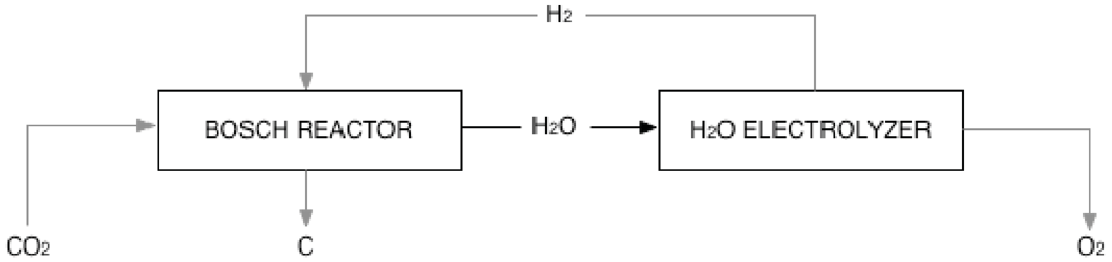


Figure 2 Bosch process for atmosphere revitalization

The CO_2 and H_2O 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 CO_2 and H_2O co-electrolysis process to produce oxygen and syngas (CO and H_2 mixture) for terrestrial (energy production) application. The technology is a combined process that involves steam electrolysis, CO_2 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 CO_2 and H_2O co-electrolysis concept in conjunction with the methanation reactor is shown in Figure 3.

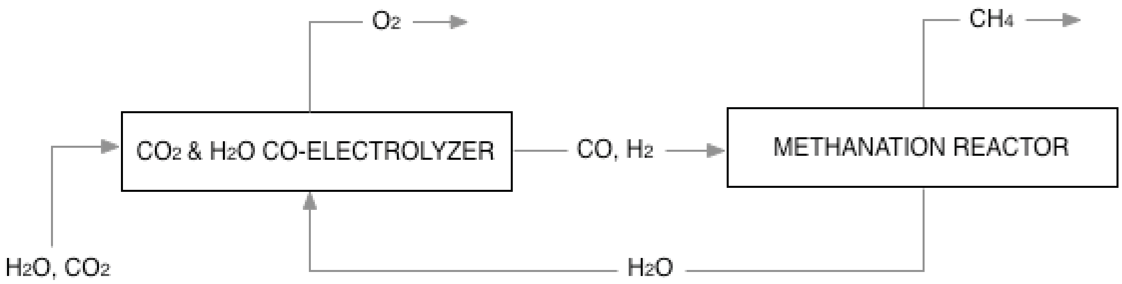


Figure 3 Co-electrolysis process for atmosphere revitalization

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 H_2O and CO_2 in terms of electrical efficiency. Compared to pure CO_2 electrolysis, co-electrolysis using a solid-oxide cell utilizes considerably less electrical energy (only as much as the H_2O 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, CH_4. 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 CO_2). A mathematical analysis is being performed under this project to evaluate INL's co-electrolysis process as a CO_2 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 CO_2 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 CO_2 from a compressor. One example of NASA's potential atmosphere revitalization architecture is shown in Figure 4.

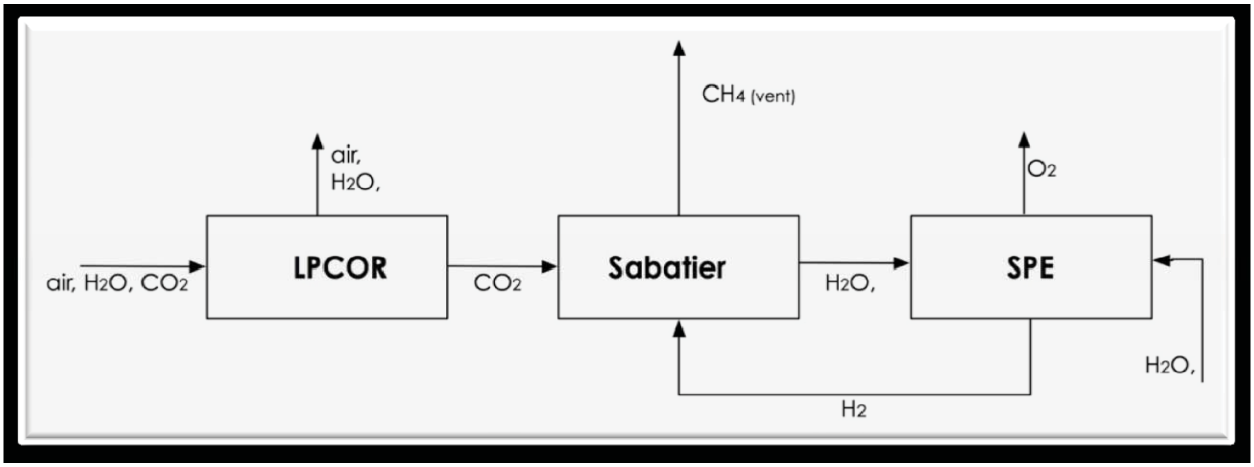


Figure 4 Currently considered CO2 reduction process for closed-loop life support, by NASA

The metabolic CO_2 from the cabin is removed and compressed using the LPCOR (Low-Power CO_2 Removal) technology and is delivered to a Sabatier reactor. Products of the Sabatier reaction (CH_4 and H_2O) are separated, H_2O is directed to an SPE (solid polymer electrolyte) water electrolysis unit, and CH_4 is vented (or stored for fuel). The oxygen from the electrolysis unit is released to the cabin and the H_2 is recycled to the Sabatier reactor.

If the Sabatier and SPE processes are replaced with the CO_2 and H_2O co-electrolysis process in the atmosphere revitalization scheme, additional downstream processors have to be implemented to recover and recycle H_2 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.

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

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

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

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

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.

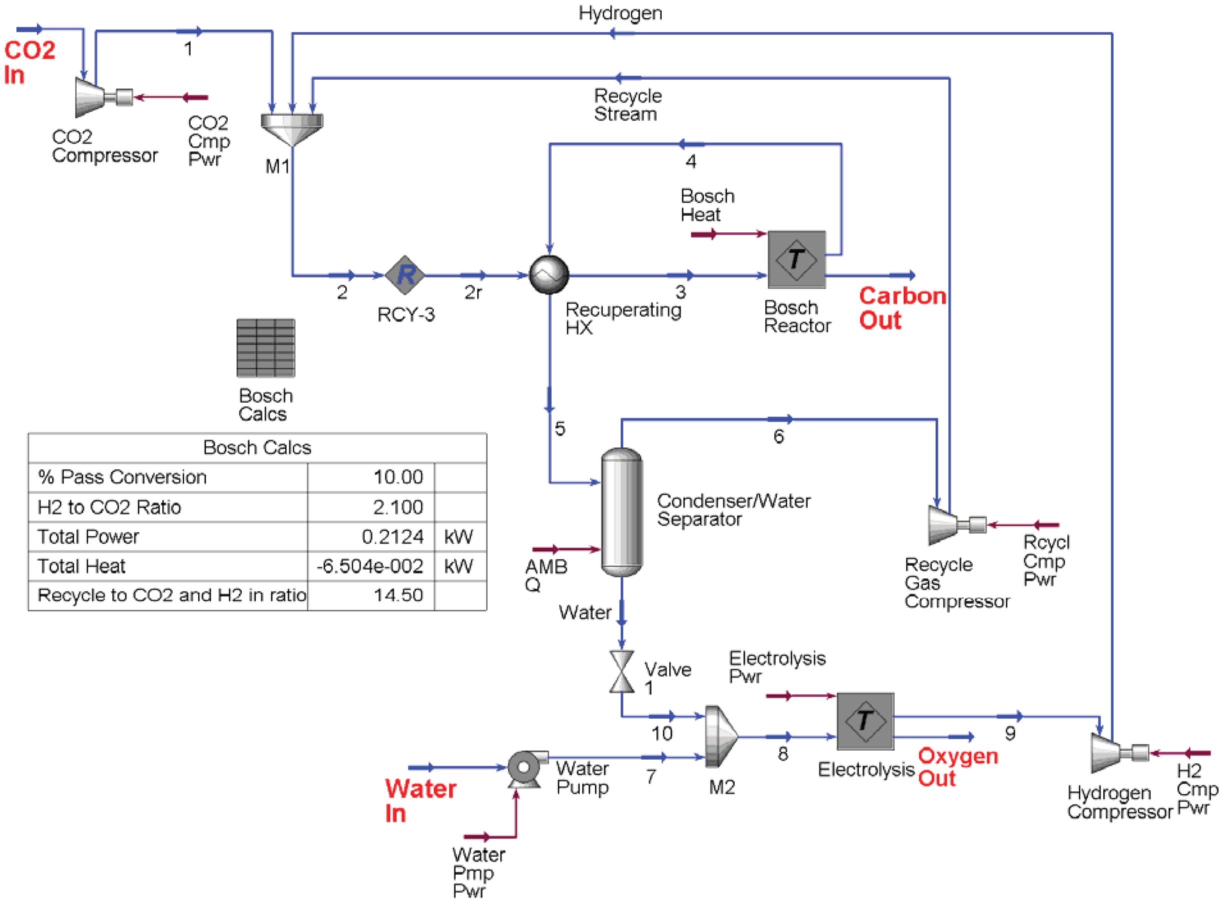
The SPE electrolysis process is modeled as a conversion reactor that splits 100% of the water coming in based on the following equation, Figure 7.

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

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.



Bosch Calcs		
% Pass Conversion	10.00	
H2 to CO2 Ratio	2.100	
Total Power	0.2124	kW
Total Heat	-6.504e-002	kW
Recycle to CO2 and H2 in ratio	14.50	

Figure 5 Process flow diagram of Bosch process

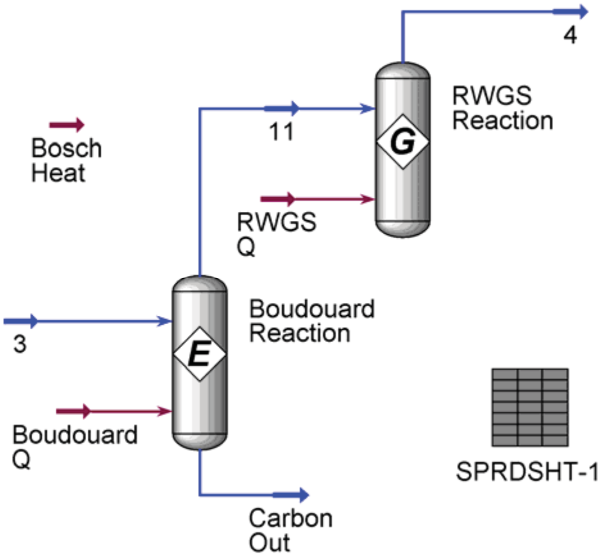


Figure 6 Process flow diagram of Bosch reactor

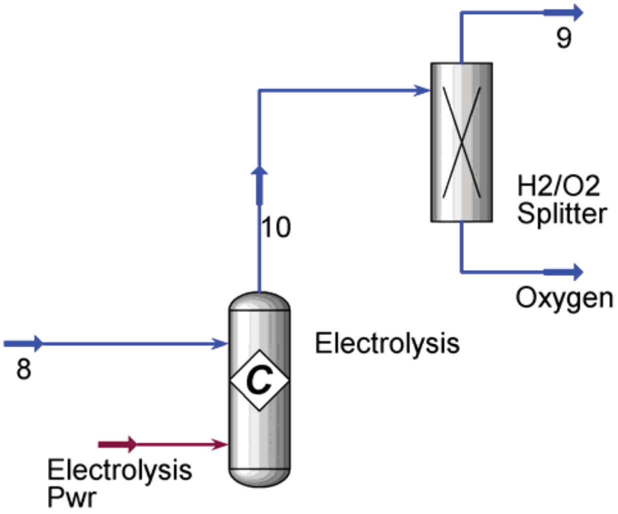
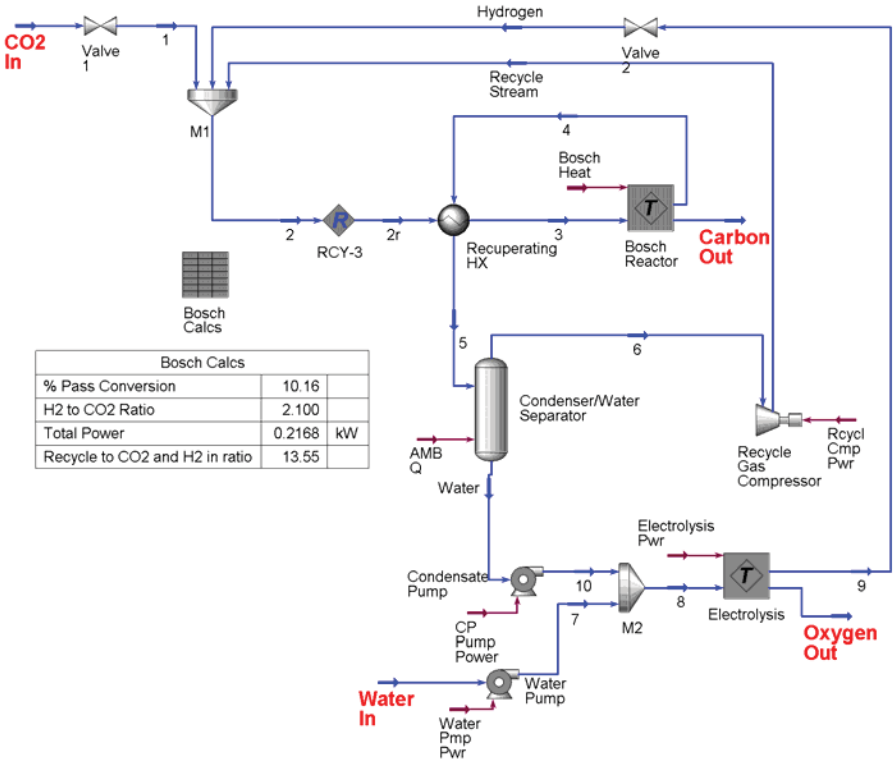
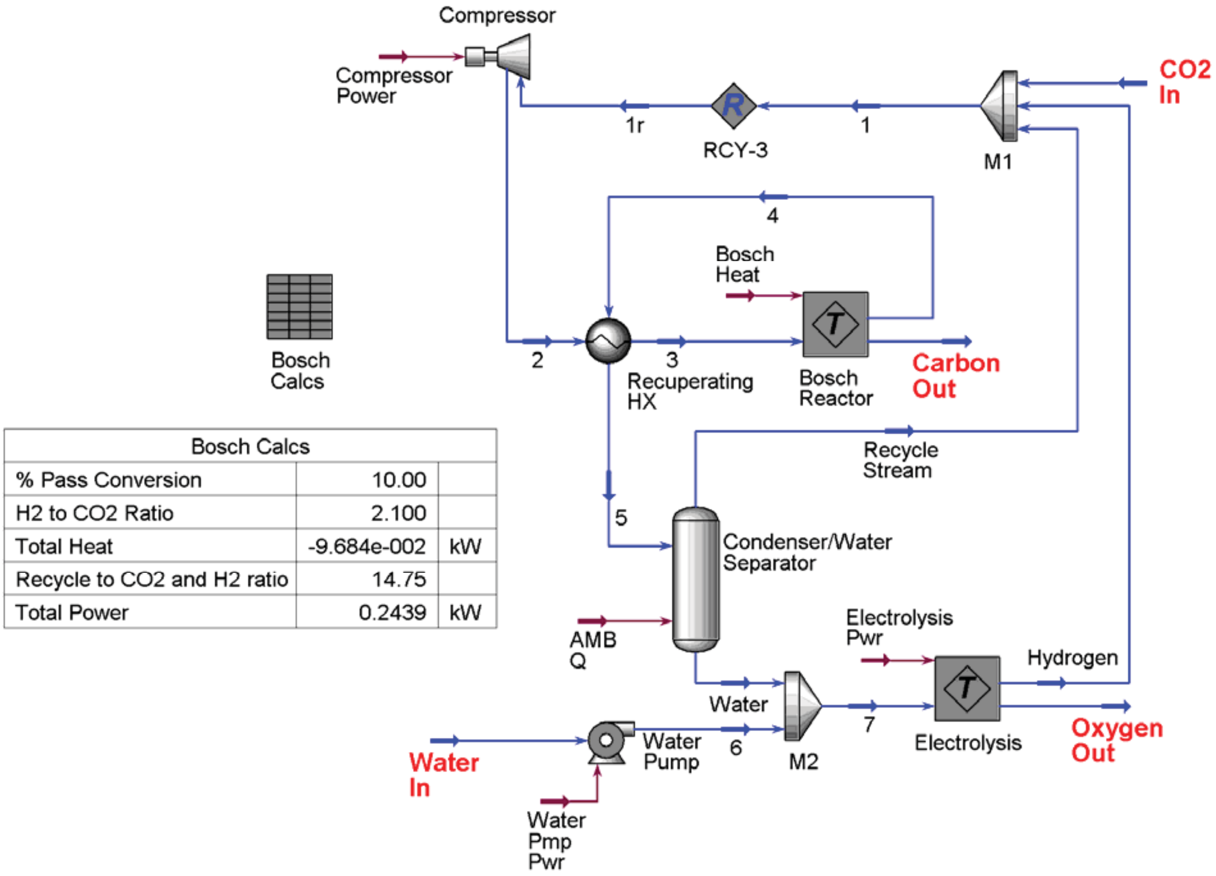


Figure 7 Process flow diagram of electrolysis module



Bosch Calcs		
% Pass Conversion	10.16	
H2 to CO2 Ratio	2.100	
Total Power	0.2168	kW
Recycle to CO2 and H2 in ratio	13.55	

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



Bosch Calcs		
% Pass Conversion	10.00	
H2 to CO2 Ratio	2.100	
Total Heat	-9.684e-002	kW
Recycle to CO2 and H2 ratio	14.75	
Total Power	0.2439	kW

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.

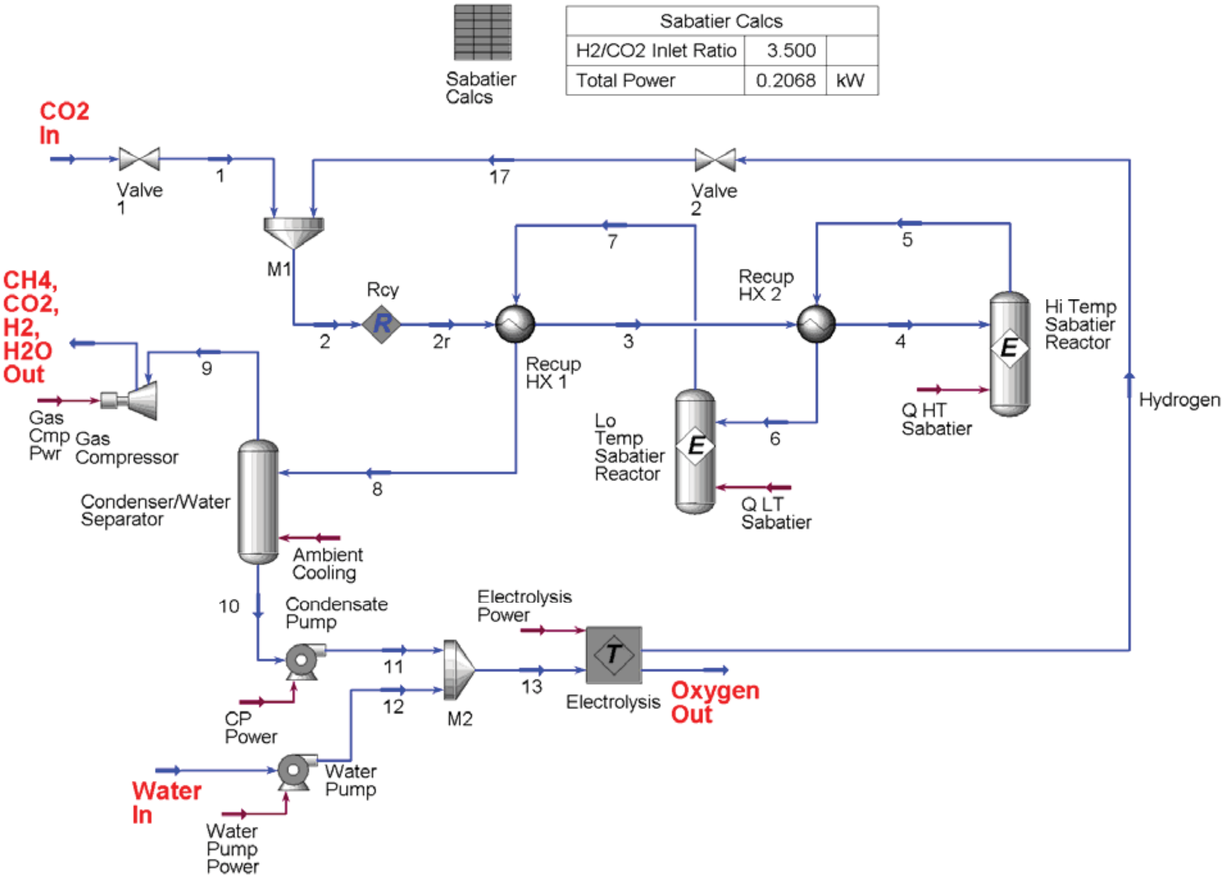


Figure 10 Process flow diagram of base Sabatier process

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 CO_2-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:

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

where the $y_{0,j}$ values represent the cold inlet mole fractions of CO, CO_2, H_2, and H_2O, 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 $y_{1,j}$ values. There are three governing chemical balance equations for carbon, hydrogen, and oxygen corresponding to Eqn. (5):

$$y_{0,CO} + y_{0,CO2} = y_{1,CO} + y_{1,CO2} \tag{6}$$

$$2y_{0,H2} + 2y_{0,H2O} = 2y_{1,H2} + 2y_{1,H2O} \tag{7}$$

$$y_{0,CO} + 2y_{0,CO2} + y_{0,H2O} = y_{1,CO} + 2y_{1,CO2} + y_{1,H2O} \tag{8}$$

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

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

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:

$$V_N = \frac{-\Delta G_{f,H_2O}(T)}{2F} - \frac{R_u T}{2F}\ln\left[\left(\frac{y_{1,H2O}}{y_{1,H2}\,y_{O2}^{1/2}}\right)\left(\frac{P}{P_{std}}\right)^{-1/2}\right] = \frac{-\Delta G_{f,CO_2}(T)}{2F} - \frac{R_u T}{2F}\ln\left[\left(\frac{y_{1,CO2}}{y_{1,CO}\,y_{O2}^{1/2}}\right)\left(\frac{P}{P_{std}}\right)^{-1/2}\right] \tag{10}$$

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 CO_2-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 CO_2/steam mixture. Accordingly, the oxygen balance equation becomes:

$$y_{1,CO} + 2y_{1,CO2} + y_{1,H2O} = y_{2,CO} + 2y_{2,CO2} + y_{2,H2O} + \Delta n_O \tag{11}$$

where Δn_O is the relative molar rate of monatomic oxygen removal from the CO_2/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-CO_2 electrolysis, the thermal neutral voltage is given by

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

where $\Delta H_{R,j}(T)$ is the enthalpy of reaction for electrolysis of pure component j (H_2O or CO_2) at temperature T. At 800°C, $V_{tn,H2O} = 1.29$ V and $V_{tn,CO2} = 1.46$ 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 CO_2 and CO, the co-electrolysis thermal neutral voltage will be closer to the pure-CO_2 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 CO_2), a thermal neutral voltage value of ~1.34 V is typical. The energy equation for the co-electrolysis process can be written as:

$$\dot{Q} - \dot{W} = \sum_P \dot{N}_i [\Delta H^o_{f_i} + H_i(T_P) - H^o_i] - \sum_R \dot{N}_i [\Delta H^o_{f_i} + H_i(T_R) - H^o_i] \tag{14}$$

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, $\Delta H^o_{f_i}$ is the standard-state enthalpy of formation of each reactant or product and $H_i(T) - H^o_i$ 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:

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

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:

$$\overline{V}_N(T_P) = \frac{1}{2F(T_P - T_R)(y_{2,O_2} - y_{1,O_2})[y_{2,H_2}(T_P) - y_{1,H_2}]} \times$$

$$\int_{T_R}^{T_P} \int_{y_{1,O2}}^{y_{2,O2}} \int_{y_{1,H2}}^{y_{2,H2}(T_P)} \Delta G_{R,H_2O}(T) + R_u T \ln\left(\frac{1 - y_{H_2} - y_{0,CO_2} - y_{N_2}}{y_{H_2} y_{O_2}^{1/2}} \right) dy_{H_2}\, dy_{O_2}\, dT \tag{17}$$

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).

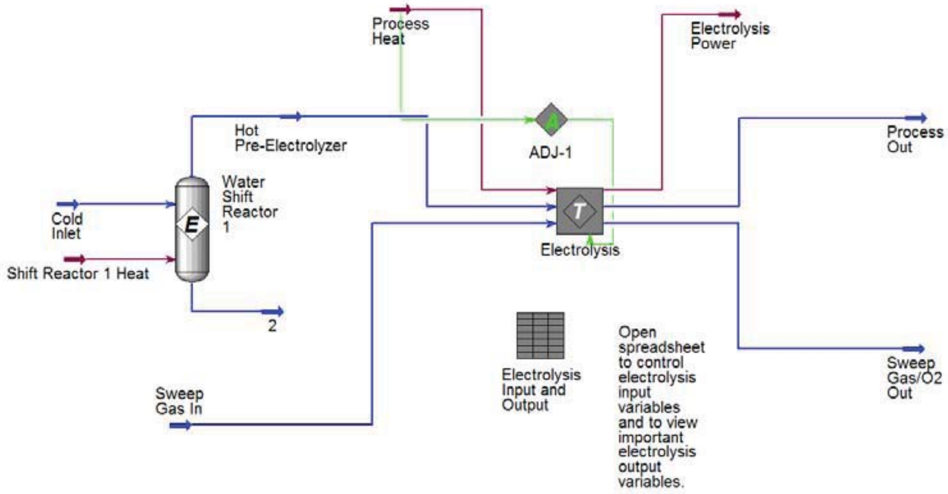
The solution methodology described above can be applied to any specified electrolyzer heat loss or gain. For adiabatic operation, $Q = 0$. Alternately, if the heat loss or gain from the operating electrolyzer is known from a separate heat transfer analysis for a given operating point, the value of that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



Open spreadsheet to control electrolysis input variables and to view important electrolysis output variables.

Figure 11 Process flow diagram external to the electrolysis module

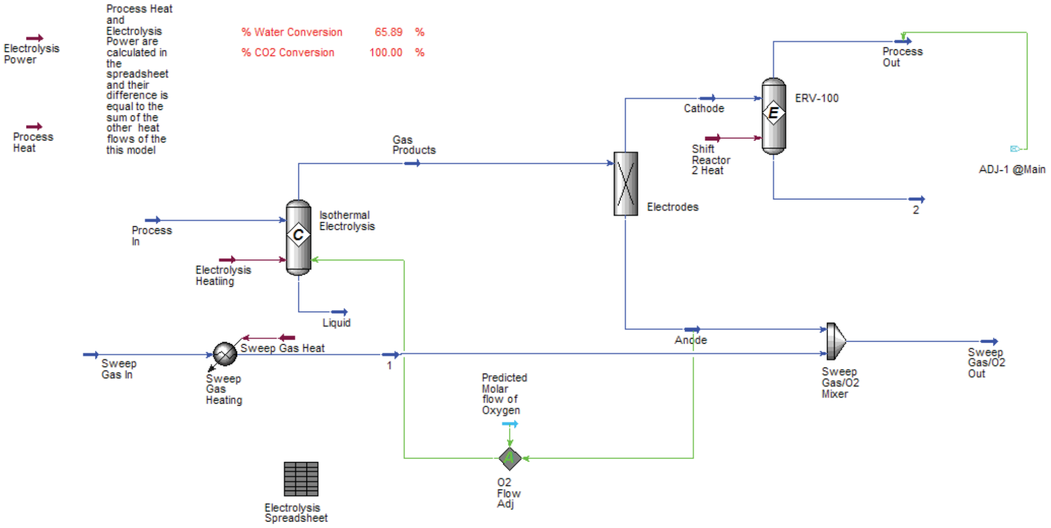


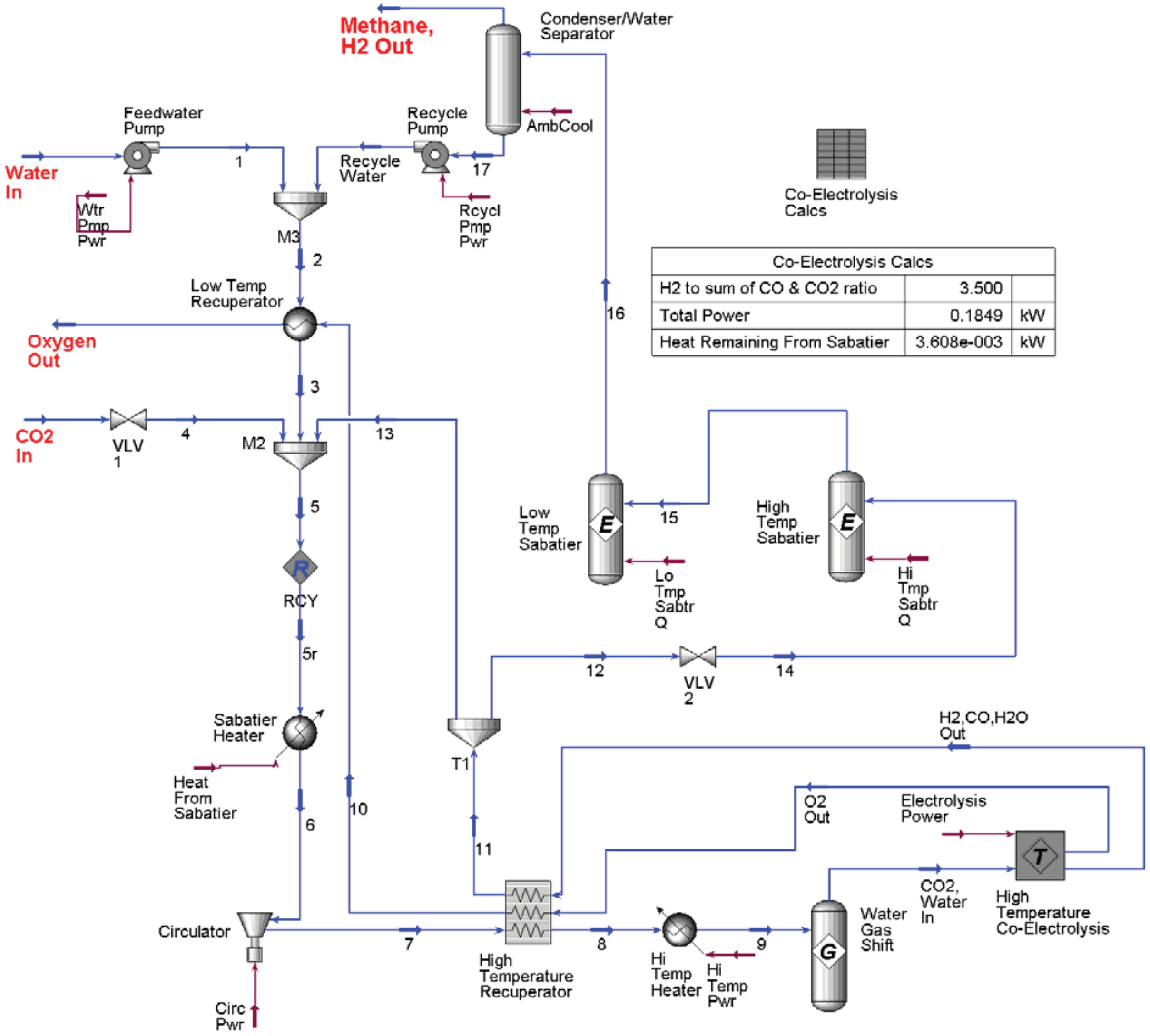
Figure 12 Process flow diagram for electrolysis module

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 CO_2, the reactor will calculate the heat of reaction. The percent conversion of steam and/or CO_2 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

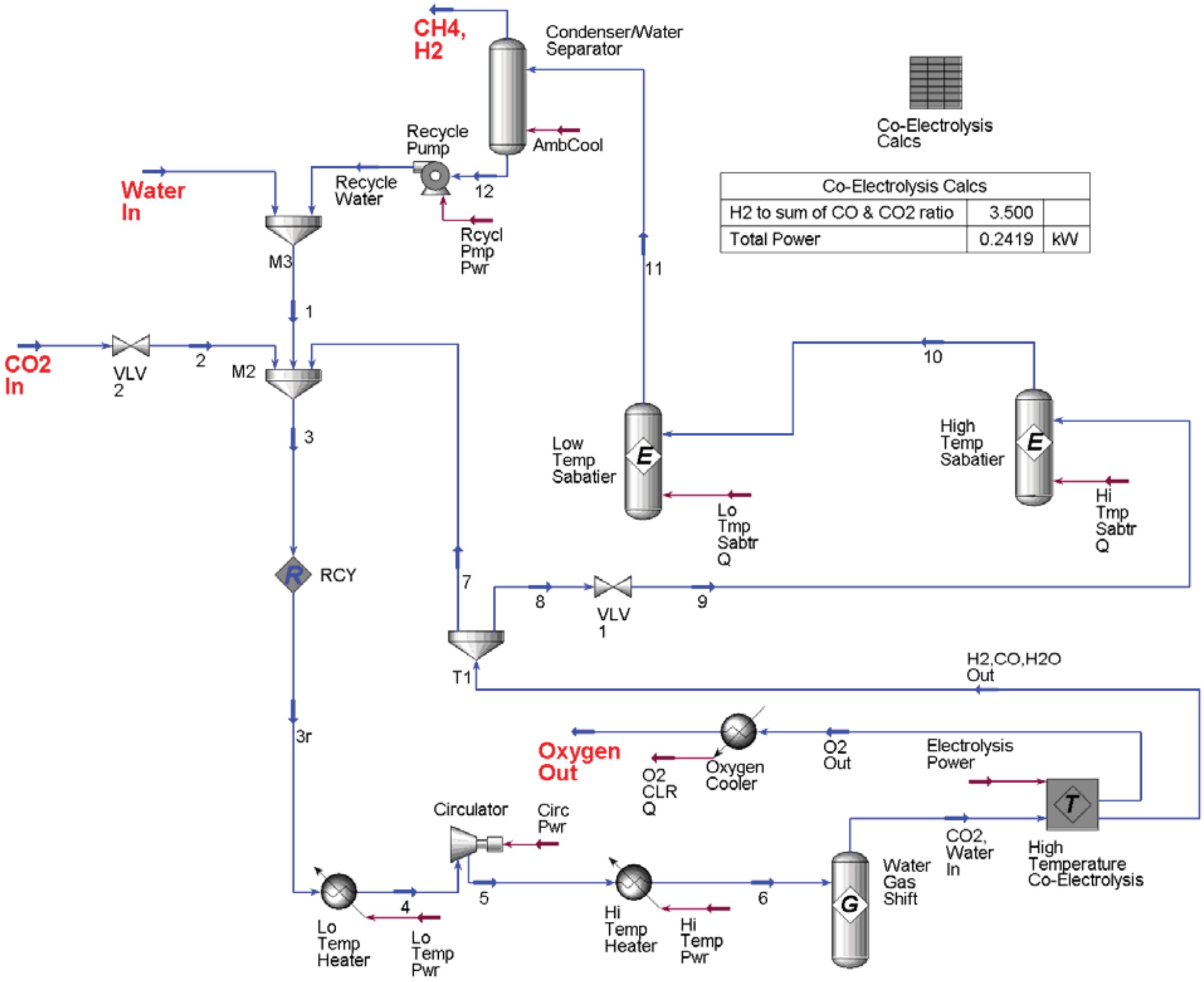
The Sabatier process model was modified by removing the electrolysis module and replacing it with the co-electrolysis module. The overall process was modified as well in that water is mixed with the incoming carbon dioxide before the co-electrolysis process, see Figure13. Recycled water is combined with 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.



Co-Electrolysis Calcs		
H2 to sum of CO & CO2 ratio	3.500	
Total Power	0.1849	kW
Heat Remaining From Sabatier	3.608e-003	kW

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.



Co-Electrolysis Calcs		
H2 to sum of CO & CO2 ratio	3.500	
Total Power	0.2419	kW

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.

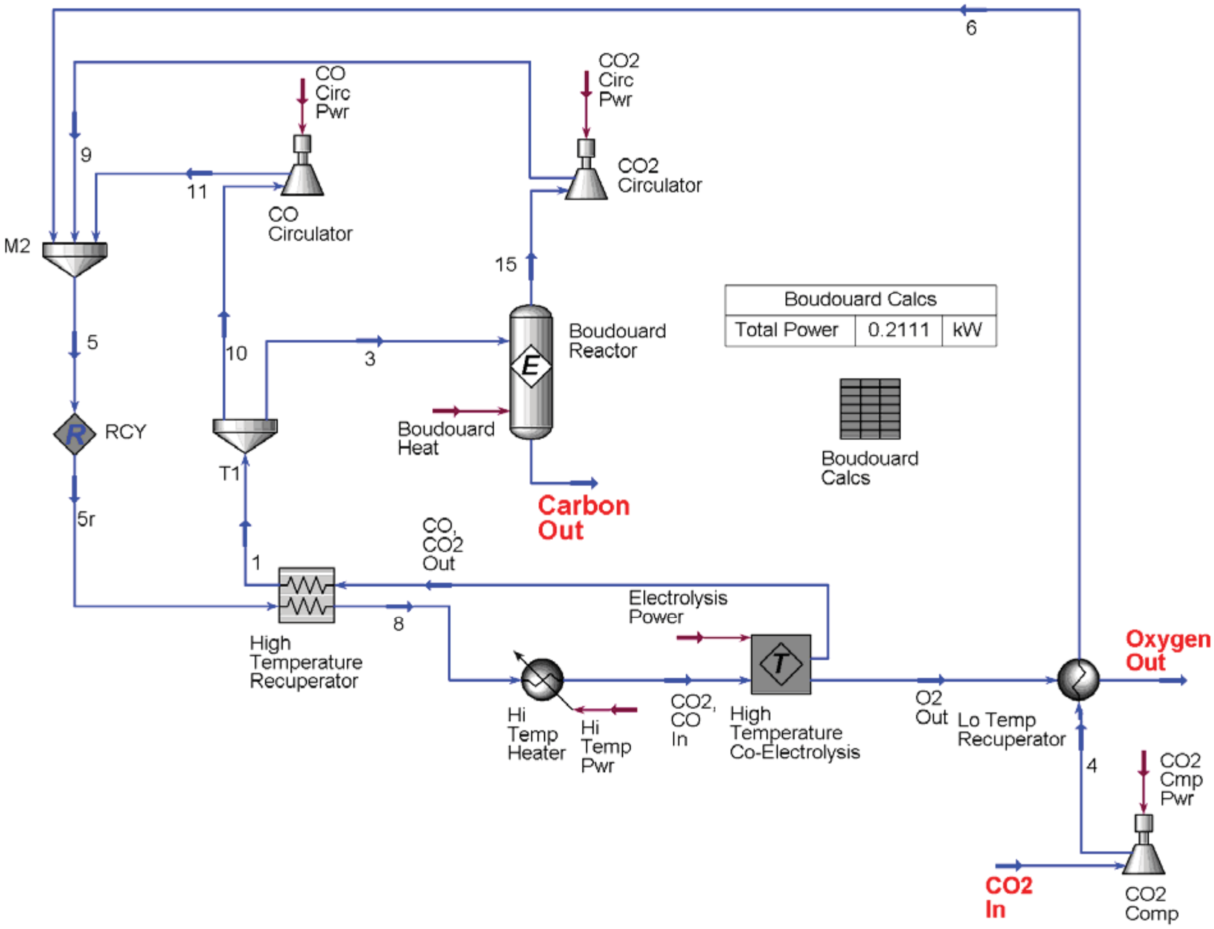


Figure 15 Process flow diagram of Boudouard process with co-electrolysis

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.

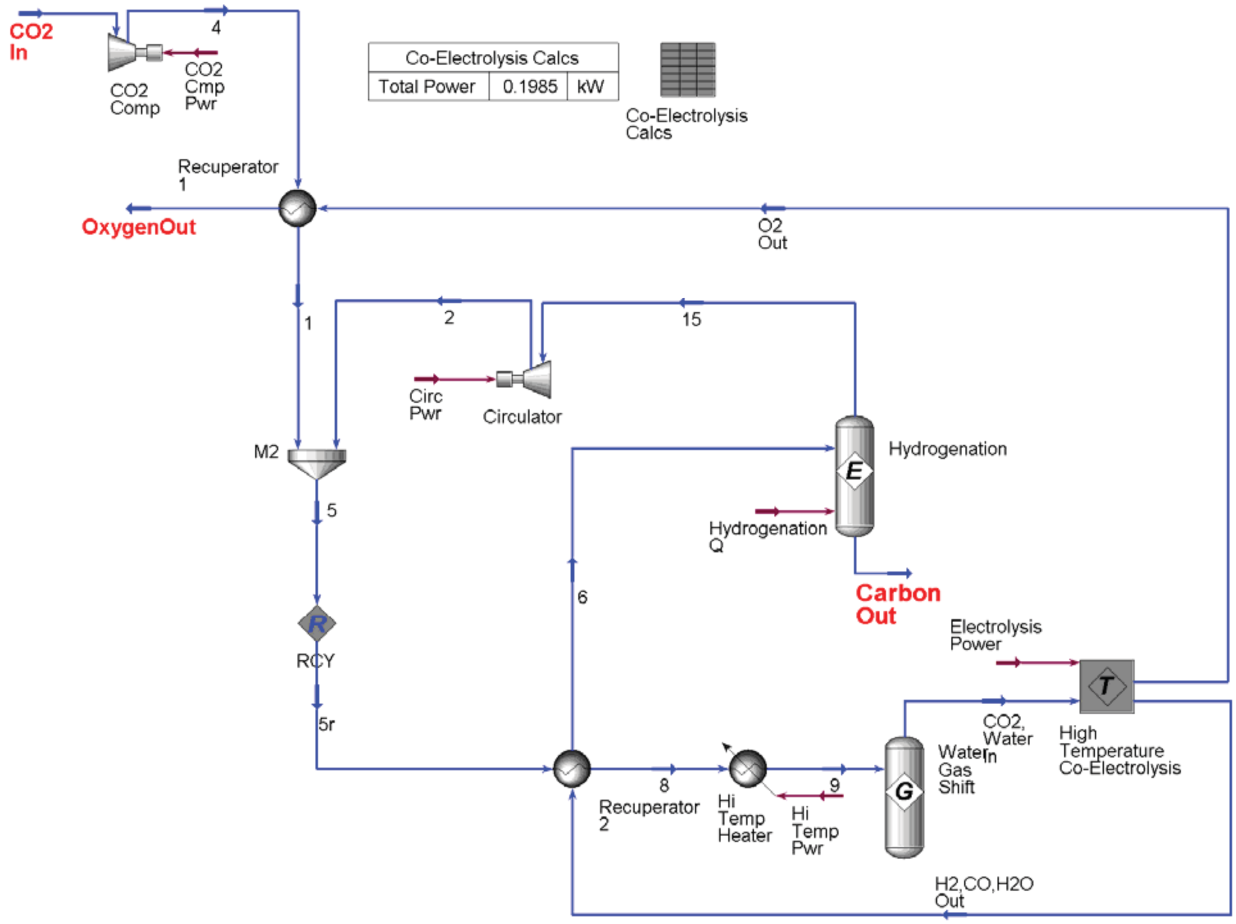


Figure 16 Process flow diagram of hydrogenation process with co-electrolysis

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 CO_2 are the Boudouard with co-electrolysis and Hydrogenation with co-electrolysis processes which also have no water input. The Bosch processes have slightly less CO_2 flows but also have small amounts of water. The lowest CO_2 flow rates are the Sabatier processes with and without co-electrolysis, but they also have the highest water flow rates. The CO_2 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 CO_2 which requires more power to split than water.

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

	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

	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	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 CO_2 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

	Condensers		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

	Condensers		Reactors		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	C	CO	CO_2	CH_4	Total	C	CO	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 (gmole/hr)					Carbon Out %			
Bosch Process with 3 Compressors	CO_2	C	CO	CO_2	CH_4	Total	C	CO	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 CO_2. If the fuel cell is operated in the electrolysis mode, the names and function of the electrodes are reversed as shown in Figure 17a.

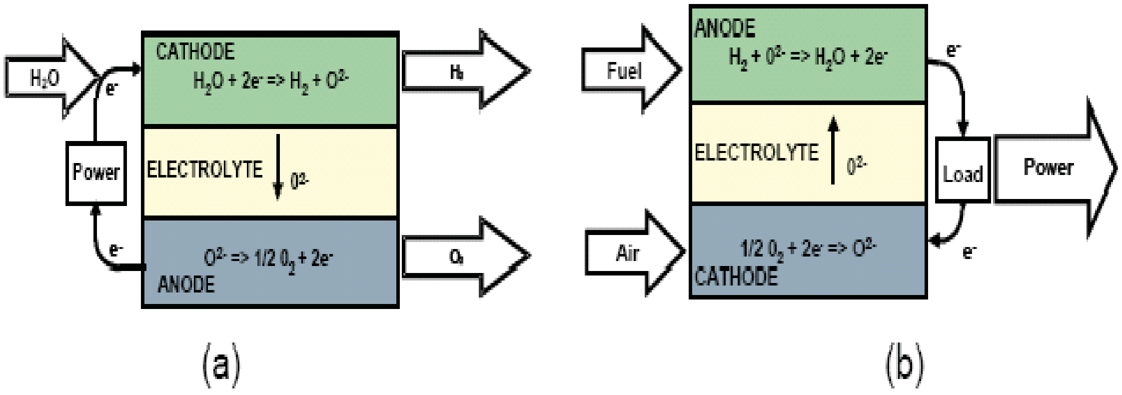


Figure 17 (a) Solid oxide electrolysis cell (SOEC); (b) solid oxide fuel cell (SOFC) operating in reverse compared to an SOEC [Guan, et al. 2006]

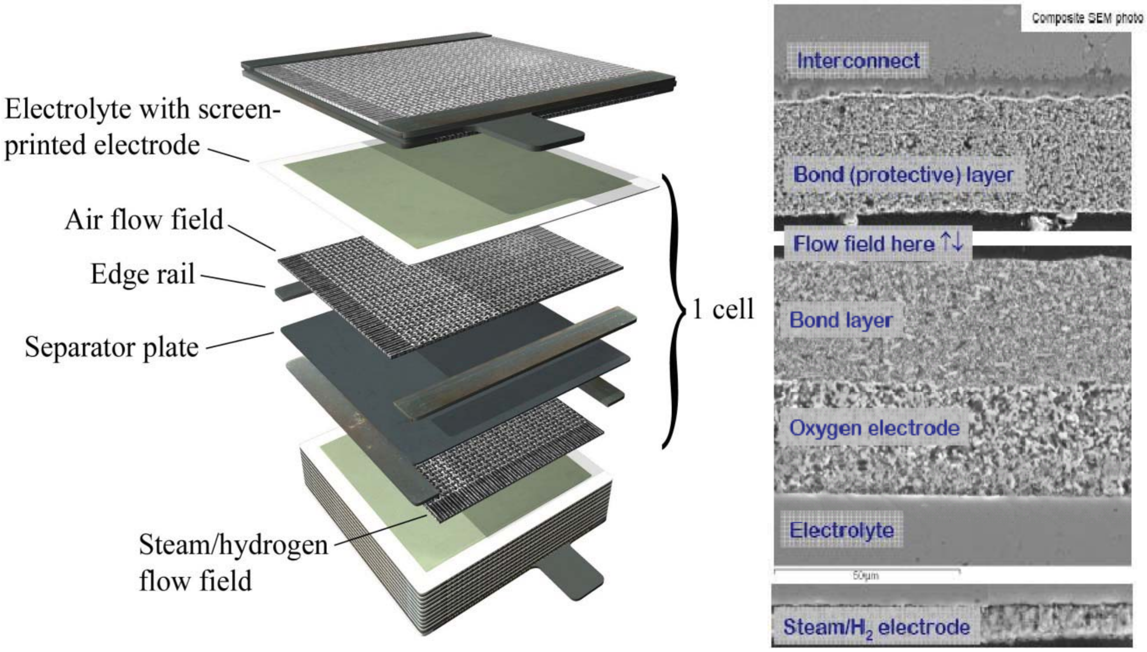


Figure 18 Ceramatec solid oxide cell/stack construction; (scanning electron microscopy figure on the right taken from Carter et al. 2008)

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/H_2 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 (**cer**amic-**met**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 700–1,100ºC 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 O_2-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 ~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/O_2-Electrode Side Bond Layer

An O_2-electrode side protective bond layer is shown in Figure 18. Because, it is next to the O_2-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 O_2-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 O_2 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 O_2-electrode and LSC bond layer, which can prevent solid state Cr from diffusing into the O_2-electrode. For this reason, the O_2-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-ZrO_2/8YSZ) 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 SiO_2 was detected at the Ni/YSZ H_2-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 ZrO_2 remained stable at the present Scandia doping level.

4.2.5 Steam/H_2-Electrode

Overall, many researchers agree that the contribution of a steam/H_2-electrode to SOEC degradation is much less than that of other cell components. ANL also observed Si as a capping layer on steam/H_2-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 H_2-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-H_2 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/H_2-electrode side is not degrading,
- Air and steam/H_2 flow fields (flow channels) are not degrading,
- Five cell components are suspect:
    - Bond layer on O_2-electrode-Cr poisoning and dissociation
    - O_2-electrode-microstructural changes and delamination
    - Loss of electrical/ionic conductivity of electrolyte
    - Interconnect-generation of contaminants

- Steam/H_2- 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-t_0). 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]:

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

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.

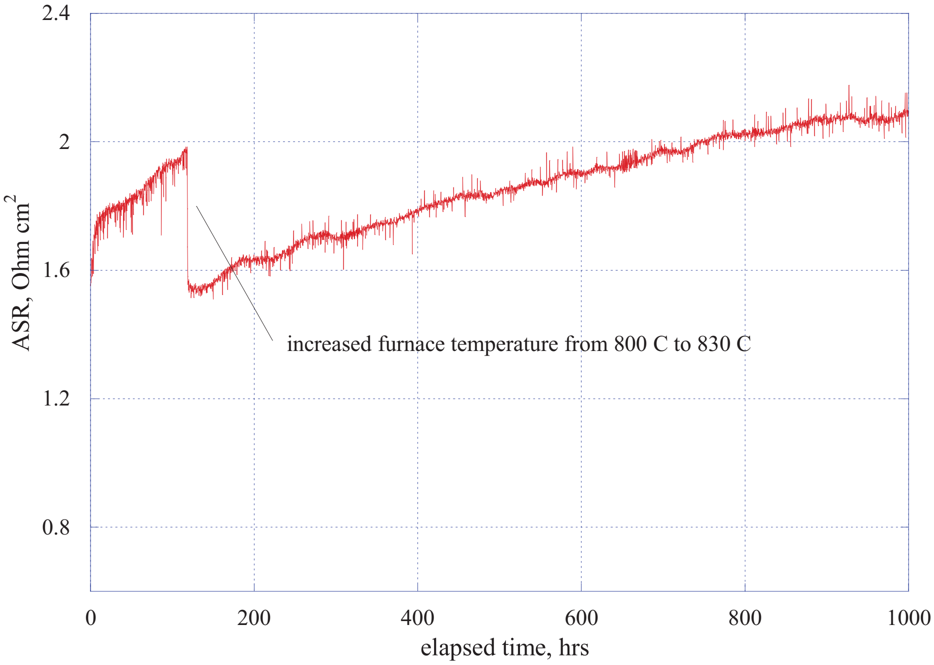


Figure 19 Area-specific resistance of a 25-cell stack as a function of time for a 1,000-hour test [O'Brien et al. 2007]

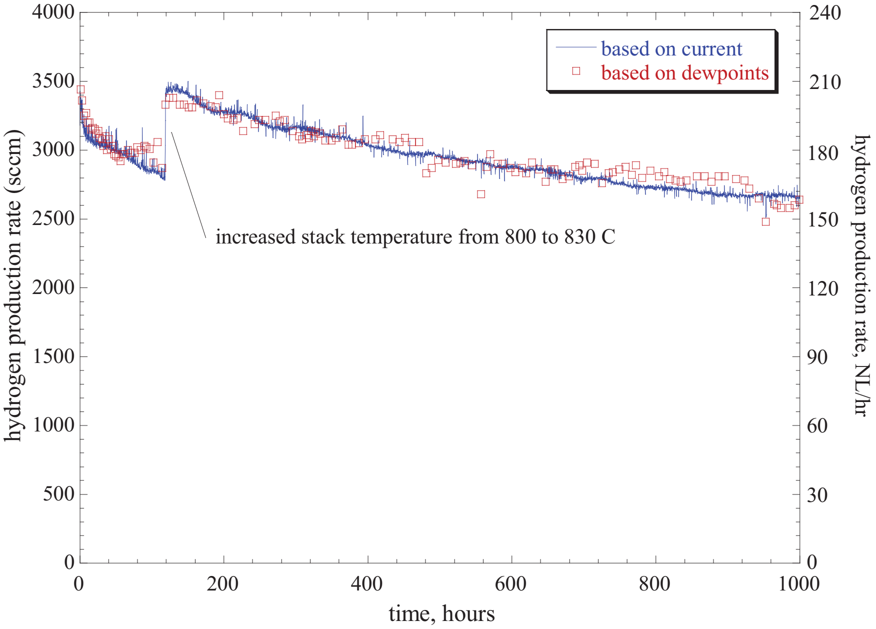


Figure 20 Hydrogen production rates during 1,000-hour long-term test [O'Brien et al. 2007]

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.

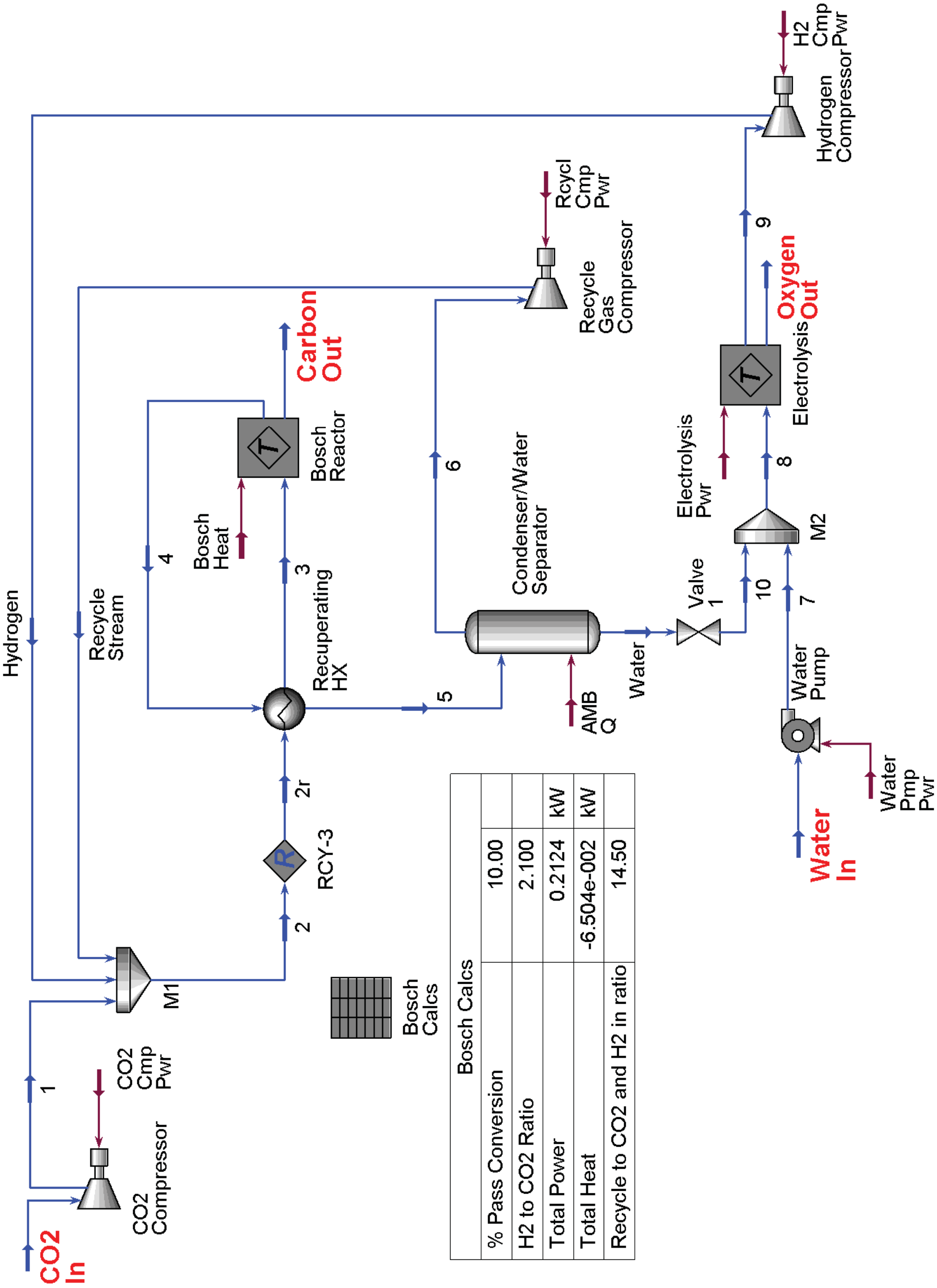
Appendix A

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



Bosch Calcs		
% Pass Conversion	10.00	
H2 to CO2 Ratio	2.100	
Total Power	0.2124	kW
Total Heat	-6.504e-002	kW
Recycle to CO2 and H2 in ratio	14.50	

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

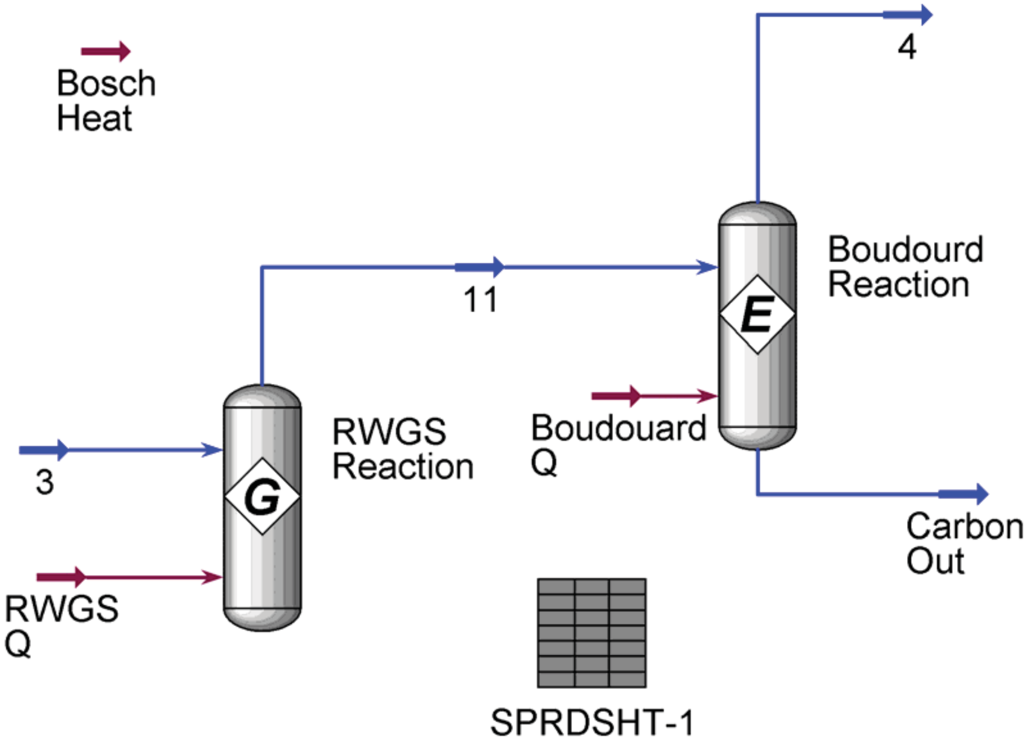


Figure A - 2 Process flow diagram of Bosch reactor

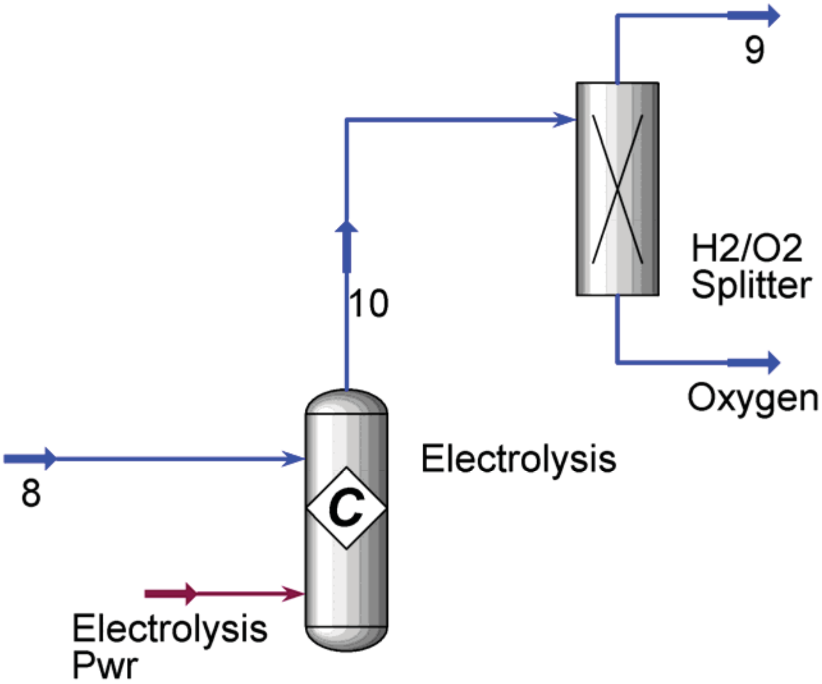


Figure A - 3 Process flow diagram of electrolysis module

INL
Calgary, Alberta
CANADA

Case Name:	C:\NASA Final\Bosch 3-Comp v_2.hsc
Unit Set:	NASA2
Date/Time:	Mon Aug 23 10:20:55 2010

Workbook: Case (Main)

Streams

Name	CO2 In	1	Hydrogen	Recycle Stream	2
Vapour Fraction	1.0000	1.0000	1.0000	1.0000	1.0000
Temperature (C)	21.111 *	45.103	91.537	34.609	37.371
Pressure (kPa)	131.00 *	172.37 *	172.37	172.37	172.37
Molar Flow (gmole/h)	1.2404	1.2404	2.6054	49.471	53.317
Mass Flow (kg/d)	1.3102 *	1.3102	0.12633	20.826	22.262
Liquid Volume Flow (m3/h)	6.614e-005	6.614e-005	7.519e-005	1.917e-003	2.059e-003
Heat Flow (kW)	-0.1358	-0.1354	1.344e-003	-1.406	-1.540
Molar Enthalpy (kJ/kgmole)	-3.940e+005	-3.931e+005	1857	-1.023e+005	-1.040e+005

Name	2r	3	Carbon Out	4	5
Vapour Fraction	1.0000	1.0000	1.0000 *	1.0000	1.0000
Temperature (C)	37.396 *	620.26 *	650.00	650.00	62.396
Pressure (kPa)	172.37 *	169.37	163.37	163.37	160.37
Molar Flow (gmole/h)	53.298	53.298	1.2214	52.001	52.001
Mass Flow (kg/d)	22.272 *	22.272	0.35208	21.920	21.920
Liquid Volume Flow (m3/h)	2.058e-003	2.058e-003	8.934e-006	1.963e-003	1.963e-003
Heat Flow (kW)	-1.543	-1.225	3.473e-003	-1.245	-1.563
Molar Enthalpy (kJ/kgmole)	-1.042e+005	-8.276e+004	1.024e+004	-8.621e+004	-1.082e+005

Name	6	Water	Water In	7	8
Vapour Fraction	1.0000	0.0000	0.0000	0.0000	0.0000
Temperature (C)	25.000 *	25.000	21.111 *	21.112	24.897
Pressure (kPa)	157.37	157.37	101.32 *	107.32 *	107.32
Molar Flow (gmole/h)	49.471	2.5291	7.6325e-002	7.6325e-002	2.6054
Mass Flow (kg/d)	20.826	1.0936	3.3000e-002 *	3.3000e-002	1.1266
Liquid Volume Flow (m3/h)	1.917e-003	4.566e-005	1.378e-006	1.378e-006	4.704e-005
Heat Flow (kW)	-1.411	-0.2005	-6.057e-003	-6.057e-003	-0.2066
Molar Enthalpy (kJ/kgmole)	-1.026e+005	-2.854e+005	-2.857e+005	-2.857e+005	-2.854e+005

Name	Oxygen Out	9	10	CO2 Cmp Pwr	AMB Q
Vapour Fraction	1.0000	1.0000	0.0000	---	---
Temperature (C)	24.996	24.897	25.011	---	---
Pressure (kPa)	101.32	101.32	107.32	---	---
Molar Flow (gmole/h)	1.3025	2.6054	2.5291	---	---
Mass Flow (kg/d)	1.0003	0.12633	1.0936	---	---
Liquid Volume Flow (m3/h)	3.664e-005	7.519e-005	4.566e-005	---	---
Heat Flow (kW)	-3.500e-006	-3.110e-005	-0.2005	3.154e-004	-4.846e-002
Molar Enthalpy (kJ/kgmole)	-9.675	-42.97	-2.854e+005	---	---

Name	Rcycl Cmp Pwr	H2 Cmp Pwr	Bosch Heat	Electrolysis Pwr	Water Pmp Pwr
Vapour Fraction	---	---	---	---	---
Temperature (C)	---	---	---	---	---
Pressure (kPa)	---	---	---	---	---
Molar Flow (gmole/h)	---	---	---	---	---
Mass Flow (kg/d)	---	---	---	---	---
Liquid Volume Flow (m3/h)	---	---	---	---	---
Heat Flow (kW)	4.180e-003	1.375e-003	-1.658e-002	0.2065	3.025e-009
Molar Enthalpy (kJ/kgmole)	---	---	---	---	---

Composition

Name	CO2 In	1	2	2r	3
Comp Mole Frac (Carbon)	0.00000 *	0.00000	0.00000	0.00000 *	0.00000
Comp Mole Frac (Oxygen)	0.00000 *	0.00000	0.00000	0.00000 *	0.00000
Comp Mole Frac (H2O)	0.00000 *	0.00000	0.01859	0.01858 *	0.01858
Comp Mole Frac (Methane)	0.00000 *	0.00000	0.19444	0.19380 *	0.19380
Comp Mole Frac (CO)	0.00000 *	0.00000	0.22924	0.22911 *	0.22911
Comp Mole Frac (Hydrogen)	0.00000 *	0.00000	0.40538	0.40554 *	0.40554
Comp Mole Frac (CO2)	1.00000 *	1.00000	0.15235	0.15297 *	0.15297

* Specified by user.

Workbook: Case (Main) (continued)

Composition (continued)

Name	Carbon Out	4	5	6	Recycle Stream
Comp Mole Frac (Carbon)	1.00000	0.00000	0.00000	0.00000	0.00000
Comp Mole Frac (Oxygen)	0.00000	0.00000	0.00000	0.00000	0.00000
Comp Mole Frac (H2O)	0.00000	0.06769	0.06769	0.02003	0.02003
Comp Mole Frac (Methane)	0.00000	0.19936	0.19936	0.20955	0.20955
Comp Mole Frac (CO)	0.00000	0.23505	0.23505	0.24706	0.24706
Comp Mole Frac (Hydrogen)	0.00000	0.36555	0.36555	0.38423	0.38423
Comp Mole Frac (CO2)	0.00000	0.13236	0.13236	0.13912	0.13912

Name	Water	Water In	7	8	9
Comp Mole Frac (Carbon)	0.00000	0.00000 *	0.00000	0.00000	0.00000
Comp Mole Frac (Oxygen)	0.00000	0.00000 *	0.00000	0.00000	0.00000
Comp Mole Frac (H2O)	0.99989	1.00000 *	1.00000	0.99990	0.00000
Comp Mole Frac (Methane)	0.00000	0.00000 *	0.00000	0.00000	0.00000
Comp Mole Frac (CO)	0.00000	0.00000 *	0.00000	0.00000	0.00000
Comp Mole Frac (Hydrogen)	0.00000	0.00000 *	0.00000	0.00000	0.99990
Comp Mole Frac (CO2)	0.00010	0.00000 *	0.00000	0.00010	0.00010

Name	Oxygen Out	Hydrogen	10		
Comp Mole Frac (Carbon)	0.00000	0.00000	0.00000		
Comp Mole Frac (Oxygen)	1.00000	0.00000	0.00000		
Comp Mole Frac (H2O)	0.00000	0.00000	0.99989		
Comp Mole Frac (Methane)	0.00000	0.00000	0.00000		
Comp Mole Frac (CO)	0.00000	0.00000	0.00000		
Comp Mole Frac (Hydrogen)	0.00000	0.99990	0.00000		
Comp Mole Frac (CO2)	0.00000	0.00010	0.00010		

Heat Exchangers

Name		Recuperating HX				
Duty	(kW)	0.3173				
Tube Inlet Temperature	(C)	37.40 *				
Tube Outlet Temperature	(C)	620.3 *				
Shell Inlet Temperature	(C)	650.0				
Shell Outlet Temperature	(C)	62.40				
UA	(W/C)	11.54				
LMTD	(C)	27.49				
Minimum Approach	(C)	25.00				

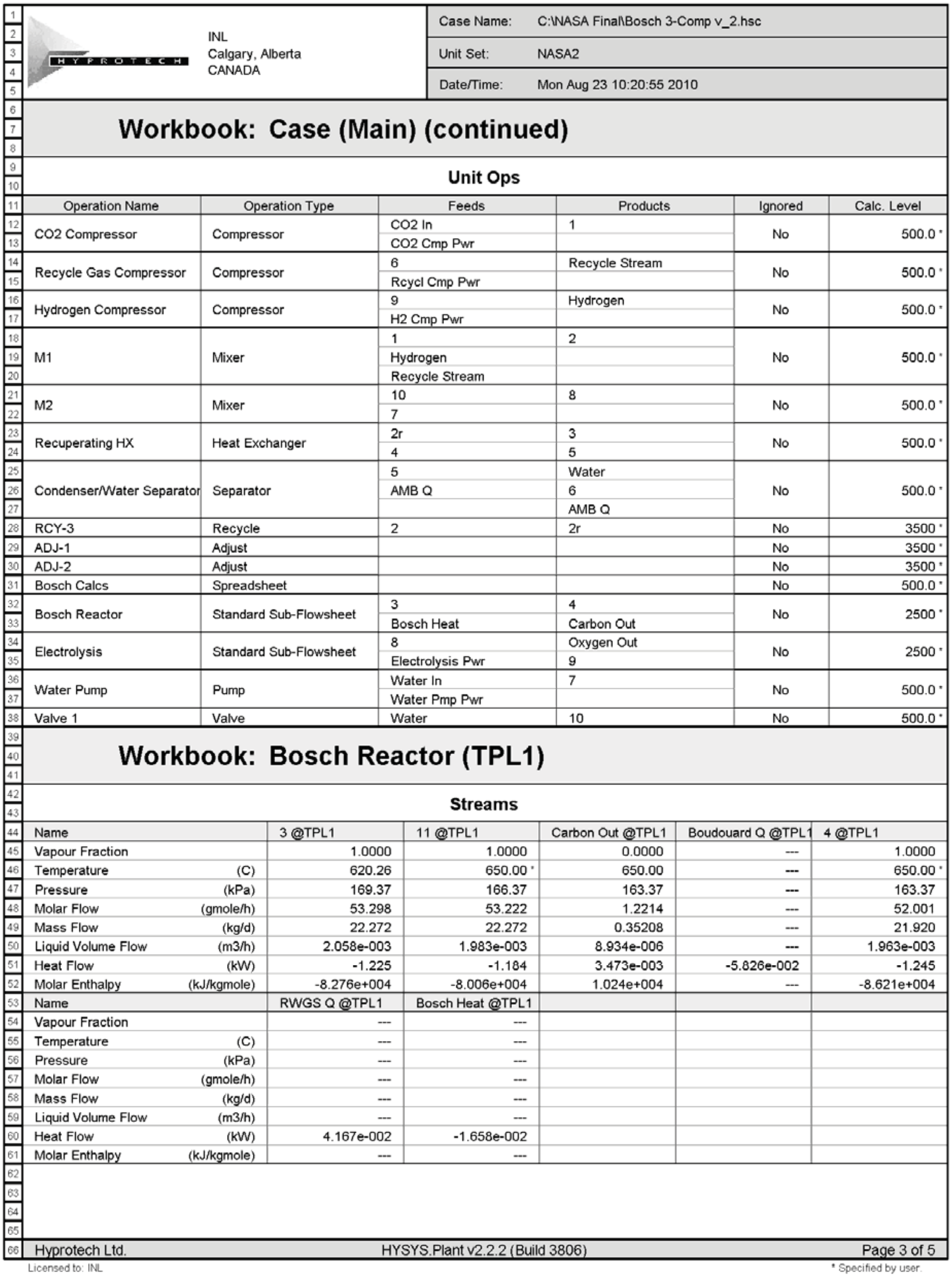
Compressors

Name		CO2 Compressor	Recycle Gas Compre	Hydrogen Compress		
Feed Pressure	(kPa)	131.0 *	157.4	101.3		
Product Pressure	(kPa)	172.4 *	172.4	172.4		
Molar Flow	(gmole/h)	1.240	49.47	2.605		
Energy	(kW)	3.154e-004	4.180e-003	1.375e-003		
Adiabatic Efficiency		75 *	75 *	75 *		
Polytropic Efficiency		76	75	77		

Pumps

Name		Water Pump				
Delta P	(kPa)	6.000				
Energy	(kW)	3.025e-009				
Feed Pressure	(kPa)	101.3 *				
Product Pressure	(kPa)	107.3 *				
Molar Flow	(gmole/h)	7.632e-002				
Adiabatic Efficiency	(%)	75.00 *				

* Specified by user.



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CANADA

Case Name:	C:\NASA Final\Bosch 3-Comp v_2.hsc
Unit Set:	NASA2
Date/Time:	Mon Aug 23 10:20:55 2010

Workbook: Case (Main) (continued)

Unit Ops

Operation Name	Operation Type	Feeds	Products	Ignored	Calc. Level
CO2 Compressor	Compressor	CO2 In CO2 Cmp Pwr	1	No	500.0 *
Recycle Gas Compressor	Compressor	6 Rcycl Cmp Pwr	Recycle Stream	No	500.0 *
Hydrogen Compressor	Compressor	9 H2 Cmp Pwr	Hydrogen	No	500.0 *
M1	Mixer	1 Hydrogen Recycle Stream	2	No	500.0 *
M2	Mixer	10 7	8	No	500.0 *
Recuperating HX	Heat Exchanger	2r 4	3 5	No	500.0 *
Condenser/Water Separator	Separator	5 AMB Q	Water 6 AMB Q	No	500.0 *
RCY-3	Recycle	2	2r	No	3500 *
ADJ-1	Adjust			No	3500 *
ADJ-2	Adjust			No	3500 *
Bosch Calcs	Spreadsheet			No	500.0 *
Bosch Reactor	Standard Sub-Flowsheet	3 Bosch Heat	4 Carbon Out	No	2500 *
Electrolysis	Standard Sub-Flowsheet	8 Electrolysis Pwr	Oxygen Out 9	No	2500 *
Water Pump	Pump	Water In Water Pmp Pwr	7	No	500.0 *
Valve 1	Valve	Water	10	No	500.0 *

Workbook: Bosch Reactor (TPL1)

Streams

Name		3 @TPL1	11 @TPL1	Carbon Out @TPL1	Boudouard Q @TPL1	4 @TPL1
Vapour Fraction		1.0000	1.0000	0.0000	---	1.0000
Temperature	(C)	620.26	650.00 *	650.00	---	650.00 *
Pressure	(kPa)	169.37	166.37	163.37	---	163.37
Molar Flow	(gmole/h)	53.298	53.222	1.2214	---	52.001
Mass Flow	(kg/d)	22.272	22.272	0.35208	---	21.920
Liquid Volume Flow	(m3/h)	2.058e-003	1.983e-003	8.934e-006	---	1.963e-003
Heat Flow	(kW)	-1.225	-1.184	3.473e-003	-5.826e-002	-1.245
Molar Enthalpy	(kJ/kgmole)	-8.276e+004	-8.006e+004	1.024e+004	---	-8.621e+004

Name		RWGS Q @TPL1	Bosch Heat @TPL1			
Vapour Fraction		---	---			
Temperature	(C)	---	---			
Pressure	(kPa)	---	---			
Molar Flow	(gmole/h)	---	---			
Mass Flow	(kg/d)	---	---			
Liquid Volume Flow	(m3/h)	---	---			
Heat Flow	(kW)	4.167e-002	-1.658e-002			
Molar Enthalpy	(kJ/kgmole)	---	---			

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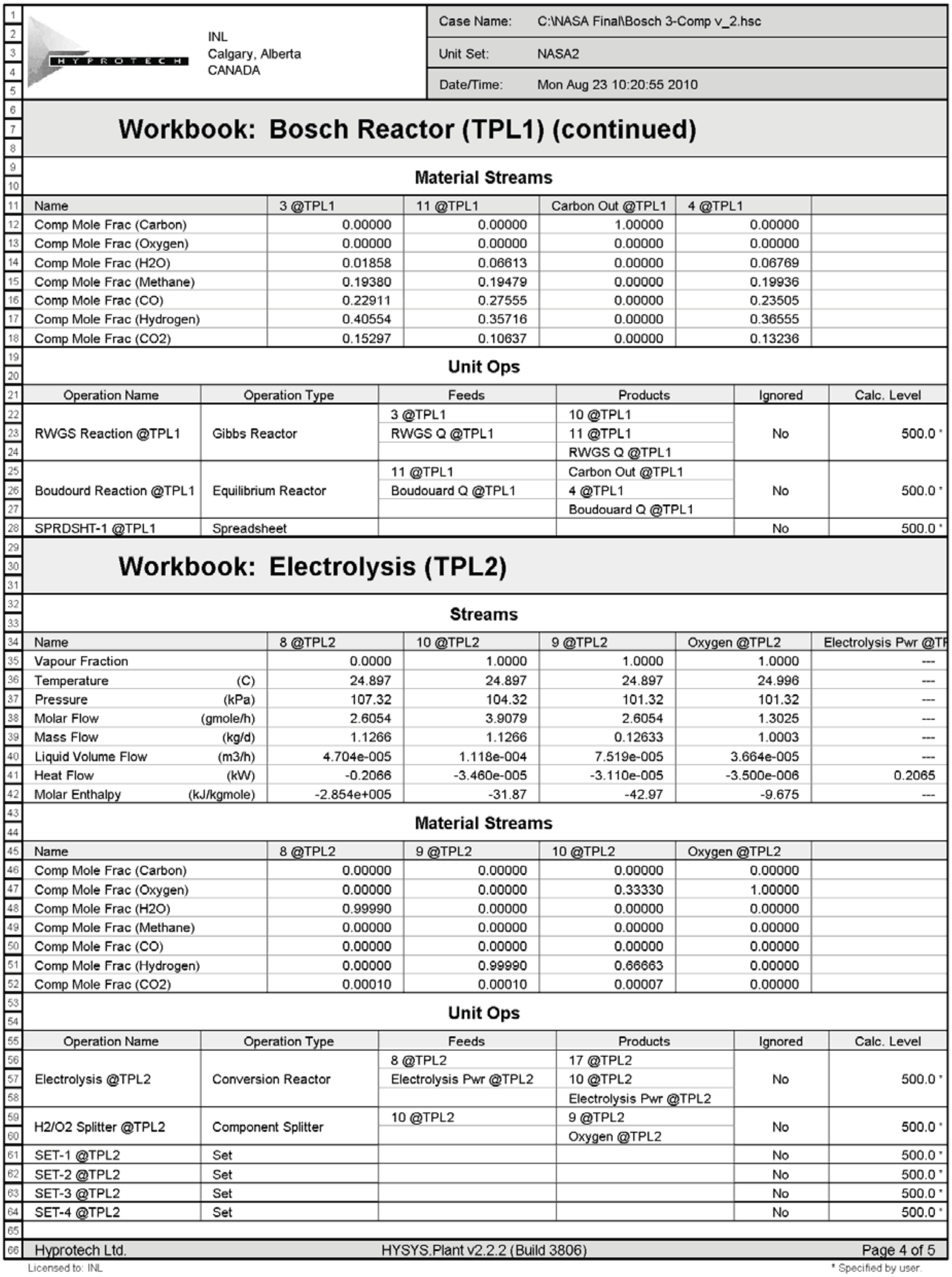

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Case Name: C:\NASA Final\Bosch 3-Comp v_2.hsc
Unit Set: NASA2
Date/Time: Mon Aug 23 10:20:55 2010

Workbook: Bosch Reactor (TPL1) (continued)

Material Streams

Name	3 @TPL1	11 @TPL1	Carbon Out @TPL1	4 @TPL1	
Comp Mole Frac (Carbon)	0.00000	0.00000	1.00000	0.00000	
Comp Mole Frac (Oxygen)	0.00000	0.00000	0.00000	0.00000	
Comp Mole Frac (H2O)	0.01858	0.06613	0.00000	0.06769	
Comp Mole Frac (Methane)	0.19380	0.19479	0.00000	0.19936	
Comp Mole Frac (CO)	0.22911	0.27555	0.00000	0.23505	
Comp Mole Frac (Hydrogen)	0.40554	0.35716	0.00000	0.36555	
Comp Mole Frac (CO2)	0.15297	0.10637	0.00000	0.13236	

Unit Ops

Operation Name	Operation Type	Feeds	Products	Ignored	Calc. Level
RWGS Reaction @TPL1	Gibbs Reactor	3 @TPL1 RWGS Q @TPL1	10 @TPL1 11 @TPL1 RWGS Q @TPL1	No	500.0 *
Boudourd Reaction @TPL1	Equilibrium Reactor	11 @TPL1 Boudouard Q @TPL1	Carbon Out @TPL1 4 @TPL1 Boudouard Q @TPL1	No	500.0 *
SPRDSHT-1 @TPL1	Spreadsheet			No	500.0 *

Workbook: Electrolysis (TPL2)

Streams

Name		8 @TPL2	10 @TPL2	9 @TPL2	Oxygen @TPL2	Electrolysis Pwr @T
Vapour Fraction		0.0000	1.0000	1.0000	1.0000	---
Temperature	(C)	24.897	24.897	24.897	24.996	---
Pressure	(kPa)	107.32	104.32	101.32	101.32	---
Molar Flow	(gmole/h)	2.6054	3.9079	2.6054	1.3025	---
Mass Flow	(kg/d)	1.1266	1.1266	0.12633	1.0003	---
Liquid Volume Flow	(m3/h)	4.704e-005	1.118e-004	7.519e-005	3.664e-005	---
Heat Flow	(kW)	-0.2066	-3.460e-005	-3.110e-005	-3.500e-006	0.2065
Molar Enthalpy	(kJ/kgmole)	-2.854e+005	-31.87	-42.97	-9.675	---

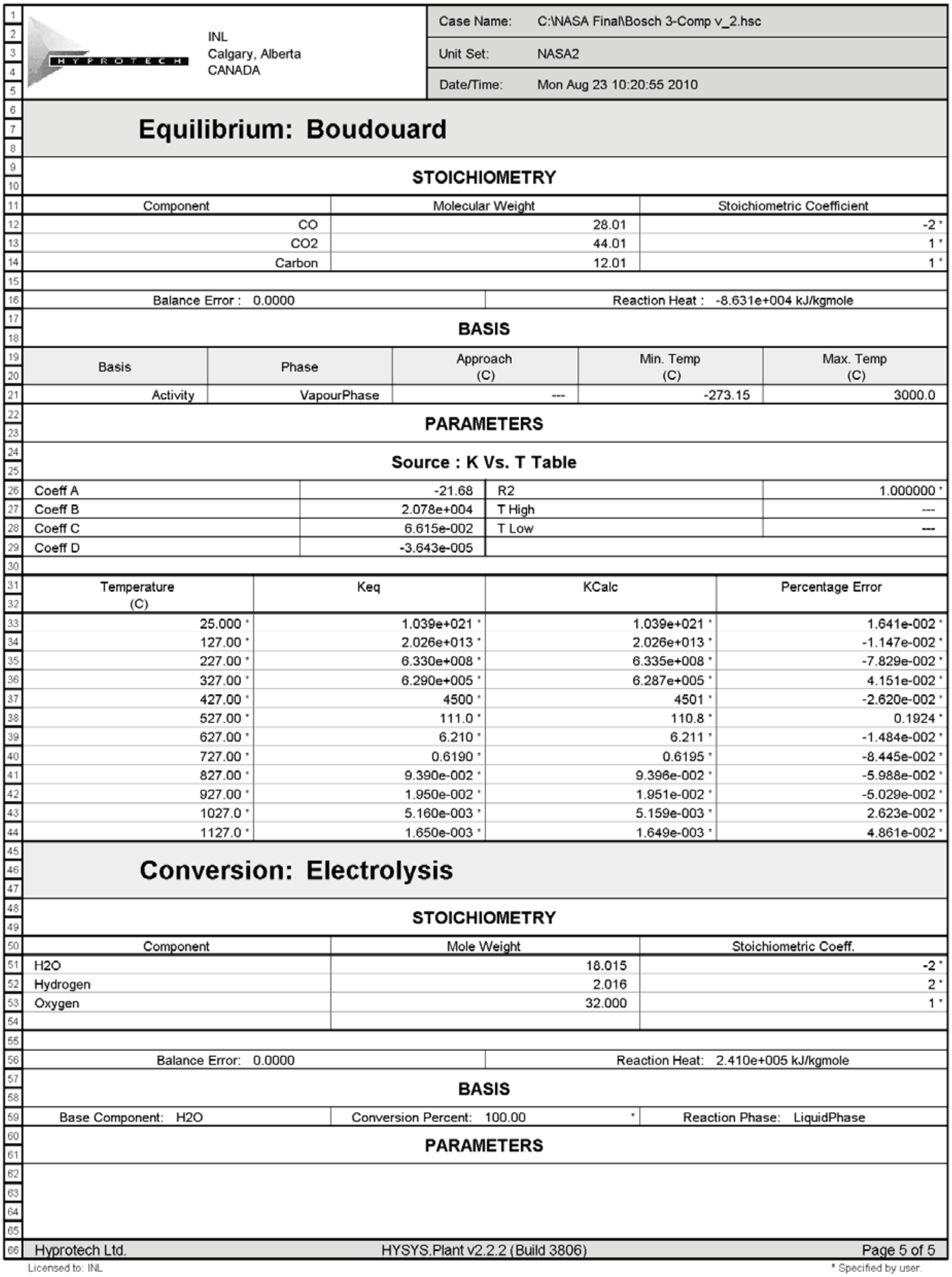
Material Streams

Name	8 @TPL2	9 @TPL2	10 @TPL2	Oxygen @TPL2	
Comp Mole Frac (Carbon)	0.00000	0.00000	0.00000	0.00000	
Comp Mole Frac (Oxygen)	0.00000	0.00000	0.33330	1.00000	
Comp Mole Frac (H2O)	0.99990	0.00000	0.00000	0.00000	
Comp Mole Frac (Methane)	0.00000	0.00000	0.00000	0.00000	
Comp Mole Frac (CO)	0.00000	0.00000	0.00000	0.00000	
Comp Mole Frac (Hydrogen)	0.00000	0.99990	0.66663	0.00000	
Comp Mole Frac (CO2)	0.00010	0.00010	0.00007	0.00000	

Unit Ops

Operation Name	Operation Type	Feeds	Products	Ignored	Calc. Level
Electrolysis @TPL2	Conversion Reactor	8 @TPL2 Electrolysis Pwr @TPL2	17 @TPL2 10 @TPL2 Electrolysis Pwr @TPL2	No	500.0 *
H2/O2 Splitter @TPL2	Component Splitter	10 @TPL2	9 @TPL2 Oxygen @TPL2	No	500.0 *
SET-1 @TPL2	Set			No	500.0 *
SET-2 @TPL2	Set			No	500.0 *
SET-3 @TPL2	Set			No	500.0 *
SET-4 @TPL2	Set			No	500.0 *

* Specified by user.



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Case Name:	C:\NASA Final\Bosch 3-Comp v_2.hsc
Unit Set:	NASA2
Date/Time:	Mon Aug 23 10:20:55 2010

Equilibrium: Boudouard

STOICHIOMETRY

Component	Molecular Weight	Stoichiometric Coefficient
CO	28.01	-2 *
CO2	44.01	1 *
Carbon	12.01	1 *

Balance Error : 0.0000 | Reaction Heat : -8.631e+004 kJ/kgmole

BASIS

Basis	Phase	Approach (C)	Min. Temp (C)	Max. Temp (C)
Activity	VapourPhase	---	-273.15	3000.0

PARAMETERS

Source : K Vs. T Table

Coeff A	-21.68	R2	1.000000 *
Coeff B	2.078e+004	T High	---
Coeff C	6.615e-002	T Low	---
Coeff D	-3.643e-005		

Temperature (C)	Keq	KCalc	Percentage Error
25.000 *	1.039e+021 *	1.039e+021 *	1.641e-002 *
127.00 *	2.026e+013 *	2.026e+013 *	-1.147e-002 *
227.00 *	6.330e+008 *	6.335e+008 *	-7.829e-002 *
327.00 *	6.290e+005 *	6.287e+005 *	4.151e-002 *
427.00 *	4500 *	4501 *	-2.620e-002 *
527.00 *	111.0 *	110.8 *	0.1924 *
627.00 *	6.210 *	6.211 *	-1.484e-002 *
727.00 *	0.6190 *	0.6195 *	-8.445e-002 *
827.00 *	9.390e-002 *	9.396e-002 *	-5.988e-002 *
927.00 *	1.950e-002 *	1.951e-002 *	-5.029e-002 *
1027.0 *	5.160e-003 *	5.159e-003 *	2.623e-002 *
1127.0 *	1.650e-003 *	1.649e-003 *	4.861e-002 *

Conversion: Electrolysis

STOICHIOMETRY

Component	Mole Weight	Stoichiometric Coeff.
H2O	18.015	-2 *
Hydrogen	2.016	2 *
Oxygen	32.000	1 *

Balance Error: 0.0000 | Reaction Heat: 2.410e+005 kJ/kgmole

BASIS

Base Component: H2O | Conversion Percent: 100.00 * | Reaction Phase: LiquidPhase

PARAMETERS

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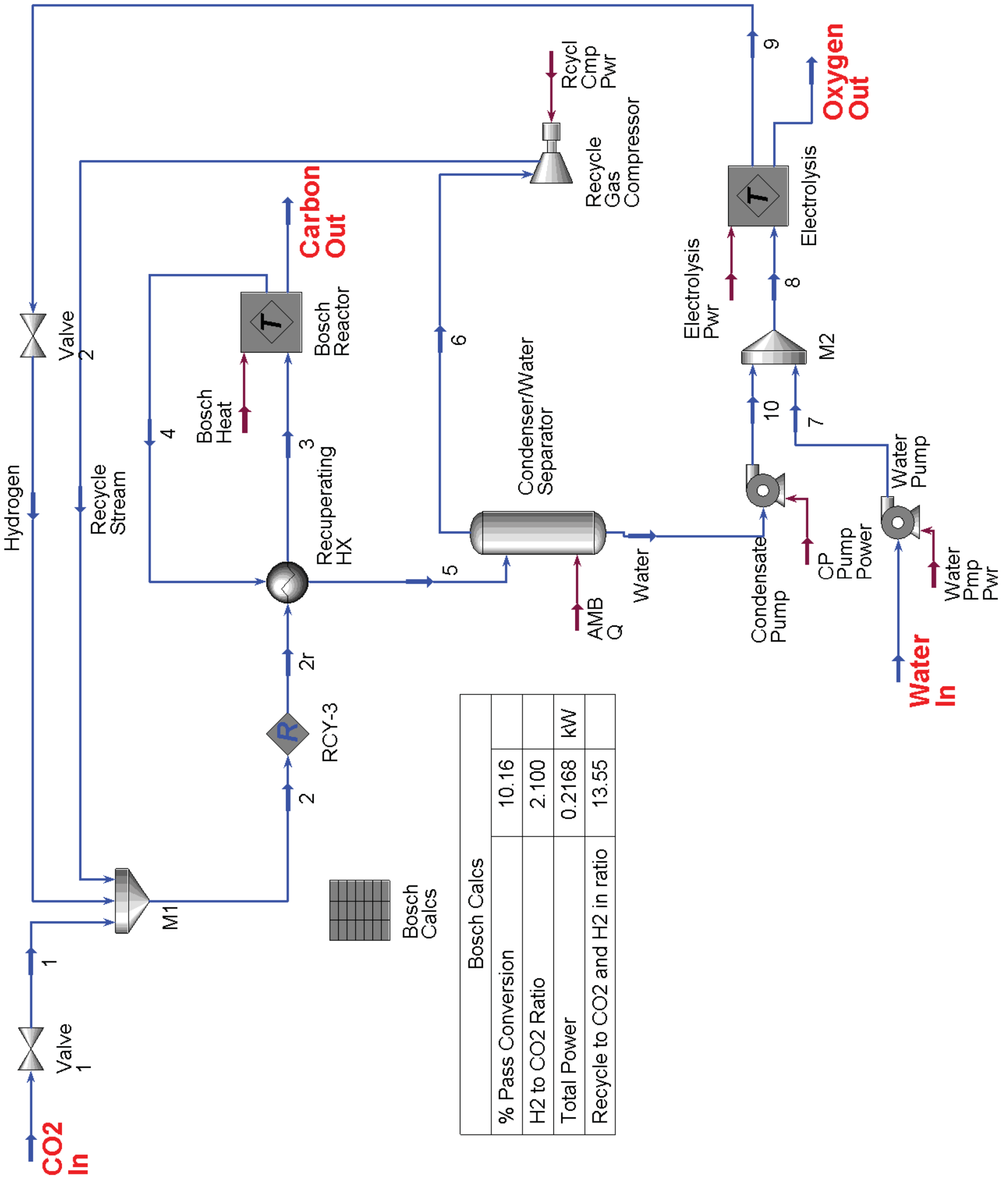
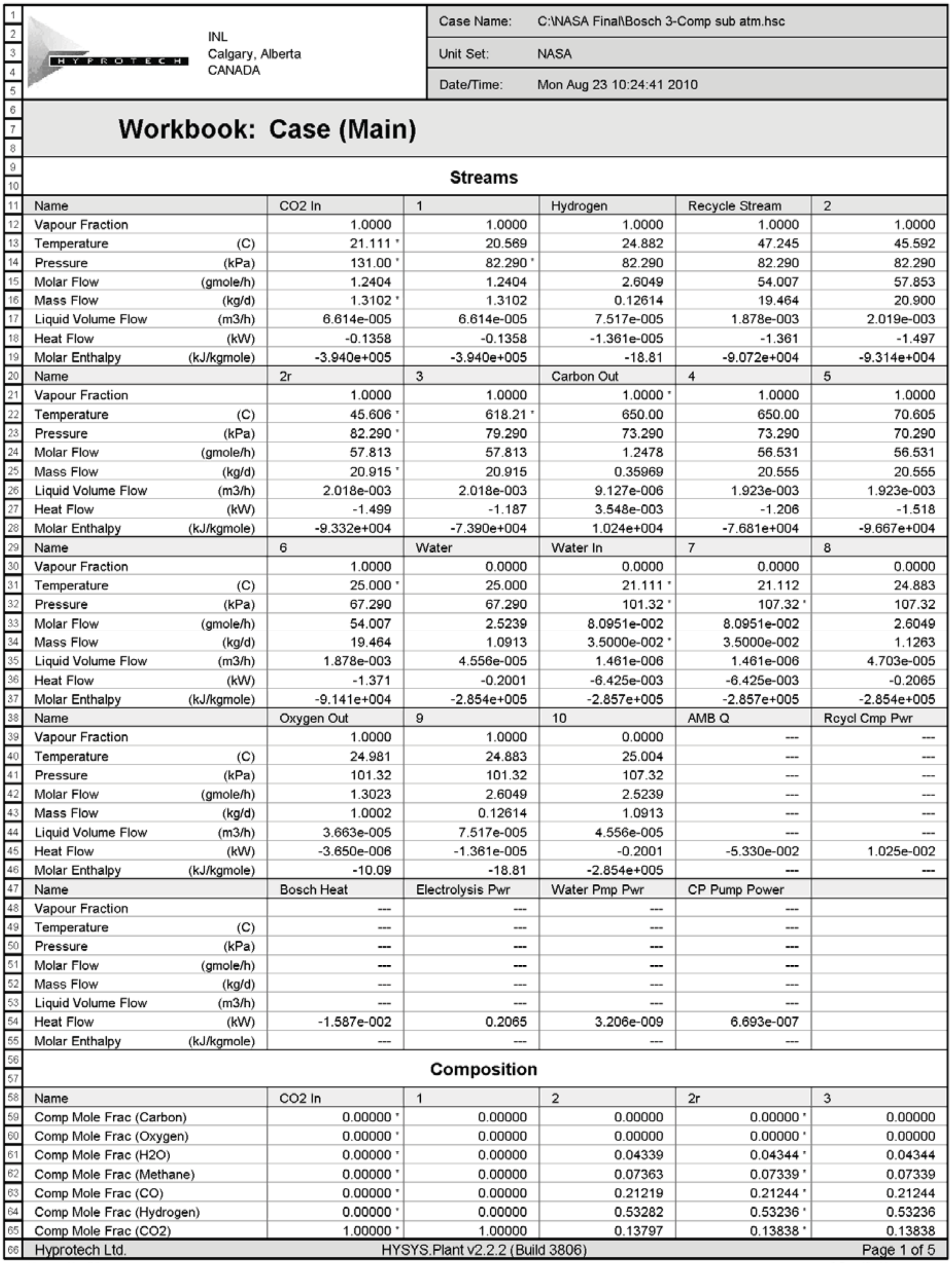
A.2 Bosch Process with 3 Compressors with Sub Atmospheric Conditions



Bosch Calcs		
% Pass Conversion	10.16	
H2 to CO2 Ratio	2.100	
Total Power	0.2168	kW
Recycle to CO2 and H2 in ratio	13.55	

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



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Calgary, Alberta
CANADA

Case Name: C:\NASA Final\Bosch 3-Comp sub atm.hsc
Unit Set: NASA
Date/Time: Mon Aug 23 10:24:41 2010

Workbook: Case (Main)

Streams

Name		CO2 In	1	Hydrogen	Recycle Stream	2
Vapour Fraction		1.0000	1.0000	1.0000	1.0000	1.0000
Temperature	(C)	21.111 *	20.569	24.882	47.245	45.592
Pressure	(kPa)	131.00 *	82.290 *	82.290	82.290	82.290
Molar Flow	(gmole/h)	1.2404	1.2404	2.6049	54.007	57.853
Mass Flow	(kg/d)	1.3102 *	1.3102	0.12614	19.464	20.900
Liquid Volume Flow	(m3/h)	6.614e-005	6.614e-005	7.517e-005	1.878e-003	2.019e-003
Heat Flow	(kW)	-0.1358	-0.1358	-1.361e-005	-1.361	-1.497
Molar Enthalpy	(kJ/kgmole)	-3.940e+005	-3.940e+005	-18.81	-9.072e+004	-9.314e+004
Name		2r	3	Carbon Out	4	5
Vapour Fraction		1.0000	1.0000	1.0000 *	1.0000	1.0000
Temperature	(C)	45.606 *	618.21 *	650.00	650.00	70.605
Pressure	(kPa)	82.290 *	79.290	73.290	73.290	70.290
Molar Flow	(gmole/h)	57.813	57.813	1.2478	56.531	56.531
Mass Flow	(kg/d)	20.915 *	20.915	0.35969	20.555	20.555
Liquid Volume Flow	(m3/h)	2.018e-003	2.018e-003	9.127e-006	1.923e-003	1.923e-003
Heat Flow	(kW)	-1.499	-1.187	3.548e-003	-1.206	-1.518
Molar Enthalpy	(kJ/kgmole)	-9.332e+004	-7.390e+004	1.024e+004	-7.681e+004	-9.667e+004
Name		6	Water	Water In	7	8
Vapour Fraction		1.0000	0.0000	0.0000	0.0000	0.0000
Temperature	(C)	25.000 *	25.000	21.111 *	21.112	24.883
Pressure	(kPa)	67.290	67.290	101.32 *	107.32 *	107.32
Molar Flow	(gmole/h)	54.007	2.5239	8.0951e-002	8.0951e-002	2.6049
Mass Flow	(kg/d)	19.464	1.0913	3.5000e-002 *	3.5000e-002	1.1263
Liquid Volume Flow	(m3/h)	1.878e-003	4.556e-005	1.461e-006	1.461e-006	4.703e-005
Heat Flow	(kW)	-1.371	-0.2001	-6.425e-003	-6.425e-003	-0.2065
Molar Enthalpy	(kJ/kgmole)	-9.141e+004	-2.854e+005	-2.857e+005	-2.857e+005	-2.854e+005
Name		Oxygen Out	9	10	AMB Q	Rcycl Cmp Pwr
Vapour Fraction		1.0000	1.0000	0.0000	---	---
Temperature	(C)	24.981	24.883	25.004	---	---
Pressure	(kPa)	101.32	101.32	107.32	---	---
Molar Flow	(gmole/h)	1.3023	2.6049	2.5239	---	---
Mass Flow	(kg/d)	1.0002	0.12614	1.0913	---	---
Liquid Volume Flow	(m3/h)	3.663e-005	7.517e-005	4.556e-005	---	---
Heat Flow	(kW)	-3.650e-006	-1.361e-005	-0.2001	-5.330e-002	1.025e-002
Molar Enthalpy	(kJ/kgmole)	-10.09	-18.81	-2.854e+005	---	---
Name		Bosch Heat	Electrolysis Pwr	Water Pmp Pwr	CP Pump Power	
Vapour Fraction		---	---	---	---	
Temperature	(C)	---	---	---	---	
Pressure	(kPa)	---	---	---	---	
Molar Flow	(gmole/h)	---	---	---	---	
Mass Flow	(kg/d)	---	---	---	---	
Liquid Volume Flow	(m3/h)	---	---	---	---	
Heat Flow	(kW)	-1.587e-002	0.2065	3.206e-009	6.693e-007	
Molar Enthalpy	(kJ/kgmole)	---	---	---	---	

Composition

Name	CO2 In	1	2	2r	3
Comp Mole Frac (Carbon)	0.00000 *	0.00000	0.00000	0.00000 *	0.00000
Comp Mole Frac (Oxygen)	0.00000 *	0.00000	0.00000	0.00000 *	0.00000
Comp Mole Frac (H2O)	0.00000 *	0.00000	0.04339	0.04344 *	0.04344
Comp Mole Frac (Methane)	0.00000 *	0.00000	0.07363	0.07339 *	0.07339
Comp Mole Frac (CO)	0.00000 *	0.00000	0.21219	0.21244 *	0.21244
Comp Mole Frac (Hydrogen)	0.00000 *	0.00000	0.53282	0.53236 *	0.53236
Comp Mole Frac (CO2)	1.00000 *	1.00000	0.13797	0.13838 *	0.13838

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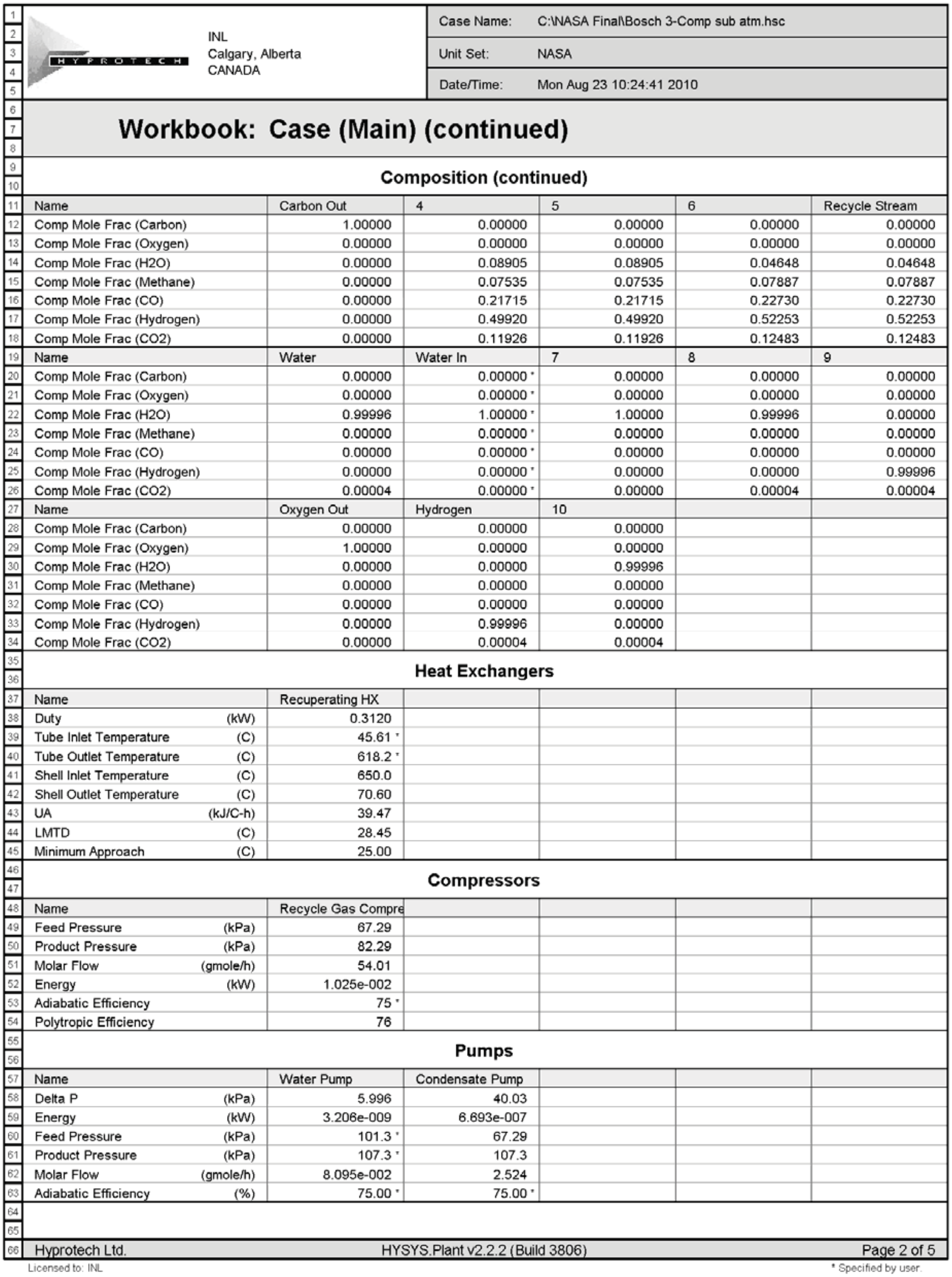

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Case Name:	C:\NASA Final\Bosch 3-Comp sub atm.hsc
Unit Set:	NASA
Date/Time:	Mon Aug 23 10:24:41 2010

Workbook: Case (Main) (continued)

Composition (continued)

Name	Carbon Out	4	5	6	Recycle Stream
Comp Mole Frac (Carbon)	1.00000	0.00000	0.00000	0.00000	0.00000
Comp Mole Frac (Oxygen)	0.00000	0.00000	0.00000	0.00000	0.00000
Comp Mole Frac (H2O)	0.00000	0.08905	0.08905	0.04648	0.04648
Comp Mole Frac (Methane)	0.00000	0.07535	0.07535	0.07887	0.07887
Comp Mole Frac (CO)	0.00000	0.21715	0.21715	0.22730	0.22730
Comp Mole Frac (Hydrogen)	0.00000	0.49920	0.49920	0.52253	0.52253
Comp Mole Frac (CO2)	0.00000	0.11926	0.11926	0.12483	0.12483
Name	**Water**	**Water In**	**7**	**8**	**9**
Comp Mole Frac (Carbon)	0.00000	0.00000 *	0.00000	0.00000	0.00000
Comp Mole Frac (Oxygen)	0.00000	0.00000 *	0.00000	0.00000	0.00000
Comp Mole Frac (H2O)	0.99996	1.00000 *	1.00000	0.99996	0.00000
Comp Mole Frac (Methane)	0.00000	0.00000 *	0.00000	0.00000	0.00000
Comp Mole Frac (CO)	0.00000	0.00000 *	0.00000	0.00000	0.00000
Comp Mole Frac (Hydrogen)	0.00000	0.00000 *	0.00000	0.00000	0.99996
Comp Mole Frac (CO2)	0.00004	0.00000 *	0.00000	0.00004	0.00004
Name	**Oxygen Out**	**Hydrogen**	**10**		
Comp Mole Frac (Carbon)	0.00000	0.00000	0.00000		
Comp Mole Frac (Oxygen)	1.00000	0.00000	0.00000		
Comp Mole Frac (H2O)	0.00000	0.00000	0.99996		
Comp Mole Frac (Methane)	0.00000	0.00000	0.00000		
Comp Mole Frac (CO)	0.00000	0.00000	0.00000		
Comp Mole Frac (Hydrogen)	0.00000	0.99996	0.00000		
Comp Mole Frac (CO2)	0.00000	0.00004	0.00004		

Heat Exchangers

Name		Recuperating HX
Duty	(kW)	0.3120
Tube Inlet Temperature	(C)	45.61 *
Tube Outlet Temperature	(C)	618.2 *
Shell Inlet Temperature	(C)	650.0
Shell Outlet Temperature	(C)	70.60
UA	(kJ/C-h)	39.47
LMTD	(C)	28.45
Minimum Approach	(C)	25.00

Compressors

Name		Recycle Gas Compre
Feed Pressure	(kPa)	67.29
Product Pressure	(kPa)	82.29
Molar Flow	(gmole/h)	54.01
Energy	(kW)	1.025e-002
Adiabatic Efficiency		75 *
Polytropic Efficiency		76

Pumps

Name		Water Pump	Condensate Pump
Delta P	(kPa)	5.996	40.03
Energy	(kW)	3.206e-009	6.693e-007
Feed Pressure	(kPa)	101.3 *	67.29
Product Pressure	(kPa)	107.3 *	107.3
Molar Flow	(gmole/h)	8.095e-002	2.524
Adiabatic Efficiency	(%)	75.00 *	75.00 *

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Case Name:	C:\NASA Final\Bosch 3-Comp sub atm.hsc
Unit Set:	NASA
Date/Time:	Mon Aug 23 10:24:41 2010

Workbook: Case (Main) (continued)

Unit Ops

Operation Name	Operation Type	Feeds	Products	Ignored	Calc. Level
Recycle Gas Compressor	Compressor	6 Rcycl Cmp Pwr	Recycle Stream	No	500.0 *
M1	Mixer	1 Recycle Stream Hydrogen	2	No	500.0 *
M2	Mixer	10 7	8	No	500.0 *
Recuperating HX	Heat Exchanger	2r 4	3 5	No	500.0 *
Condenser/Water Separator	Separator	5 AMB Q	Water 6 AMB Q	No	500.0 *
RCY-3	Recycle	2	2r	No	3500 *
ADJ-1	Adjust			No	3500 *
ADJ-2	Adjust			No	3500 *
ADJ-3	Adjust			No	3500 *
Bosch Calcs	Spreadsheet			No	500.0 *
Bosch Reactor	Standard Sub-Flowsheet	3 Bosch Heat	4 Carbon Out	No	2500 *
Electrolysis	Standard Sub-Flowsheet	8 Electrolysis Pwr	Oxygen Out 9	No	2500 *
Water Pump	Pump	Water In Water Pmp Pwr	7	No	500.0 *
Condensate Pump	Pump	Water CP Pump Power	10	No	500.0 *
Valve 1	Valve	CO2 In	1	No	500.0 *
Valve 2	Valve	9	Hydrogen	No	500.0 *

Workbook: Bosch Reactor (TPL1)

Streams

Name		3 @TPL1	11 @TPL1	Carbon Out @TPL1	Boudouard Q @TPL1	4 @TPL1
Vapour Fraction		1.0000	1.0000	0.0000	---	1.0000
Temperature	(C)	618.21	650.00 *	650.00	---	650.00 *
Pressure	(kPa)	79.290	76.290	73.290	---	73.290
Molar Flow	(gmole/h)	57.813	57.779	1.2478	---	56.531
Mass Flow	(kg/d)	20.915	20.915	0.35969	---	20.555
Liquid Volume Flow	(m3/h)	2.018e-003	1.944e-003	9.127e-006	---	1.923e-003
Heat Flow	(kW)	-1.187	-1.143	3.548e-003	-5.951e-002	-1.206
Molar Enthalpy	(kJ/kgmole)	-7.390e+004	-7.122e+004	1.024e+004	---	-7.681e+004
Name		RWGS Q @TPL1	Bosch Heat @TPL1			
Vapour Fraction		---	---			
Temperature	(C)	---	---			
Pressure	(kPa)	---	---			
Molar Flow	(gmole/h)	---	---			
Mass Flow	(kg/d)	---	---			
Liquid Volume Flow	(m3/h)	---	---			
Heat Flow	(kW)	4.364e-002	-1.587e-002			
Molar Enthalpy	(kJ/kgmole)	---	---			

* Specified by user.

Workbook: Bosch Reactor (TPL1) (continued)

Material Streams

Name	3 @TPL1	11 @TPL1	Carbon Out @TPL1	4 @TPL1	
Comp Mole Frac (Carbon)	0.00000	0.00000	1.00000	0.00000	
Comp Mole Frac (Oxygen)	0.00000	0.00000	0.00000	0.00000	
Comp Mole Frac (H2O)	0.04344	0.08713	0.00000	0.08905	
Comp Mole Frac (Methane)	0.07339	0.07372	0.00000	0.07535	
Comp Mole Frac (CO)	0.21244	0.25565	0.00000	0.21715	
Comp Mole Frac (Hydrogen)	0.53236	0.48842	0.00000	0.49920	
Comp Mole Frac (CO2)	0.13838	0.09509	0.00000	0.11926	

Unit Ops

Operation Name	Operation Type	Feeds	Products	Ignored	Calc. Level
RWGS Reaction @TPL1	Gibbs Reactor	3 @TPL1 RWGS Q @TPL1	10 @TPL1 11 @TPL1 RWGS Q @TPL1	No	500.0 *
Boudourd Reaction @TPL1	Equilibrium Reactor	11 @TPL1 Boudouard Q @TPL1	Carbon Out @TPL1 4 @TPL1 Boudouard Q @TPL1	No	500.0 *
SPRDSHT-1 @TPL1	Spreadsheet			No	500.0 *

Workbook: Electrolysis (TPL2)

Streams

Name	8 @TPL2	10 @TPL2	9 @TPL2	Oxygen Out @TPL2	Electrolysis Pwr @T
Vapour Fraction	0.0000	1.0000	1.0000	1.0000	---
Temperature (C)	24.883	24.883	24.883	24.981	---
Pressure (kPa)	107.32	104.32	101.32	101.32	---
Molar Flow (gmole/h)	2.6049	3.9072	2.6049	1.3023	---
Mass Flow (kg/d)	1.1263	1.1263	0.12614	1.0002	---
Liquid Volume Flow (m3/h)	4.703e-005	1.118e-004	7.517e-005	3.663e-005	---
Heat Flow (kW)	-0.2065	-1.726e-005	-1.361e-005	-3.650e-006	0.2065
Molar Enthalpy (kJ/kgmole)	-2.854e+005	-15.90	-18.81	-10.09	---

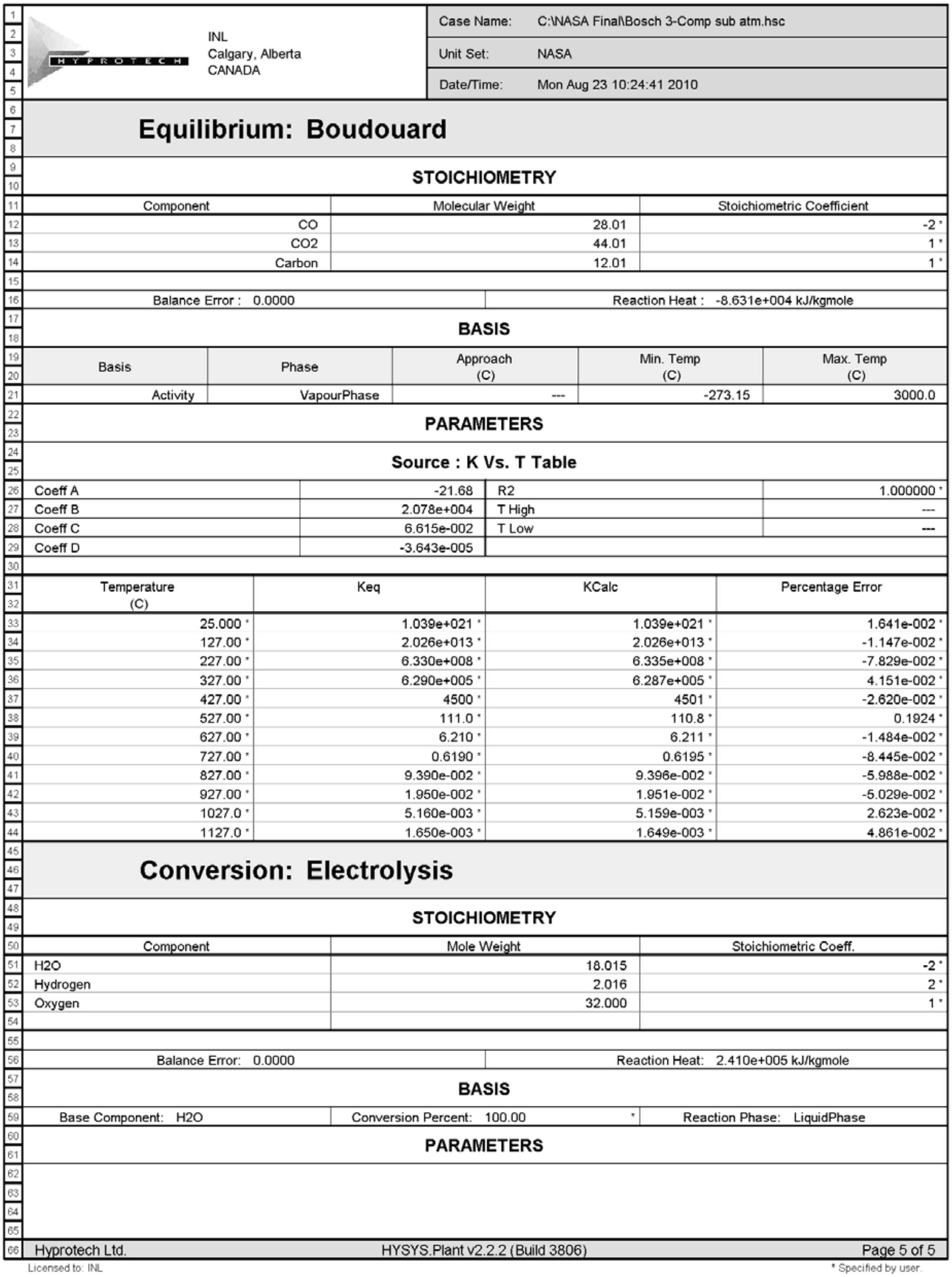
Material Streams

Name	8 @TPL2	9 @TPL2	10 @TPL2	Oxygen Out @TPL2	
Comp Mole Frac (Carbon)	0.00000	0.00000	0.00000	0.00000	
Comp Mole Frac (Oxygen)	0.00000	0.00000	0.33331	1.00000	
Comp Mole Frac (H2O)	0.99996	0.00000	0.00000	0.00000	
Comp Mole Frac (Methane)	0.00000	0.00000	0.00000	0.00000	
Comp Mole Frac (CO)	0.00000	0.00000	0.00000	0.00000	
Comp Mole Frac (Hydrogen)	0.00000	0.99996	0.66666	0.00000	
Comp Mole Frac (CO2)	0.00004	0.00004	0.00003	0.00000	

Unit Ops

Operation Name	Operation Type	Feeds	Products	Ignored	Calc. Level
Electrolysis @TPL2	Conversion Reactor	8 @TPL2 Electrolysis Pwr @TPL2	17 @TPL2 10 @TPL2 Electrolysis Pwr @TPL2	No	500.0 *
H2/O2 Splitter @TPL2	Component Splitter	10 @TPL2	9 @TPL2 Oxygen Out @TPL2	No	500.0 *
SET-1 @TPL2	Set			No	500.0 *
SET-2 @TPL2	Set			No	500.0 *
SET-3 @TPL2	Set			No	500.0 *
SET-4 @TPL2	Set			No	500.0 *

* Specified by user.



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Calgary, Alberta
CANADA

Case Name:	C:\NASA Final\Bosch 3-Comp sub atm.hsc
Unit Set:	NASA
Date/Time:	Mon Aug 23 10:24:41 2010

Equilibrium: Boudouard

STOICHIOMETRY

Component	Molecular Weight	Stoichiometric Coefficient
CO	28.01	-2 *
CO2	44.01	1 *
Carbon	12.01	1 *

Balance Error : 0.0000

Reaction Heat : -8.631e+004 kJ/kgmole

BASIS

Basis	Phase	Approach (C)	Min. Temp (C)	Max. Temp (C)
Activity	VapourPhase	---	-273.15	3000.0

PARAMETERS

Source : K Vs. T Table

Coeff A	-21.68	R2	1.000000 *
Coeff B	2.078e+004	T High	---
Coeff C	6.615e-002	T Low	---
Coeff D	-3.643e-005		

Temperature (C)	Keq	KCalc	Percentage Error
25.000 *	1.039e+021 *	1.039e+021 *	1.641e-002 *
127.00 *	2.026e+013 *	2.026e+013 *	-1.147e-002 *
227.00 *	6.330e+008 *	6.335e+008 *	-7.829e-002 *
327.00 *	6.290e+005 *	6.287e+005 *	4.151e-002 *
427.00 *	4500 *	4501 *	-2.620e-002 *
527.00 *	111.0 *	110.8 *	0.1924 *
627.00 *	6.210 *	6.211 *	-1.484e-002 *
727.00 *	0.6190 *	0.6195 *	-8.445e-002 *
827.00 *	9.390e-002 *	9.396e-002 *	-5.988e-002 *
927.00 *	1.950e-002 *	1.951e-002 *	-5.029e-002 *
1027.0 *	5.160e-003 *	5.159e-003 *	2.623e-002 *
1127.0 *	1.650e-003 *	1.649e-003 *	4.861e-002 *

Conversion: Electrolysis

STOICHIOMETRY

Component	Mole Weight	Stoichiometric Coeff.
H2O	18.015	-2 *
Hydrogen	2.016	2 *
Oxygen	32.000	1 *

Balance Error: 0.0000

Reaction Heat: 2.410e+005 kJ/kgmole

BASIS

Base Component: H2O	Conversion Percent: 100.00 *	Reaction Phase: LiquidPhase

PARAMETERS

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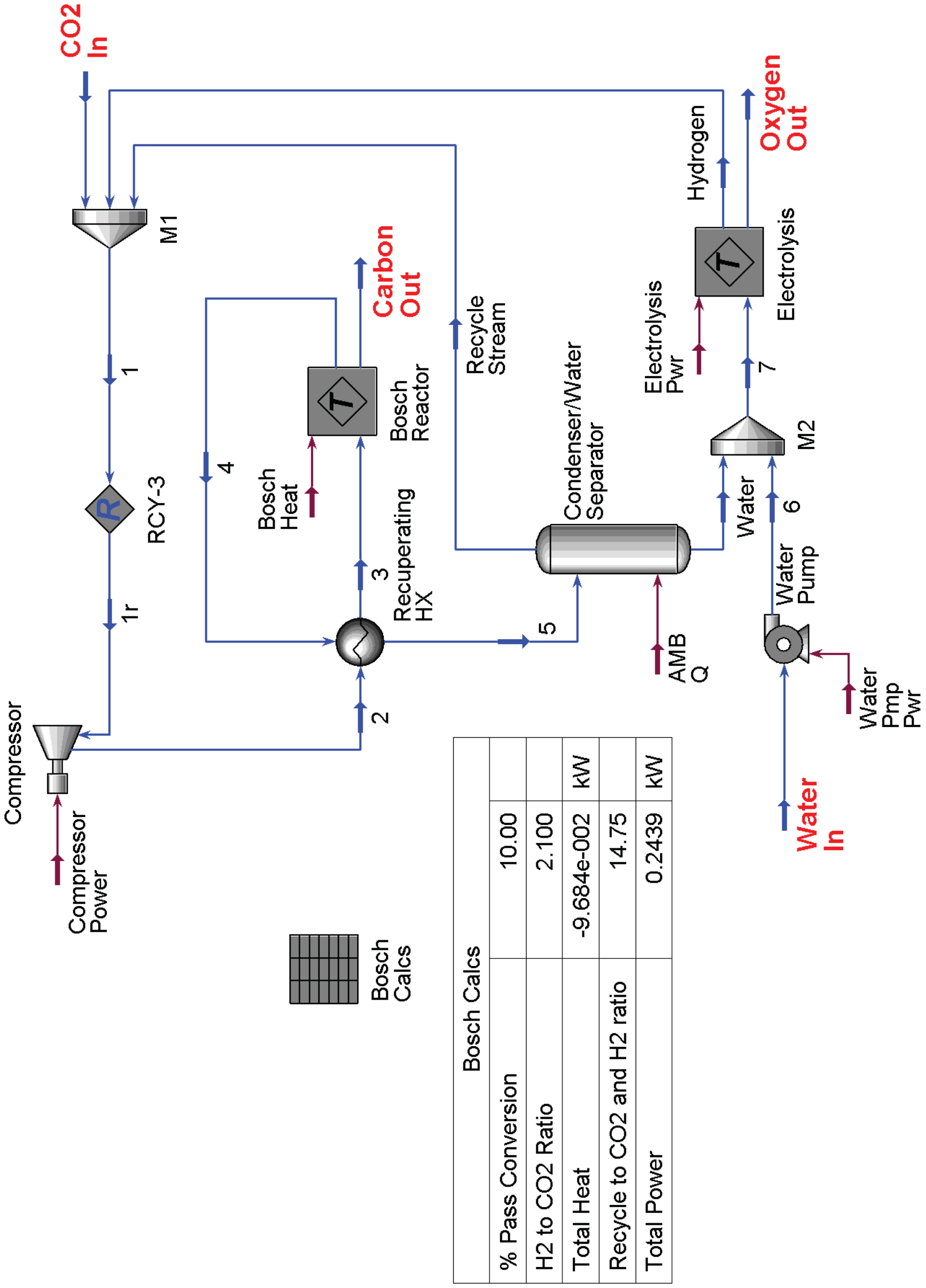
* Specified by user.

A.3 Bosch Process with 1 Compressor



Bosch Calcs		
% Pass Conversion	10.00	
H2 to CO2 Ratio	2.100	
Total Heat	-9.684e-002	kW
Recycle to CO2 and H2 ratio	14.75	
Total Power	0.2439	kW

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

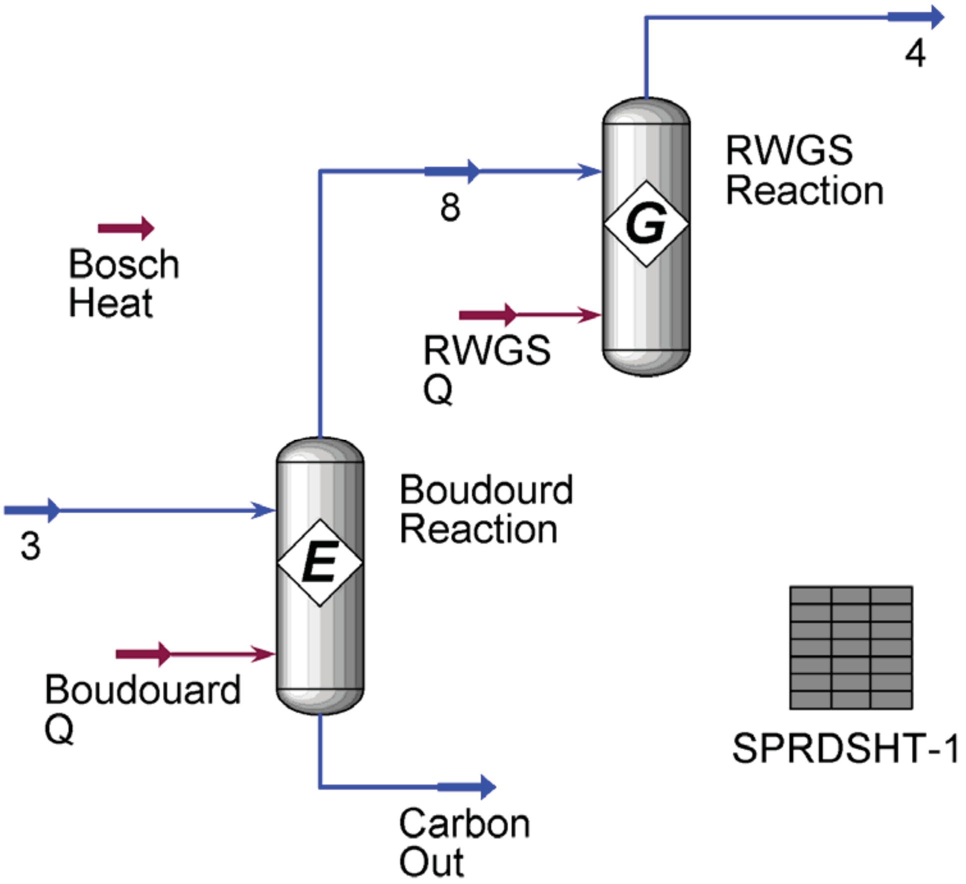


Figure A - 6 Process flow diagram of Bosch Reactor within Bosch process with 1 compressor

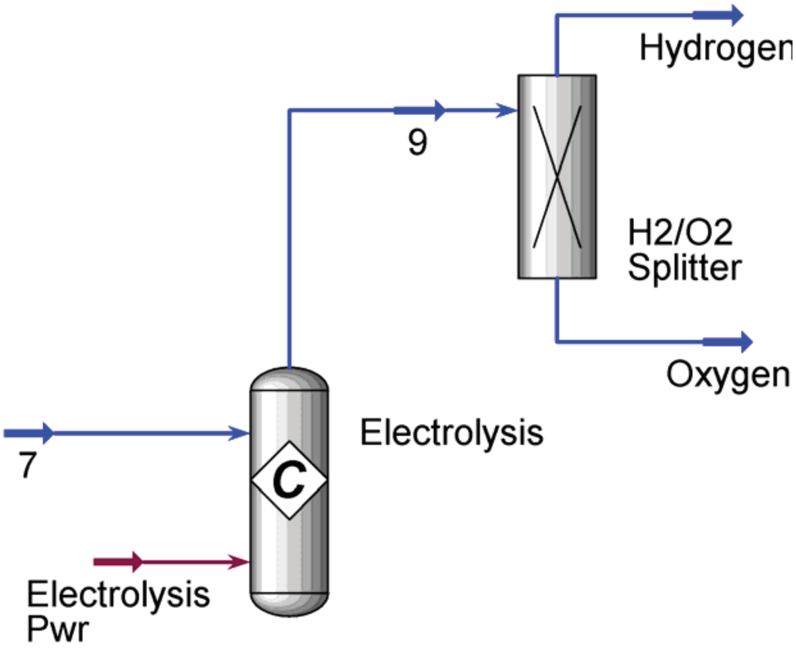


Figure A - 7 Process flow diagram of Electrolysis Module within Bosch process with 1 compressor

Workbook: Case (Main)

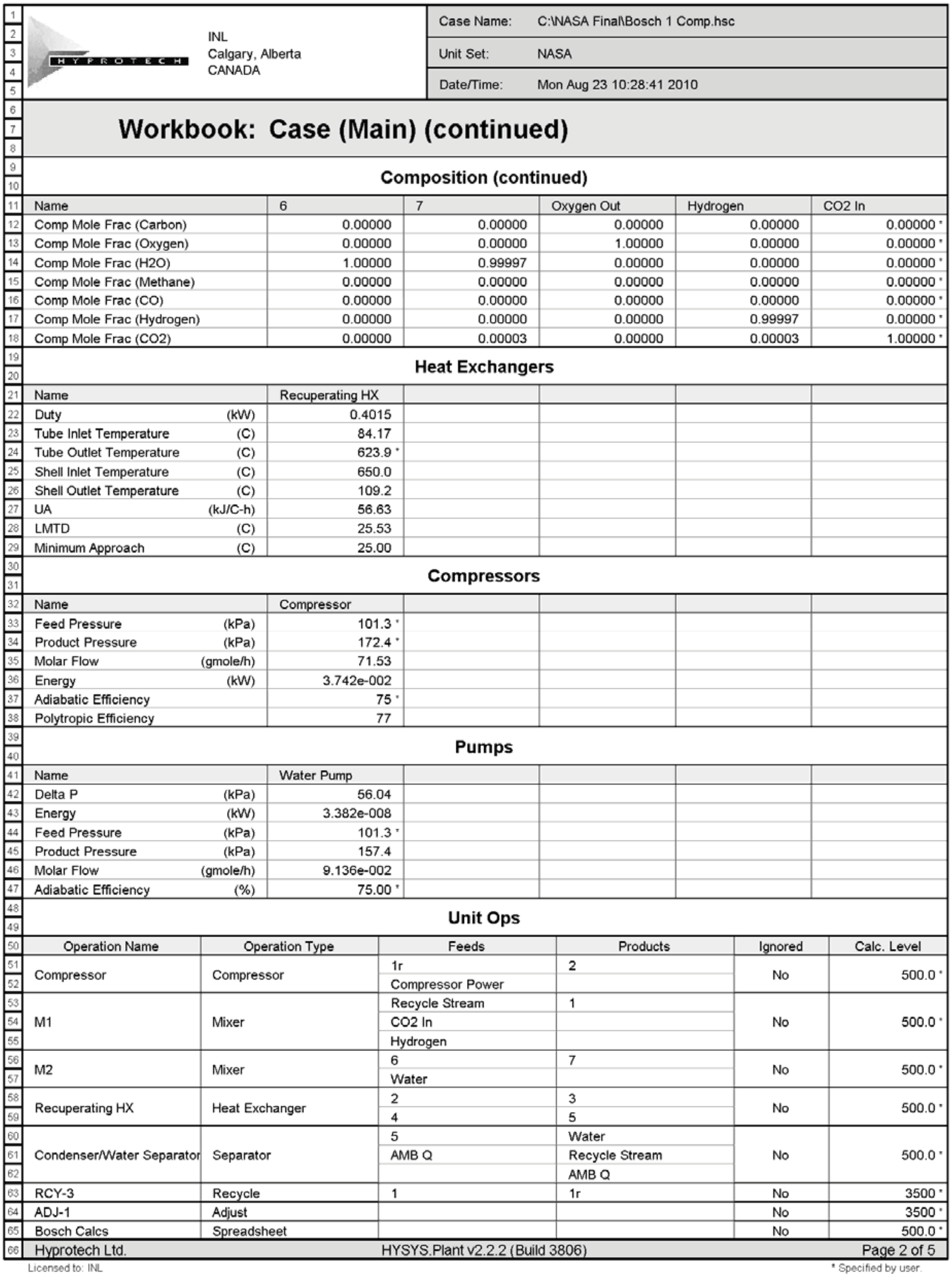
Streams

Name	1	1r	Compressor Power	2	3
Vapour Fraction	1.0000	1.0000	---	1.0000	1.0000
Temperature (C)	24.794	24.792 *	---	84.170	623.87 *
Pressure (kPa)	101.32	101.32 *	---	172.37 *	169.37
Molar Flow (gmole/h)	71.552	71.525	---	71.525	71.525
Mass Flow (kg/d)	22.610	22.613 *	---	22.613	22.613
Liquid Volume Flow (m3/h)	2.718e-003	2.716e-003	---	2.716e-003	2.716e-003
Heat Flow (kW)	-1.352	-1.353	3.742e-002	-1.316	-0.9141
Molar Enthalpy (kJ/kgmole)	-6.804e+004	-6.810e+004	---	-6.622e+004	-4.601e+004
Name	**Bosch Heat**	**4**	**Carbon Out**	**5**	**AMB Q**
Vapour Fraction	---	1.0000	0.0000 *	1.0000	---
Temperature (C)	---	650.00	650.00	109.17	---
Pressure (kPa)	---	163.37	166.37	160.37	---
Molar Flow (gmole/h)	---	70.221	1.2227	70.221	---
Mass Flow (kg/d)	---	22.261	0.35246	22.261	---
Liquid Volume Flow (m3/h)	---	2.622e-003	8.944e-006	2.622e-003	---
Heat Flow (kW)	-1.326e-002	-0.9308	3.477e-003	-1.332	-8.357e-002
Molar Enthalpy (kJ/kgmole)	---	-4.772e+004	1.024e+004	-6.831e+004	---
Name	**Recycle Stream**	**Water**	**Water In**	**Water Pmp Pwr**	**6**
Vapour Fraction	1.0000	0.0000	0.0000	---	0.0000
Temperature (C)	25.000 *	25.000	21.111 *	---	21.116
Pressure (kPa)	157.37	157.37	101.32 *	---	157.37
Molar Flow (gmole/h)	67.708	2.5129	9.1359e-002	---	9.1359e-002
Mass Flow (kg/d)	21.174	1.0865	3.9500e-002 *	---	3.9500e-002
Liquid Volume Flow (m3/h)	2.576e-003	4.536e-005	1.649e-006	---	1.649e-006
Heat Flow (kW)	-1.217	-0.1992	-7.251e-003	3.382e-008	-7.251e-003
Molar Enthalpy (kJ/kgmole)	-6.469e+004	-2.854e+005	-2.857e+005	---	-2.857e+005
Name	**7**	**Electrolysis Pwr**	**Hydrogen**	**Oxygen Out**	**CO2 In**
Vapour Fraction	0.0000	---	1.0000	1.0000	1.0000
Temperature (C)	24.864	---	24.864	25.014	21.111 *
Pressure (kPa)	157.37	---	151.37	151.37	101.32 *
Molar Flow (gmole/h)	2.6043	---	2.6043	1.3020	1.2401
Mass Flow (kg/d)	1.1260	---	0.12609	0.99995	1.3098 *
Liquid Volume Flow (m3/h)	4.701e-005	---	7.516e-005	3.662e-005	6.613e-005
Heat Flow (kW)	-0.2065	0.2065	-1.250e-005	-5.004e-006	-0.1357
Molar Enthalpy (kJ/kgmole)	-2.854e+005	---	-17.28	-13.84	-3.940e+005

Composition

Name	1	1r	2	3	Carbon Out
Comp Mole Frac (Carbon)	0.00000	0.00000 *	0.00000	0.00000	1.00000
Comp Mole Frac (Oxygen)	0.00000	0.00000 *	0.00000	0.00000	0.00000
Comp Mole Frac (H2O)	0.01891	0.01890 *	0.01890	0.01890	0.00000
Comp Mole Frac (Methane)	0.27413	0.27366 *	0.27366	0.27366	0.00000
Comp Mole Frac (CO)	0.17063	0.17088 *	0.17088	0.17088	0.00000
Comp Mole Frac (Hydrogen)	0.47520	0.47526 *	0.47526	0.47526	0.00000
Comp Mole Frac (CO2)	0.06113	0.06130 *	0.06130	0.06130	0.00000
Name	**4**	**5**	**Recycle Stream**	**Water**	**Water In**
Comp Mole Frac (Carbon)	0.00000	0.00000	0.00000	0.00000	0.00000 *
Comp Mole Frac (Oxygen)	0.00000	0.00000	0.00000	0.00000	0.00000 *
Comp Mole Frac (H2O)	0.05505	0.05505	0.01998	0.99996	1.00000 *
Comp Mole Frac (Methane)	0.27933	0.27933	0.28970	0.00000	0.00000 *
Comp Mole Frac (CO)	0.17386	0.17386	0.18032	0.00000	0.00000 *
Comp Mole Frac (Hydrogen)	0.44712	0.44712	0.46372	0.00000	0.00000 *
Comp Mole Frac (CO2)	0.04463	0.04463	0.04628	0.00003	0.00000 *

* Specified by user.



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CANADA

Case Name:	C:\NASA Final\Bosch 1 Comp.hsc
Unit Set:	NASA
Date/Time:	Mon Aug 23 10:28:41 2010

Workbook: Case (Main) (continued)

Composition (continued)

Name	6	7	Oxygen Out	Hydrogen	CO2 In
Comp Mole Frac (Carbon)	0.00000	0.00000	0.00000	0.00000	0.00000 *
Comp Mole Frac (Oxygen)	0.00000	0.00000	1.00000	0.00000	0.00000 *
Comp Mole Frac (H2O)	1.00000	0.99997	0.00000	0.00000	0.00000 *
Comp Mole Frac (Methane)	0.00000	0.00000	0.00000	0.00000	0.00000 *
Comp Mole Frac (CO)	0.00000	0.00000	0.00000	0.00000	0.00000 *
Comp Mole Frac (Hydrogen)	0.00000	0.00000	0.00000	0.99997	0.00000 *
Comp Mole Frac (CO2)	0.00000	0.00003	0.00000	0.00003	1.00000 *

Heat Exchangers

Name		Recuperating HX
Duty	(kW)	0.4015
Tube Inlet Temperature	(C)	84.17
Tube Outlet Temperature	(C)	623.9 *
Shell Inlet Temperature	(C)	650.0
Shell Outlet Temperature	(C)	109.2
UA	(kJ/C-h)	56.63
LMTD	(C)	25.53
Minimum Approach	(C)	25.00

Compressors

Name		Compressor
Feed Pressure	(kPa)	101.3 *
Product Pressure	(kPa)	172.4 *
Molar Flow	(gmole/h)	71.53
Energy	(kW)	3.742e-002
Adiabatic Efficiency		75 *
Polytropic Efficiency		77

Pumps

Name		Water Pump
Delta P	(kPa)	56.04
Energy	(kW)	3.382e-008
Feed Pressure	(kPa)	101.3 *
Product Pressure	(kPa)	157.4
Molar Flow	(gmole/h)	9.136e-002
Adiabatic Efficiency	(%)	75.00 *

Unit Ops

Operation Name	Operation Type	Feeds	Products	Ignored	Calc. Level
Compressor	Compressor	1r Compressor Power	2	No	500.0 *
M1	Mixer	Recycle Stream CO2 In Hydrogen	1	No	500.0 *
M2	Mixer	6 Water	7	No	500.0 *
Recuperating HX	Heat Exchanger	2 4	3 5	No	500.0 *
Condenser/Water Separator	Separator	5 AMB Q	Water Recycle Stream AMB Q	No	500.0 *
RCY-3	Recycle	1	1r	No	3500 *
ADJ-1	Adjust			No	3500 *
Bosch Calcs	Spreadsheet			No	500.0 *

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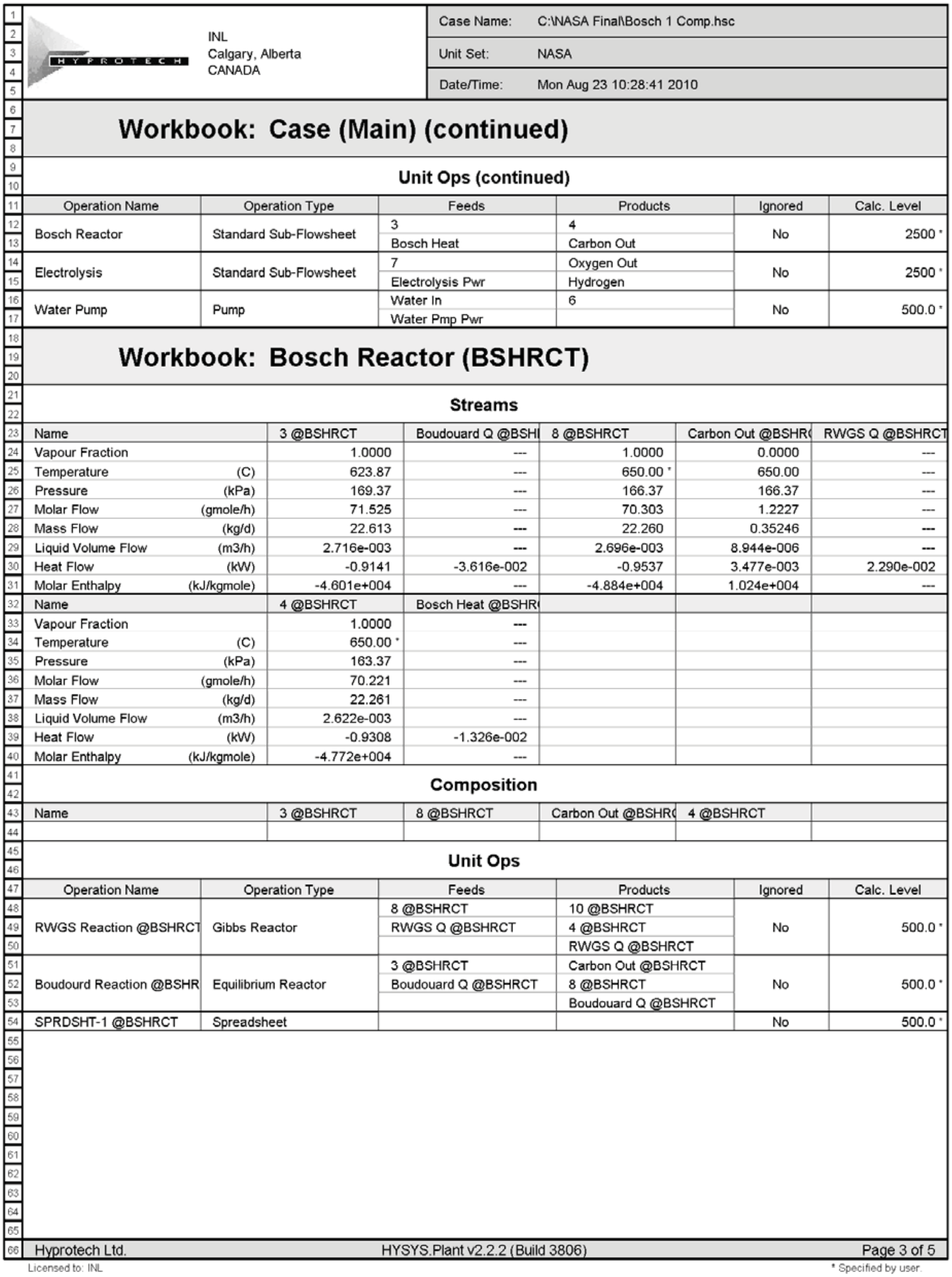

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Calgary, Alberta
CANADA

Case Name:	C:\NASA Final\Bosch 1 Comp.hsc
Unit Set:	NASA
Date/Time:	Mon Aug 23 10:28:41 2010

Workbook: Case (Main) (continued)

Unit Ops (continued)

Operation Name	Operation Type	Feeds	Products	Ignored	Calc. Level
Bosch Reactor	Standard Sub-Flowsheet	3 Bosch Heat	4 Carbon Out	No	2500 *
Electrolysis	Standard Sub-Flowsheet	7 Electrolysis Pwr	Oxygen Out Hydrogen	No	2500 *
Water Pump	Pump	Water In Water Pmp Pwr	6	No	500.0 *

Workbook: Bosch Reactor (BSHRCT)

Streams

Name		3 @BSHRCT	Boudouard Q @BSHI	8 @BSHRCT	Carbon Out @BSHR(	RWGS Q @BSHRCT
Vapour Fraction		1.0000	---	1.0000	0.0000	---
Temperature	(C)	623.87	---	650.00 *	650.00	---
Pressure	(kPa)	169.37	---	166.37	166.37	---
Molar Flow	(gmole/h)	71.525	---	70.303	1.2227	---
Mass Flow	(kg/d)	22.613	---	22.260	0.35246	---
Liquid Volume Flow	(m3/h)	2.716e-003	---	2.696e-003	8.944e-006	---
Heat Flow	(kW)	-0.9141	-3.616e-002	-0.9537	3.477e-003	2.290e-002
Molar Enthalpy	(kJ/kgmole)	-4.601e+004	---	-4.884e+004	1.024e+004	---
Name		4 @BSHRCT	Bosch Heat @BSHR(			
Vapour Fraction		1.0000	---			
Temperature	(C)	650.00 *	---			
Pressure	(kPa)	163.37	---			
Molar Flow	(gmole/h)	70.221	---			
Mass Flow	(kg/d)	22.261	---			
Liquid Volume Flow	(m3/h)	2.622e-003	---			
Heat Flow	(kW)	-0.9308	-1.326e-002			
Molar Enthalpy	(kJ/kgmole)	-4.772e+004	---			

Composition

Name	3 @BSHRCT	8 @BSHRCT	Carbon Out @BSHR(	4 @BSHRCT	

Unit Ops

Operation Name	Operation Type	Feeds	Products	Ignored	Calc. Level
RWGS Reaction @BSHRCT	Gibbs Reactor	8 @BSHRCT RWGS Q @BSHRCT	10 @BSHRCT 4 @BSHRCT RWGS Q @BSHRCT	No	500.0 *
Boudourd Reaction @BSHR	Equilibrium Reactor	3 @BSHRCT Boudouard Q @BSHRCT	Carbon Out @BSHRCT 8 @BSHRCT Boudouard Q @BSHRCT	No	500.0 *
SPRDSHT-1 @BSHRCT	Spreadsheet			No	500.0 *

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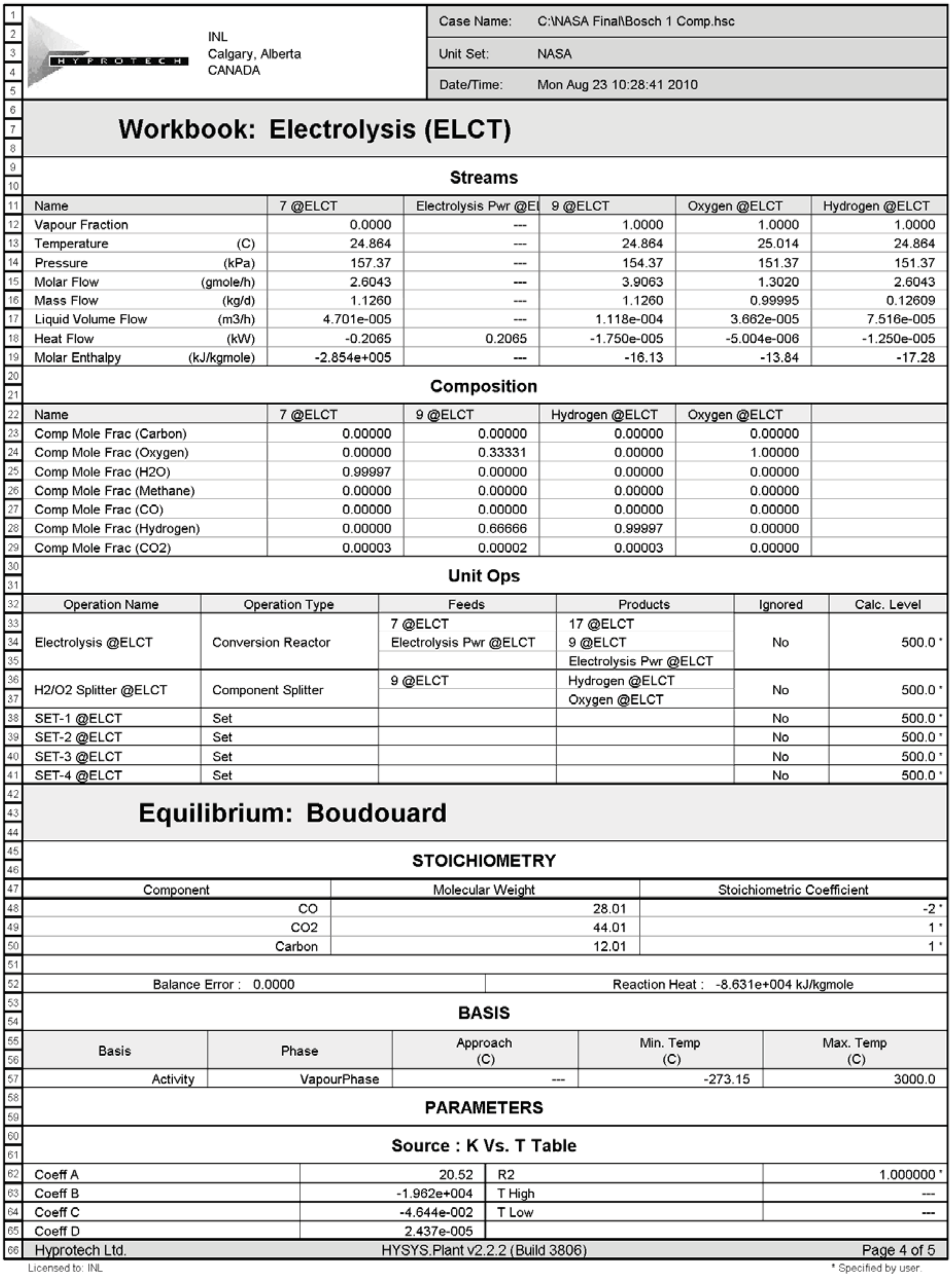

INL Calgary, Alberta CANADA	Case Name: C:\NASA Final\Bosch 1 Comp.hsc Unit Set: NASA Date/Time: Mon Aug 23 10:28:41 2010

Workbook: Electrolysis (ELCT)

Streams

Name		7 @ELCT	Electrolysis Pwr @El	9 @ELCT	Oxygen @ELCT	Hydrogen @ELCT
Vapour Fraction		0.0000	---	1.0000	1.0000	1.0000
Temperature	(C)	24.864	---	24.864	25.014	24.864
Pressure	(kPa)	157.37	---	154.37	151.37	151.37
Molar Flow	(gmole/h)	2.6043	---	3.9063	1.3020	2.6043
Mass Flow	(kg/d)	1.1260	---	1.1260	0.99995	0.12609
Liquid Volume Flow	(m3/h)	4.701e-005	---	1.118e-004	3.662e-005	7.516e-005
Heat Flow	(kW)	-0.2065	0.2065	-1.750e-005	-5.004e-006	-1.250e-005
Molar Enthalpy	(kJ/kgmole)	-2.854e+005	---	-16.13	-13.84	-17.28

Composition

Name	7 @ELCT	9 @ELCT	Hydrogen @ELCT	Oxygen @ELCT	
Comp Mole Frac (Carbon)	0.00000	0.00000	0.00000	0.00000	
Comp Mole Frac (Oxygen)	0.00000	0.33331	0.00000	1.00000	
Comp Mole Frac (H2O)	0.99997	0.00000	0.00000	0.00000	
Comp Mole Frac (Methane)	0.00000	0.00000	0.00000	0.00000	
Comp Mole Frac (CO)	0.00000	0.00000	0.00000	0.00000	
Comp Mole Frac (Hydrogen)	0.00000	0.66666	0.99997	0.00000	
Comp Mole Frac (CO2)	0.00003	0.00002	0.00003	0.00000	

Unit Ops

Operation Name	Operation Type	Feeds	Products	Ignored	Calc. Level
Electrolysis @ELCT	Conversion Reactor	7 @ELCT Electrolysis Pwr @ELCT	17 @ELCT 9 @ELCT Electrolysis Pwr @ELCT	No	500.0 *
H2/O2 Splitter @ELCT	Component Splitter	9 @ELCT	Hydrogen @ELCT Oxygen @ELCT	No	500.0 *
SET-1 @ELCT	Set			No	500.0 *
SET-2 @ELCT	Set			No	500.0 *
SET-3 @ELCT	Set			No	500.0 *
SET-4 @ELCT	Set			No	500.0 *

Equilibrium: Boudouard

STOICHIOMETRY

Component	Molecular Weight	Stoichiometric Coefficient
CO	28.01	-2 *
CO2	44.01	1 *
Carbon	12.01	1 *

Balance Error : 0.0000

Reaction Heat : -8.631e+004 kJ/kgmole

BASIS

Basis	Phase	Approach (C)	Min. Temp (C)	Max. Temp (C)
Activity	VapourPhase	---	-273.15	3000.0

PARAMETERS

Source : K Vs. T Table

Coeff A	20.52	R2	1.000000 *
Coeff B	-1.962e+004	T High	---
Coeff C	-4.644e-002	T Low	---
Coeff D	2.437e-005		

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Equilibrium: Boudouard (continued)

PARAMETERS

Source : K Vs. T Table

Temperature (C)	Keq	KCalc	Percentage Error
25.000 *	1.640e-020 *	1.640e-020 *	-2.452e-002 *
127.00 *	3.140e-013 *	3.139e-013 *	3.731e-002 *
227.00 *	5.650e-009 *	5.648e-009 *	3.529e-002 *
327.00 *	3.880e-006 *	3.879e-006 *	3.547e-002 *
427.00 *	4.120e-004 *	4.120e-004 *	-1.092e-002 *
527.00 *	1.360e-002 *	1.363e-002 *	-0.2546 *
627.00 *	0.2075 *	0.2073 *	6.258e-002 *
727.00 *	1.830 *	1.829 *	6.516e-002 *
827.00 *	10.87 *	10.86 *	5.621e-002 *
927.00 *	47.97 *	47.95 *	4.263e-002 *
1027.0 *	168.5 *	168.4 *	1.777e-002 *
1127.0 *	494.5 *	494.5 *	-1.079e-002 *
1227.0 *	1257 *	1258 *	-5.204e-002 *

Conversion: Electrolysis

STOICHIOMETRY

Component	Mole Weight	Stoichiometric Coeff.
H2O	18.015	-2 *
Hydrogen	2.016	2 *
Oxygen	32.000	1 *

Balance Error: 0.0000

Reaction Heat: 2.410e+005 kJ/kgmole

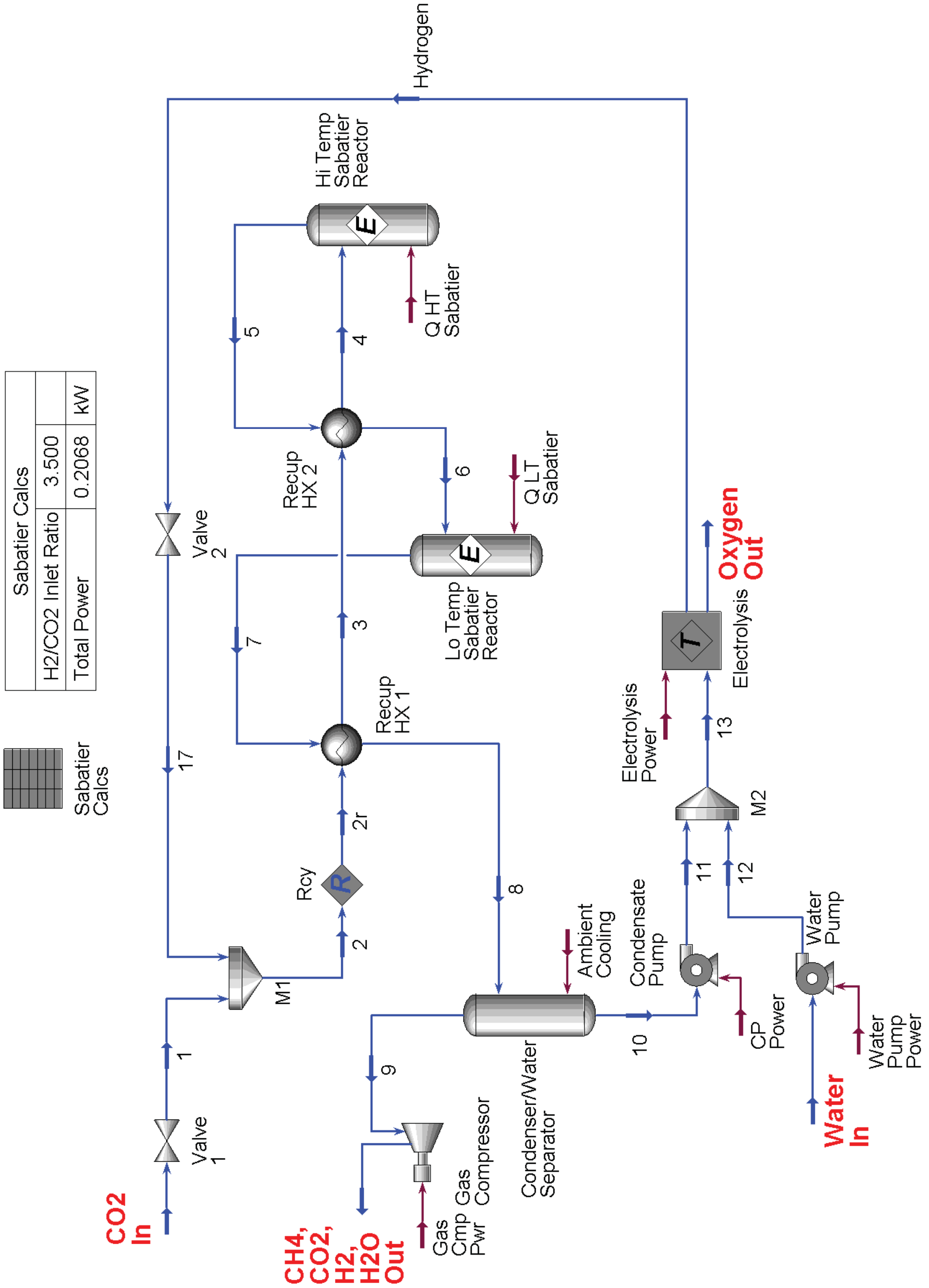
BASIS

Base Component: H2O	Conversion Percent: 100.00 *	Reaction Phase: LiquidPhase

PARAMETERS

* Specified by user.

A.4 Base Sabatier Process



Sabatier Calcs		
H2/CO2 Inlet Ratio	3.500	
Total Power	0.2068	kW

Figure A - 8 Process flow diagram of base Sabatier process

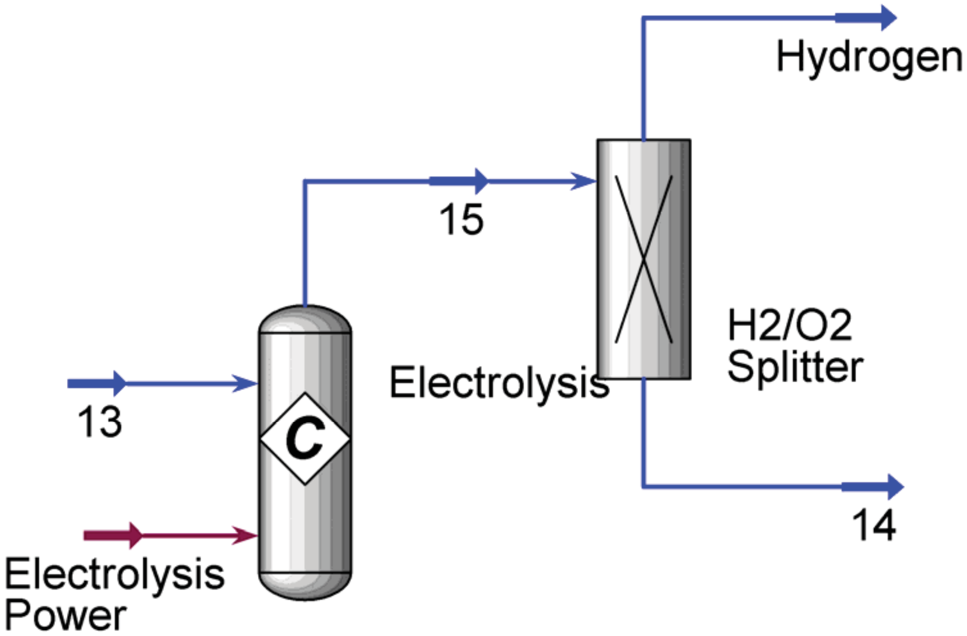
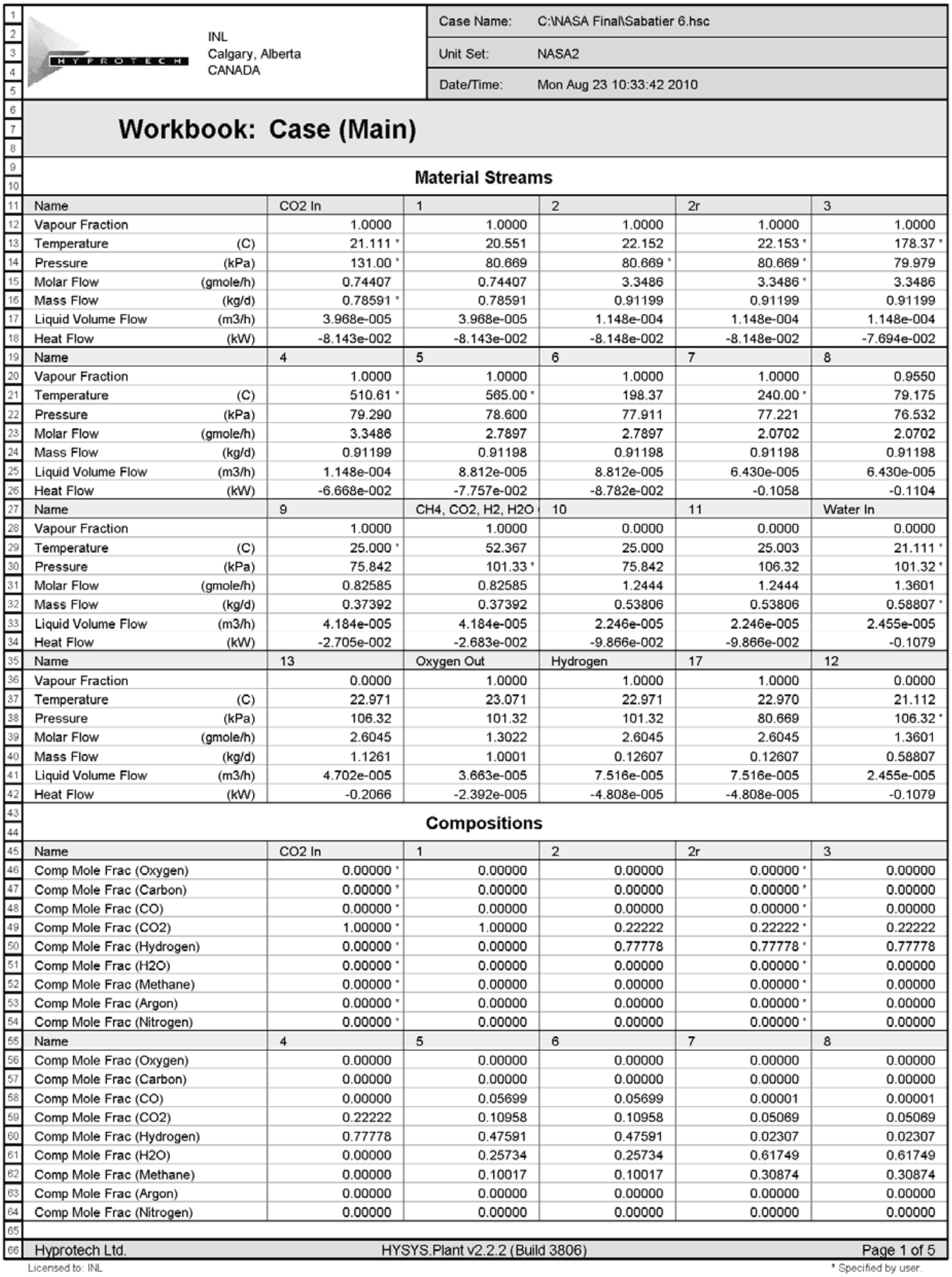


Figure A - 9 Process flow diagram of Electrolysis module within Sabatier process



INL
Calgary, Alberta
CANADA

Case Name: C:\NASA Final\Sabatier 6.hsc
Unit Set: NASA2
Date/Time: Mon Aug 23 10:33:42 2010

Workbook: Case (Main)

Material Streams

Name	CO2 In	1	2	2r	3
Vapour Fraction	1.0000	1.0000	1.0000	1.0000	1.0000
Temperature (C)	21.111 *	20.551	22.152	22.153 *	178.37 *
Pressure (kPa)	131.00 *	80.669	80.669 *	80.669 *	79.979
Molar Flow (gmole/h)	0.74407	0.74407	3.3486	3.3486 *	3.3486
Mass Flow (kg/d)	0.78591 *	0.78591	0.91199	0.91199	0.91199
Liquid Volume Flow (m3/h)	3.968e-005	3.968e-005	1.148e-004	1.148e-004	1.148e-004
Heat Flow (kW)	-8.143e-002	-8.143e-002	-8.148e-002	-8.148e-002	-7.694e-002
Name	4	5	6	7	8
Vapour Fraction	1.0000	1.0000	1.0000	1.0000	0.9550
Temperature (C)	510.61 *	565.00 *	198.37	240.00 *	79.175
Pressure (kPa)	79.290	78.600	77.911	77.221	76.532
Molar Flow (gmole/h)	3.3486	2.7897	2.7897	2.0702	2.0702
Mass Flow (kg/d)	0.91199	0.91198	0.91198	0.91198	0.91198
Liquid Volume Flow (m3/h)	1.148e-004	8.812e-005	8.812e-005	6.430e-005	6.430e-005
Heat Flow (kW)	-6.668e-002	-7.757e-002	-8.782e-002	-0.1058	-0.1104
Name	9	CH4, CO2, H2, H2O	10	11	Water In
Vapour Fraction	1.0000	1.0000	0.0000	0.0000	0.0000
Temperature (C)	25.000 *	52.367	25.000	25.003	21.111 *
Pressure (kPa)	75.842	101.33 *	75.842	106.32	101.32 *
Molar Flow (gmole/h)	0.82585	0.82585	1.2444	1.2444	1.3601
Mass Flow (kg/d)	0.37392	0.37392	0.53806	0.53806	0.58807 *
Liquid Volume Flow (m3/h)	4.184e-005	4.184e-005	2.246e-005	2.246e-005	2.455e-005
Heat Flow (kW)	-2.705e-002	-2.683e-002	-9.866e-002	-9.866e-002	-0.1079
Name	13	Oxygen Out	Hydrogen	17	12
Vapour Fraction	0.0000	1.0000	1.0000	1.0000	0.0000
Temperature (C)	22.971	23.071	22.971	22.970	21.112
Pressure (kPa)	106.32	101.32	101.32	80.669	106.32 *
Molar Flow (gmole/h)	2.6045	1.3022	2.6045	2.6045	1.3601
Mass Flow (kg/d)	1.1261	1.0001	0.12607	0.12607	0.58807
Liquid Volume Flow (m3/h)	4.702e-005	3.663e-005	7.516e-005	7.516e-005	2.455e-005
Heat Flow (kW)	-0.2066	-2.392e-005	-4.808e-005	-4.808e-005	-0.1079

Compositions

Name	CO2 In	1	2	2r	3
Comp Mole Frac (Oxygen)	0.00000 *	0.00000	0.00000	0.00000 *	0.00000
Comp Mole Frac (Carbon)	0.00000 *	0.00000	0.00000	0.00000 *	0.00000
Comp Mole Frac (CO)	0.00000 *	0.00000	0.00000	0.00000 *	0.00000
Comp Mole Frac (CO2)	1.00000 *	1.00000	0.22222	0.22222 *	0.22222
Comp Mole Frac (Hydrogen)	0.00000 *	0.00000	0.77778	0.77778 *	0.77778
Comp Mole Frac (H2O)	0.00000 *	0.00000	0.00000	0.00000 *	0.00000
Comp Mole Frac (Methane)	0.00000 *	0.00000	0.00000	0.00000 *	0.00000
Comp Mole Frac (Argon)	0.00000 *	0.00000	0.00000	0.00000 *	0.00000
Comp Mole Frac (Nitrogen)	0.00000 *	0.00000	0.00000	0.00000 *	0.00000
Name	4	5	6	7	8
Comp Mole Frac (Oxygen)	0.00000	0.00000	0.00000	0.00000	0.00000
Comp Mole Frac (Carbon)	0.00000	0.00000	0.00000	0.00000	0.00000
Comp Mole Frac (CO)	0.00000	0.05699	0.05699	0.00001	0.00001
Comp Mole Frac (CO2)	0.22222	0.10958	0.10958	0.05069	0.05069
Comp Mole Frac (Hydrogen)	0.77778	0.47591	0.47591	0.02307	0.02307
Comp Mole Frac (H2O)	0.00000	0.25734	0.25734	0.61749	0.61749
Comp Mole Frac (Methane)	0.00000	0.10017	0.10017	0.30874	0.30874
Comp Mole Frac (Argon)	0.00000	0.00000	0.00000	0.00000	0.00000
Comp Mole Frac (Nitrogen)	0.00000	0.00000	0.00000	0.00000	0.00000

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* Specified by user.

Workbook: Case (Main) (continued)

Compositions (continued)

Name	9	CH4, CO2, H2, H2O	10	11	Water In
Comp Mole Frac (Oxygen)	0.00000	0.00000	0.00000	0.00000	0.00000 *
Comp Mole Frac (Carbon)	0.00000	0.00000	0.00000	0.00000	0.00000 *
Comp Mole Frac (CO)	0.00002	0.00002	0.00000	0.00000	0.00000 *
Comp Mole Frac (CO2)	0.12701	0.12701	0.00005	0.00005	0.00000 *
Comp Mole Frac (Hydrogen)	0.05783	0.05783	0.00000	0.00000	0.00000 *
Comp Mole Frac (H2O)	0.04120	0.04120	0.99995	0.99995	1.00000 *
Comp Mole Frac (Methane)	0.77394	0.77394	0.00000	0.00000	0.00000 *
Comp Mole Frac (Argon)	0.00000	0.00000	0.00000	0.00000	0.00000 *
Comp Mole Frac (Nitrogen)	0.00000	0.00000	0.00000	0.00000	0.00000 *

Name	13	Oxygen Out	Hydrogen	17	12
Comp Mole Frac (Oxygen)	0.00000	1.00000	0.00000	0.00000	0.00000
Comp Mole Frac (Carbon)	0.00000	0.00000	0.00000	0.00000	0.00000
Comp Mole Frac (CO)	0.00000	0.00000	0.00000	0.00000	0.00000
Comp Mole Frac (CO2)	0.00002	0.00000	0.00002	0.00002	0.00000
Comp Mole Frac (Hydrogen)	0.00000	0.00000	0.99998	0.99998	0.00000
Comp Mole Frac (H2O)	0.99998	0.00000	0.00000	0.00000	1.00000
Comp Mole Frac (Methane)	0.00000	0.00000	0.00000	0.00000	0.00000
Comp Mole Frac (Argon)	0.00000	0.00000	0.00000	0.00000	0.00000
Comp Mole Frac (Nitrogen)	0.00000	0.00000	0.00000	0.00000	0.00000

Energy Streams

Name		Q HT Sabatier	Q LT Sabatier	Ambient Cooling	Gas Cmp Pwr	CP Power
Heat Flow	(kW)	-1.088e-002	-1.801e-002	-1.534e-002	2.268e-004	2.513e-007
Name		Electrolysis Power	Water Pump Power			
Heat Flow	(kW)	0.2065	4.492e-008			

Compressors

Name		Gas Compressor				
Feed Pressure	(kPa)	75.84				
Product Pressure	(kPa)	101.3 *				
Molar Flow	(gmole/h)	0.8259				
Energy	(kW)	2.268e-004				
Adiabatic Efficiency		75 *				
Polytropic Efficiency		76				

Pumps

Name		Condensate Pump	Water Pump			
Delta P	(kPa)	30.48	5.000			
Energy	(kW)	2.513e-007	4.492e-008			
Feed Pressure	(kPa)	75.84	101.3 *			
Product Pressure	(kPa)	106.3	106.3 *			
Molar Flow	(gmole/h)	1.244	1.360			
Adiabatic Efficiency	(%)	75.00 *	75.00 *			

Heat Exchangers

Name		Recup HX 1	Recup HX 2			
Duty	(kW)	4.544e-003	1.025e-002			
Tube Inlet Temperature	(C)	22.15 *	178.4 *			
Tube Outlet Temperature	(C)	178.4 *	510.6 *			
Shell Inlet Temperature	(C)	240.0 *	565.0 *			
Shell Outlet Temperature	(C)	79.18	198.4			
UA	(W/C)	0.1229	0.2820			
LMTD	(C)	36.97	36.36			
Minimum Approach	(C)	20.00	20.00			

* Specified by user.

Workbook: Case (Main) (continued)

Unit Ops

Operation Name	Operation Type	Feeds	Products	Ignored	Calc. Level
Hi Temp Sabatier Reactor	Equilibrium Reactor	4 Q HT Sabatier	16 5 Q HT Sabatier	No	500.0 *
Lo Temp Sabatier Reactor	Equilibrium Reactor	6 Q LT Sabatier	15 7 Q LT Sabatier	No	500.0 *
Condenser/Water Separator	Separator	8 Ambient Cooling	10 9 Ambient Cooling	No	500.0 *
Rcy	Recycle	2	2r	No	3500 *
M1	Mixer	1 17	2	No	500.0 *
M2	Mixer	11 12	13	No	500.0 *
Min App Adj	Adjust			No	3500 *
ADJ-1	Adjust			No	3500 *
ADJ-2	Adjust			No	3500 *
ADJ-3	Adjust			No	3500 *
Electrolysis	Standard Sub-Flowsheet	13 Electrolysis Power	Oxygen Out Hydrogen	No	2500 *
Sabatier Calcs	Spreadsheet			No	500.0 *
Gas Compressor	Compressor	9 Gas Cmp Pwr	CH4, CO2, H2, H2O Out	No	500.0 *
Condensate Pump	Pump	10 CP Power	11	No	500.0 *
Water Pump	Pump	Water In Water Pump Power	12	No	500.0 *
Recup HX 1	Heat Exchanger	2r 7	3 8	No	500.0 *
Recup HX 2	Heat Exchanger	3 5	4 6	No	500.0 *
Valve 1	Valve	CO2 In	1	No	500.0 *
Valve 2	Valve	Hydrogen	17	No	500.0 *

Workbook: Electrolysis (TPL1)

Streams

Name		13 @TPL1	Electrolysis Power @	15 @TPL1	14 @TPL1	Hydrogen @TPL1
Vapour Fraction		0.0000	---	1.0000	1.0000	1.0000
Temperature	(C)	22.971	---	22.971	23.071	22.971
Pressure	(kPa)	106.32	---	103.82	101.32	101.32
Molar Flow	(gmole/h)	2.6045	---	3.9067	1.3022	2.6045
Mass Flow	(kg/d)	1.1261	---	1.1261	1.0001	0.12607
Liquid Volume Flow	(m3/h)	4.702e-005	---	1.118e-004	3.663e-005	7.516e-005
Heat Flow	(kW)	-0.2066	0.2065	-7.201e-005	-2.392e-005	-4.808e-005
Molar Enthalpy	(kJ/kgmole)	-2.856e+005	---	-66.36	-66.14	-66.46

* Specified by user.

Workbook: Electrolysis (TPL1) (continued)

Composition

Name	13 @TPL1	15 @TPL1	14 @TPL1	Hydrogen @TPL1	
Comp Mole Frac (Oxygen)	0.00000	0.33332	1.00000	0.00000	
Comp Mole Frac (Carbon)	0.00000	0.00000	0.00000	0.00000	
Comp Mole Frac (CO)	0.00000	0.00000	0.00000	0.00000	
Comp Mole Frac (CO2)	0.00002	0.00001	0.00000	0.00002	
Comp Mole Frac (Hydrogen)	0.00000	0.66667	0.00000	0.99998	
Comp Mole Frac (H2O)	0.99998	0.00000	0.00000	0.00000	
Comp Mole Frac (Methane)	0.00000	0.00000	0.00000	0.00000	
Comp Mole Frac (Argon)	0.00000	0.00000	0.00000	0.00000	
Comp Mole Frac (Nitrogen)	0.00000	0.00000	0.00000	0.00000	

Unit Ops

Operation Name	Operation Type	Feeds	Products	Ignored	Calc. Level
Electrolysis @TPL1	Conversion Reactor	13 @TPL1 Electrolysis Power @TPL1	2 @TPL1 15 @TPL1 Electrolysis Power @TPL1	No	500.0 *
H2/O2 Splitter @TPL1	Component Splitter	15 @TPL1	Hydrogen @TPL1 14 @TPL1	No	500.0 *
SET-1 @TPL1	Set			No	500.0 *
SET-2 @TPL1	Set			No	500.0 *
SET-3 @TPL1	Set			No	500.0 *
SET-4 @TPL1	Set			No	500.0 *

Conversion: Electrolysis

STOICHIOMETRY

Component	Mole Weight	Stoichiometric Coeff.
H2O	18.015	-1 *
Hydrogen	2.016	1 *
Oxygen	32.000	0 *

Balance Error: 0.0000 Reaction Heat: 2.410e+005 kJ/kgmole

BASIS

Base Component: H2O Conversion Percent: 100.00 * Reaction Phase: LiquidPhase

PARAMETERS

Equilibrium: Sabatier

STOICHIOMETRY

Component	Molecular Weight	Stoichiometric Coefficient
Methane	16.04	-1 *
H2O	18.02	-1 *
CO	28.01	1 *
Hydrogen	2.016	3 *

Balance Error : 0.0000 Reaction Heat : 2.053e+005 kJ/kgmole

* Specified by user.

Equilibrium: Sabatier (continued)

BASIS

Basis	Phase	Approach (C)	Min. Temp (C)	Max. Temp (C)
Activity	VapourPhase	---	-273.15	3000.0

PARAMETERS

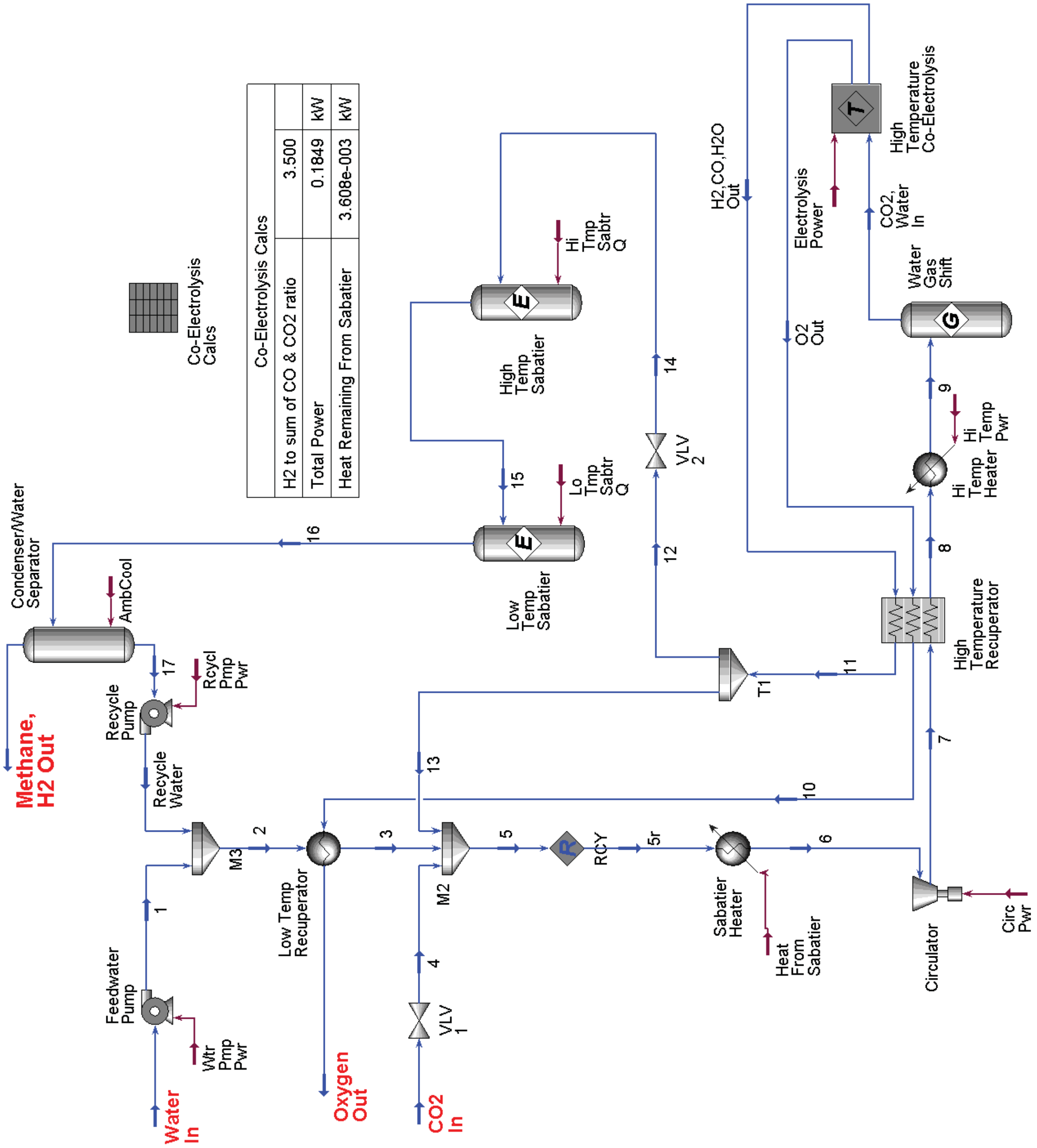
Source : K Vs. T Table

Coeff A	-20.55	R2	0.999961 *
Coeff B	-2.292e+004	T High	---
Coeff C	7.195	T Low	---
Coeff D	-2.949e-003		

Temperature (C)	Keq	KCalc	Percentage Error
93.333 *	7.813e-019 *	7.774e-019 *	0.5048 *
148.89 *	6.839e-015 *	6.854e-015 *	-0.2150 *
204.44 *	7.793e-012 *	7.849e-012 *	-0.7139 *
260.00 *	2.173e-009 *	2.184e-009 *	-0.5191 *
315.56 *	2.186e-007 *	2.187e-007 *	-3.464e-002 *
371.11 *	1.024e-005 *	1.020e-005 *	0.4196 *
426.67 *	2.659e-004 *	2.644e-004 *	0.5493 *
482.22 *	4.338e-003 *	4.325e-003 *	0.2956 *
537.78 *	4.900e-002 *	4.891e-002 *	0.1845 *
593.33 *	0.4098 *	0.4096 *	5.895e-002 *
648.89 *	2.679 *	2.676 *	0.1033 *
704.44 *	14.26 *	14.21 *	0.3276 *
760.00 *	63.43 *	63.35 *	0.1193 *
815.56 *	242.6 *	243.2 *	-0.2394 *
871.11 *	816.6 *	820.7 *	-0.5042 *
926.67 *	2464 *	2477 *	-0.5388 *
982.22 *	6755 *	6783 *	-0.4088 *
1037.8 *	1.701e+004 *	1.704e+004 *	-0.2007 *
1093.3 *	3.967e+004 *	3.970e+004 *	-8.074e-002 *
1148.9 *	8.664e+004 *	8.645e+004 *	0.2204 *
1204.4 *	1.784e+005 *	1.772e+005 *	0.6564 *

* Specified by user.

A.5 Sabatier Process with Co-electrolysis and Heat Recuperation



Co-Electrolysis Calcs		
H2 to sum of CO & CO2 ratio	3.500	
Total Power	0.1849	kW
Heat Remaining From Sabatier	3.608e-003	kW

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

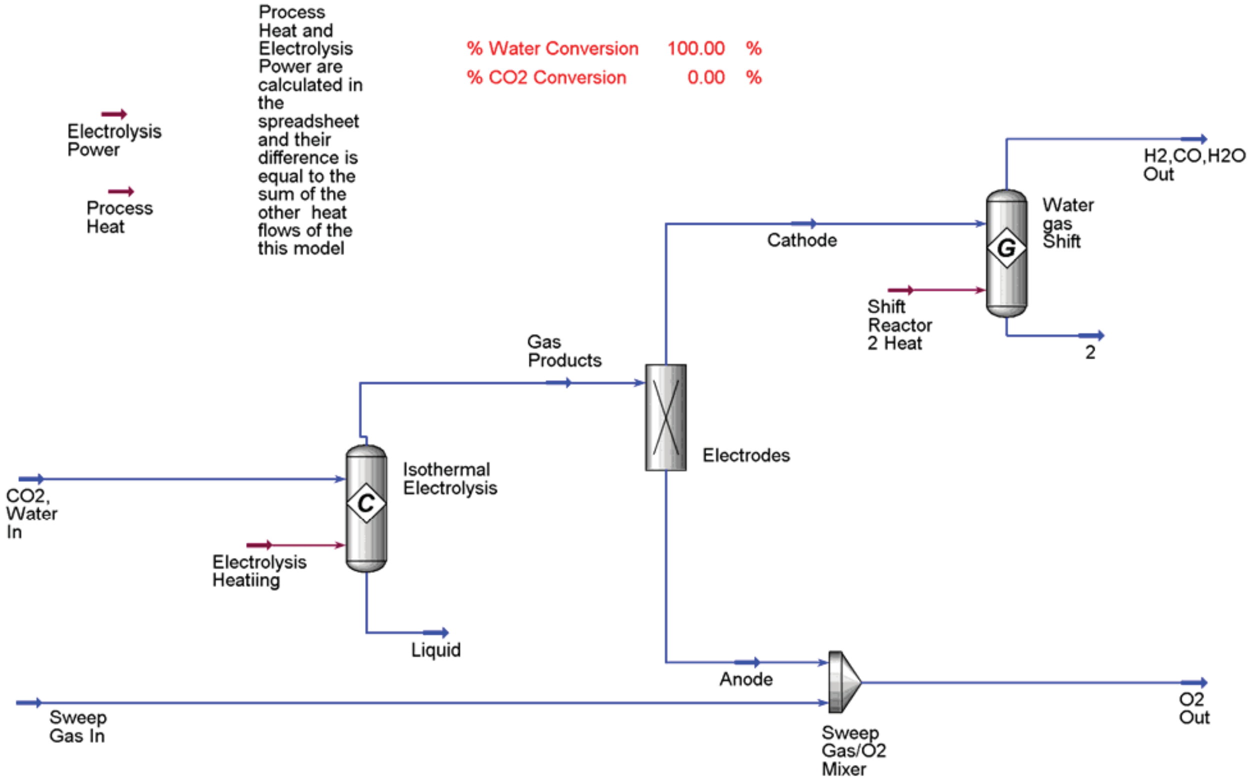


Figure A - 11 Process flow diagram of co-electrolysis module within Sabatier process with co-electrolysis and heat recuperation

INL
Calgary, Alberta
CANADA

Case Name: C:\NASA Final\NASA Co-Electrolysis 4.hsc
Unit Set: NASA
Date/Time: Mon Aug 23 10:45:17 2010

Workbook: Case (Main)

Streams

Name		1	2	3	4	5
Vapour Fraction		0.0000	0.0000	0.0000	1.0000	0.3357
Temperature	(C)	15.556	19.698	93.868	20.781	58.858
Pressure	(kPa)	102.70 *	102.70	101.33	101.33	101.33
Molar Flow	(gmole/h)	1.4299	2.5468	2.5468	0.60435	3.5882
Mass Flow	(kg/d)	0.61823	1.1011	1.1011	0.63833	1.8425
Liquid Volume Flow	(m3/h)	2.581e-005	4.597e-005	4.597e-005	3.223e-005	9.097e-005
Heat Flow	(kW)	-0.1137	-0.2022	-0.1981	-6.614e-002	-0.2718
Molar Enthalpy	(kJ/kgmole)	-2.861e+005	-2.858e+005	-2.800e+005	-3.940e+005	-2.727e+005
Name		5r	6	7	8	9
Vapour Fraction		0.3357	1.0000	1.0000	1.0000	1.0000
Temperature	(C)	58.858 *	91.597	103.98	775.00 *	800.00 *
Pressure	(kPa)	101.33 *	99.946	110.98	109.60	108.22
Molar Flow	(gmole/h)	3.5882 *	3.5882	3.5882	3.5882	3.5882
Mass Flow	(kg/d)	1.8425	1.8425	1.8425	1.8425	1.8425
Liquid Volume Flow	(m3/h)	9.097e-005	9.097e-005	9.097e-005	9.097e-005	9.097e-005
Heat Flow	(kW)	-0.2718	-0.2423	-0.2419	-0.2158	-0.2147
Molar Enthalpy	(kJ/kgmole)	-2.727e+005	-2.431e+005	-2.427e+005	-2.165e+005	-2.154e+005
Name		10	11	12	13	14
Vapour Fraction		1.0000	1.0000	1.0000	1.0000	1.0000
Temperature	(C)	409.01	129.00 *	129.00	129.00	128.98
Pressure	(kPa)	102.70	101.33	101.33	101.33	79.290 *
Molar Flow	(gmole/h)	1.3021	3.5736	3.1365	0.43706	3.1365
Mass Flow	(kg/d)	1.0000	0.84252	0.73948	0.10304	0.73948
Liquid Volume Flow	(m3/h)	3.662e-005	1.044e-004	9.164e-005	1.277e-005	9.164e-005
Heat Flow	(kW)	4.303e-003	-6.175e-002	-5.420e-002	-7.552e-003	-5.420e-002
Molar Enthalpy	(kJ/kgmole)	1.190e+004	-6.220e+004	-6.220e+004	-6.220e+004	-6.220e+004
Name		15	16	17	AmbCool	Circ Pwr
Vapour Fraction		1.0000	1.0000	0.0000	---	---
Temperature	(C)	565.00 *	150.00 *	25.000	---	---
Pressure	(kPa)	77.911	76.532	75.153	---	---
Molar Flow	(gmole/h)	2.5813	1.9425	1.1169	---	---
Mass Flow	(kg/d)	0.73947	0.73947	0.48291	---	---
Liquid Volume Flow	(m3/h)	8.033e-005	5.856e-005	2.016e-005	---	---
Heat Flow	(kW)	-6.039e-002	-8.729e-002	-8.855e-002	-1.613e-002	4.246e-004
Molar Enthalpy	(kJ/kgmole)	-8.422e+004	-1.618e+005	-2.854e+005	---	---
Name		CO2 In	CO2, Water In	Electrolysis Power	H2,CO,H2O Out	Heat From Sabatier
Vapour Fraction		1.0000	1.0000	---	1.0000	---
Temperature	(C)	21.111 *	799.25	---	800.00	---
Pressure	(kPa)	131.00 *	106.84	---	102.70	---
Molar Flow	(gmole/h)	0.60435	3.5903	---	3.5736	---
Mass Flow	(kg/d)	0.63833 *	1.8425	---	0.84252	---
Liquid Volume Flow	(m3/h)	3.223e-005	9.111e-005	---	1.044e-004	---
Heat Flow	(kW)	-6.614e-002	-0.2147	0.1834	-4.050e-002	2.949e-002
Molar Enthalpy	(kJ/kgmole)	-3.940e+005	-2.153e+005	---	-4.080e+004	---
Name		Hi Temp Pwr	Lo Tmp Sabtr Q	Methane, H2 Out	O2 Out	Oxygen Out
Vapour Fraction		---	---	1.0000	1.0000	1.0000
Temperature	(C)	---	---	25.000 *	800.00	44.698
Pressure	(kPa)	---	---	75.153	104.08	101.33
Molar Flow	(gmole/h)	---	---	0.82558	1.3021	1.3021
Mass Flow	(kg/d)	---	---	0.25656	1.0000	1.0000
Liquid Volume Flow	(m3/h)	---	---	3.840e-005	3.662e-005	3.662e-005
Heat Flow	(kW)	1.074e-003	-2.690e-002	-1.487e-002	9.140e-003	2.061e-004
Molar Enthalpy	(kJ/kgmole)	---	---	-6.484e+004	2.527e+004	569.7

* Specified by user.

Workbook: Case (Main) (continued)

Streams (continued)

Name	Rcycl Pmp Pwr	Recycle Water	Water In	Wtr Pmp Pwr	
Vapour Fraction	---	0.0000	0.0000	---	
Temperature (C)	---	25.003	15.556 *	---	
Pressure (kPa)	---	102.70	101.33 *	---	
Molar Flow (gmole/h)	---	1.1169	1.4299	---	
Mass Flow (kg/d)	---	0.48291	0.61823	---	
Liquid Volume Flow (m3/h)	---	2.016e-005	2.581e-005	---	
Heat Flow (kW)	2.038e-007	-8.855e-002	-0.1137	1.297e-008	
Molar Enthalpy (kJ/kgmole)	---	-2.854e+005	-2.861e+005	---	

Compressors

Name	Circulator				
Feed Pressure (kPa)	99.95				
Product Pressure (kPa)	111.0				
Molar Flow (gmole/h)	3.588				
Energy (kW)	4.246e-004				
Adiabatic Efficiency	75 *				
Polytropic Efficiency	75				

Composition

Name	1	2	3	4	5
Comp Mole Frac (H2O)	1.00000	1.00000	1.00000	0.00000	0.72696
Comp Mole Frac (Hydrogen)	0.00000	0.00000	0.00000	0.00000	0.08114
Comp Mole Frac (Oxygen)	0.00000	0.00000	0.00000	0.00000	0.00000
Comp Mole Frac (Argon)	0.00000	0.00000	0.00000	0.00000	0.00000
Comp Mole Frac (Nitrogen)	0.00000	0.00000	0.00000	0.00000	0.00000
Comp Mole Frac (CO2)	0.00000	0.00000	0.00000	1.00000	0.17275
Comp Mole Frac (CO)	0.00000	0.00000	0.00000	0.00000	0.01886
Comp Mole Frac (Methane)	0.00000	0.00000	0.00000	0.00000	0.00028
Comp Mole Frac (Carbon)	0.00000	0.00000	0.00000	0.00000	0.00000
Name	5r	6	7	8	9
Comp Mole Frac (H2O)	0.72696 *	0.72696	0.72696	0.72696	0.72696
Comp Mole Frac (Hydrogen)	0.08114 *	0.08114	0.08114	0.08114	0.08114
Comp Mole Frac (Oxygen)	0.00000 *	0.00000	0.00000	0.00000	0.00000
Comp Mole Frac (Argon)	0.00000 *	0.00000	0.00000	0.00000	0.00000
Comp Mole Frac (Nitrogen)	0.00000 *	0.00000	0.00000	0.00000	0.00000
Comp Mole Frac (CO2)	0.17275 *	0.17275	0.17275	0.17275	0.17275
Comp Mole Frac (CO)	0.01886 *	0.01886	0.01886	0.01886	0.01886
Comp Mole Frac (Methane)	0.00028 *	0.00028	0.00028	0.00028	0.00028
Comp Mole Frac (Carbon)	0.00000 *	0.00000	0.00000	0.00000	0.00000
Name	10	11	12	13	14
Comp Mole Frac (H2O)	0.00000	0.14115	0.14115	0.14115	0.14115
Comp Mole Frac (Hydrogen)	0.00000	0.66617	0.66617	0.66617	0.66617
Comp Mole Frac (Oxygen)	1.00000	0.00000	0.00000	0.00000	0.00000
Comp Mole Frac (Argon)	0.00000	0.00000	0.00000	0.00000	0.00000
Comp Mole Frac (Nitrogen)	0.00000	0.00000	0.00000	0.00000	0.00000
Comp Mole Frac (CO2)	0.00000	0.03553	0.03553	0.03553	0.03553
Comp Mole Frac (CO)	0.00000	0.15482	0.15482	0.15482	0.15482
Comp Mole Frac (Methane)	0.00000	0.00233	0.00233	0.00233	0.00233
Comp Mole Frac (Carbon)	0.00000	0.00000	0.00000	0.00000	0.00000

Workbook: Case (Main) (continued)

Composition (continued)

Name	15	16	17	CO2 In	CO2, Water In
Comp Mole Frac (H2O)	0.24483	0.59264	1.00000	0.00000 *	0.72538
Comp Mole Frac (Hydrogen)	0.52105	0.09624	0.00000	0.00000 *	0.08283
Comp Mole Frac (Oxygen)	0.00000	0.00000	0.00000	0.00000 *	0.00000
Comp Mole Frac (Argon)	0.00000	0.00000	0.00000	0.00000 *	0.00000
Comp Mole Frac (Nitrogen)	0.00000	0.00000	0.00000	0.00000 *	0.00000
Comp Mole Frac (CO2)	0.07740	0.00000	0.00000	1.00000 *	0.17354
Comp Mole Frac (CO)	0.04634	0.00000	0.00000	0.00000 *	0.01825
Comp Mole Frac (Methane)	0.11038	0.31112	0.00000	0.00000 *	0.00000
Comp Mole Frac (Carbon)	0.00000	0.00000	0.00000	0.00000 *	0.00000

Name	H2,CO,H2O Out	Methane, H2 Out	O2 Out	Oxygen Out	Recycle Water
Comp Mole Frac (H2O)	0.14115	0.04152	0.00000	0.00000	1.00000
Comp Mole Frac (Hydrogen)	0.66617	0.22645	0.00000	0.00000	0.00000
Comp Mole Frac (Oxygen)	0.00000	0.00000	1.00000	1.00000	0.00000
Comp Mole Frac (Argon)	0.00000	0.00000	0.00000	0.00000	0.00000
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
Comp Mole Frac (CO)	0.15482	0.00000	0.00000	0.00000	0.00000
Comp Mole Frac (Methane)	0.00233	0.73203	0.00000	0.00000	0.00000
Comp Mole Frac (Carbon)	0.00000	0.00000	0.00000	0.00000	0.00000

Name	Water In
Comp Mole Frac (H2O)	1.00000 *
Comp Mole Frac (Hydrogen)	0.00000 *
Comp Mole Frac (Oxygen)	0.00000 *
Comp Mole Frac (Argon)	0.00000 *
Comp Mole Frac (Nitrogen)	0.00000 *
Comp Mole Frac (CO2)	0.00000 *
Comp Mole Frac (CO)	0.00000 *
Comp Mole Frac (Methane)	0.00000 *
Comp Mole Frac (Carbon)	0.00000 *

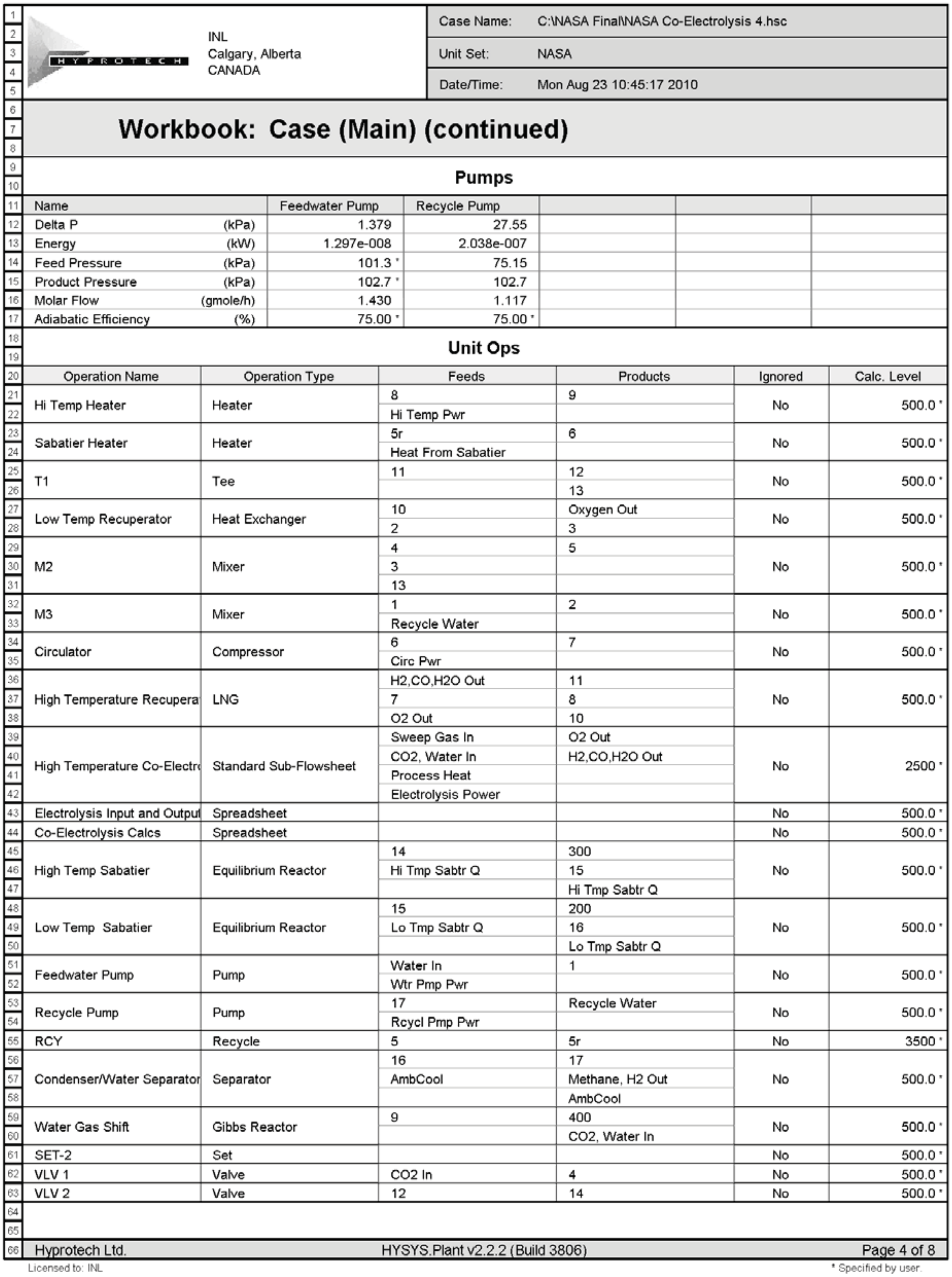
Heat Exchangers

Name		Low Temp Recuperat
Duty	(kW)	-4.097e-003
Tube Inlet Temperature	(C)	409.0
Tube Outlet Temperature	(C)	44.70
Shell Inlet Temperature	(C)	19.70
Shell Outlet Temperature	(C)	93.87
LMTD	(C)	117.5
UA	(kJ/C-h)	0.1255
Minimum Approach	(C)	25.00

Other Heat Exchangers

Name		High Temperature Re
Number of Sides		3 *
LMTD	(C)	41.41 *
UA (Calculated)	(kJ/C-h)	2.268
Hot Pinch Temperature	(C)	800.0
Cold Pinch Temperature	(C)	775.0
Minimum Approach	(C)	25.00
Exchanger Cold Duty	(kW)	2.608e-002

* Specified by user.



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CANADA

Case Name: C:\NASA Final\NASA Co-Electrolysis 4.hsc
Unit Set: NASA
Date/Time: Mon Aug 23 10:45:17 2010

Workbook: Case (Main) (continued)

Pumps

Name	Feedwater Pump	Recycle Pump			
Delta P (kPa)	1.379	27.55			
Energy (kW)	1.297e-008	2.038e-007			
Feed Pressure (kPa)	101.3 *	75.15			
Product Pressure (kPa)	102.7 *	102.7			
Molar Flow (gmole/h)	1.430	1.117			
Adiabatic Efficiency (%)	75.00 *	75.00 *			

Unit Ops

Operation Name	Operation Type	Feeds	Products	Ignored	Calc. Level
Hi Temp Heater	Heater	8 Hi Temp Pwr	9	No	500.0 *
Sabatier Heater	Heater	5r Heat From Sabatier	6	No	500.0 *
T1	Tee	11	12 13	No	500.0 *
Low Temp Recuperator	Heat Exchanger	10 2	Oxygen Out 3	No	500.0 *
M2	Mixer	4 3 13	5	No	500.0 *
M3	Mixer	1 Recycle Water	2	No	500.0 *
Circulator	Compressor	6 Circ Pwr	7	No	500.0 *
High Temperature Recupera	LNG	H2,CO,H2O Out 7 O2 Out	11 8 10	No	500.0 *
High Temperature Co-Electr	Standard Sub-Flowsheet	Sweep Gas In CO2, Water In Process Heat Electrolysis Power	O2 Out H2,CO,H2O Out	No	2500 *
Electrolysis Input and Output	Spreadsheet			No	500.0 *
Co-Electrolysis Calcs	Spreadsheet			No	500.0 *
High Temp Sabatier	Equilibrium Reactor	14 Hi Tmp Sabtr Q	300 15 Hi Tmp Sabtr Q	No	500.0 *
Low Temp Sabatier	Equilibrium Reactor	15 Lo Tmp Sabtr Q	200 16 Lo Tmp Sabtr Q	No	500.0 *
Feedwater Pump	Pump	Water In Wtr Pmp Pwr	1	No	500.0 *
Recycle Pump	Pump	17 Rcycl Pmp Pwr	Recycle Water	No	500.0 *
RCY	Recycle	5	5r	No	3500 *
Condenser/Water Separator	Separator	16 AmbCool	17 Methane, H2 Out AmbCool	No	500.0 *
Water Gas Shift	Gibbs Reactor	9	400 CO2, Water In	No	500.0 *
SET-2	Set			No	500.0 *
VLV 1	Valve	CO2 In	4	No	500.0 *
VLV 2	Valve	12	14	No	500.0 *

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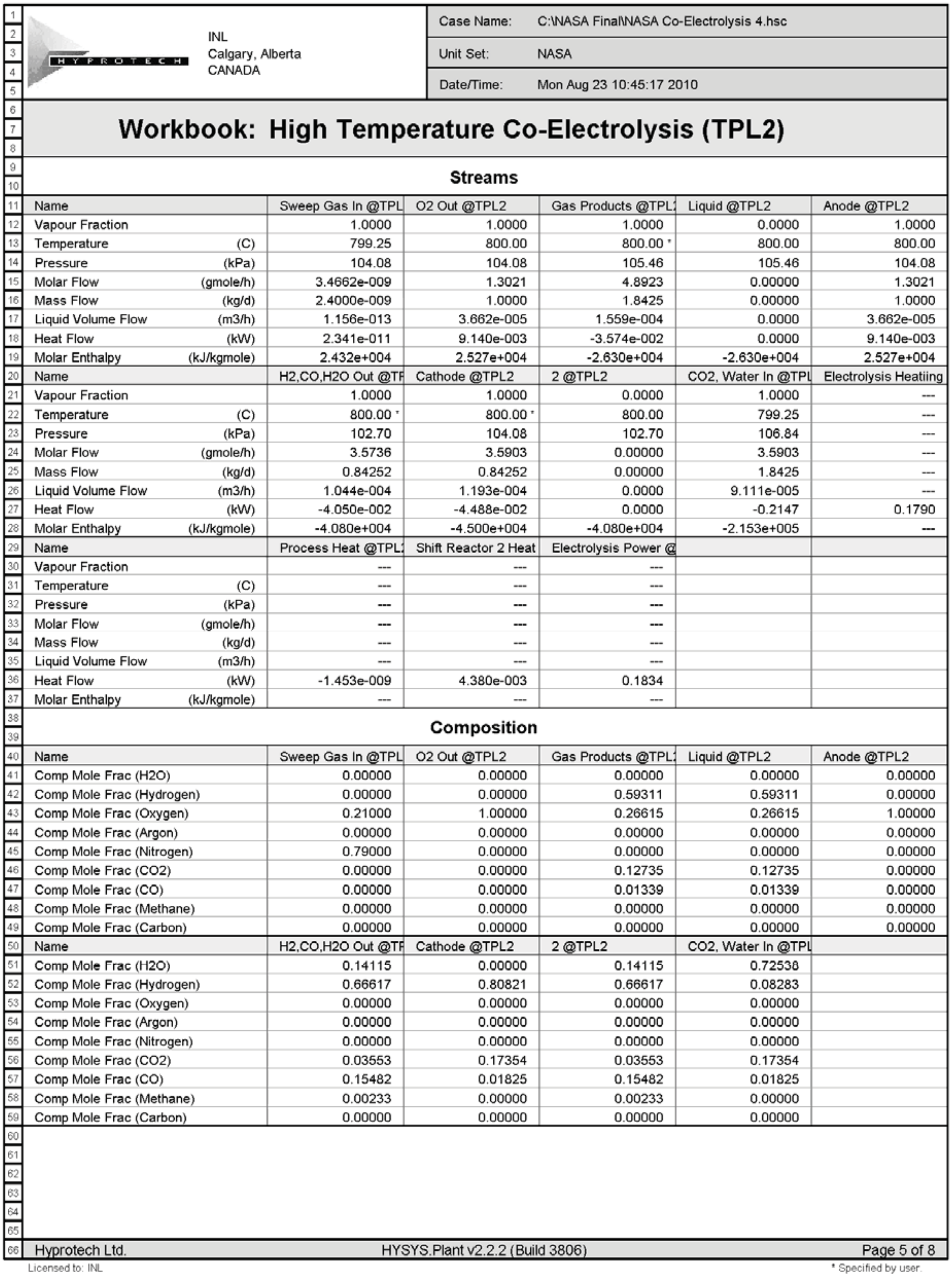

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CANADA

Case Name:	C:\NASA Final\NASA Co-Electrolysis 4.hsc
Unit Set:	NASA
Date/Time:	Mon Aug 23 10:45:17 2010

Workbook: High Temperature Co-Electrolysis (TPL2)

Streams

Name		Sweep Gas In @TPL	O2 Out @TPL2	Gas Products @TPL	Liquid @TPL2	Anode @TPL2
Vapour Fraction		1.0000	1.0000	1.0000	0.0000	1.0000
Temperature	(C)	799.25	800.00	800.00 *	800.00	800.00
Pressure	(kPa)	104.08	104.08	105.46	105.46	104.08
Molar Flow	(gmole/h)	3.4662e-009	1.3021	4.8923	0.00000	1.3021
Mass Flow	(kg/d)	2.4000e-009	1.0000	1.8425	0.00000	1.0000
Liquid Volume Flow	(m3/h)	1.156e-013	3.662e-005	1.559e-004	0.0000	3.662e-005
Heat Flow	(kW)	2.341e-011	9.140e-003	-3.574e-002	0.0000	9.140e-003
Molar Enthalpy	(kJ/kgmole)	2.432e+004	2.527e+004	-2.630e+004	-2.630e+004	2.527e+004
Name		**H2,CO,H2O Out @TF**	**Cathode @TPL2**	**2 @TPL2**	**CO2, Water In @TPL**	**Electrolysis Heating**
Vapour Fraction		1.0000	1.0000	0.0000	1.0000	---
Temperature	(C)	800.00 *	800.00 *	800.00	799.25	---
Pressure	(kPa)	102.70	104.08	102.70	106.84	---
Molar Flow	(gmole/h)	3.5736	3.5903	0.00000	3.5903	---
Mass Flow	(kg/d)	0.84252	0.84252	0.00000	1.8425	---
Liquid Volume Flow	(m3/h)	1.044e-004	1.193e-004	0.0000	9.111e-005	---
Heat Flow	(kW)	-4.050e-002	-4.488e-002	0.0000	-0.2147	0.1790
Molar Enthalpy	(kJ/kgmole)	-4.080e+004	-4.500e+004	-4.080e+004	-2.153e+005	---
Name		**Process Heat @TPL**	**Shift Reactor 2 Heat**	**Electrolysis Power @**		
Vapour Fraction		---	---	---		
Temperature	(C)	---	---	---		
Pressure	(kPa)	---	---	---		
Molar Flow	(gmole/h)	---	---	---		
Mass Flow	(kg/d)	---	---	---		
Liquid Volume Flow	(m3/h)	---	---	---		
Heat Flow	(kW)	-1.453e-009	4.380e-003	0.1834		
Molar Enthalpy	(kJ/kgmole)	---	---	---		

Composition

Name	Sweep Gas In @TPL	O2 Out @TPL2	Gas Products @TPL	Liquid @TPL2	Anode @TPL2
Comp Mole Frac (H2O)	0.00000	0.00000	0.00000	0.00000	0.00000
Comp Mole Frac (Hydrogen)	0.00000	0.00000	0.59311	0.59311	0.00000
Comp Mole Frac (Oxygen)	0.21000	1.00000	0.26615	0.26615	1.00000
Comp Mole Frac (Argon)	0.00000	0.00000	0.00000	0.00000	0.00000
Comp Mole Frac (Nitrogen)	0.79000	0.00000	0.00000	0.00000	0.00000
Comp Mole Frac (CO2)	0.00000	0.00000	0.12735	0.12735	0.00000
Comp Mole Frac (CO)	0.00000	0.00000	0.01339	0.01339	0.00000
Comp Mole Frac (Methane)	0.00000	0.00000	0.00000	0.00000	0.00000
Comp Mole Frac (Carbon)	0.00000	0.00000	0.00000	0.00000	0.00000
Name	**H2,CO,H2O Out @TF**	**Cathode @TPL2**	**2 @TPL2**	**CO2, Water In @TPL**	
Comp Mole Frac (H2O)	0.14115	0.00000	0.14115	0.72538	
Comp Mole Frac (Hydrogen)	0.66617	0.80821	0.66617	0.08283	
Comp Mole Frac (Oxygen)	0.00000	0.00000	0.00000	0.00000	
Comp Mole Frac (Argon)	0.00000	0.00000	0.00000	0.00000	
Comp Mole Frac (Nitrogen)	0.00000	0.00000	0.00000	0.00000	
Comp Mole Frac (CO2)	0.03553	0.17354	0.03553	0.17354	
Comp Mole Frac (CO)	0.15482	0.01825	0.15482	0.01825	
Comp Mole Frac (Methane)	0.00233	0.00000	0.00233	0.00000	
Comp Mole Frac (Carbon)	0.00000	0.00000	0.00000	0.00000	

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Workbook: High Temperature Co-Electrolysis (TPL2) (continued)

Equilibrium Reactors

Name					
Separator Type					
Vessel Temperature (C)					
Vessel Pressure (kPa)					
Vapour Molar Flow (gmole/h)					
Liquid Molar Flow (gmole/h)					
Heat Flow (kW)					

Gibbs Reactors

Name	Water gas Shift @TP				
Separator Type	0 *				
Vessel Temperature (C)	800.00				
Vessel Pressure (kPa)	102.70				
Vapour Molar Flow (gmole/h)	3.574				
Liquid Molar Flow (gmole/h)	0.0000				
Heat Flow (kW)	4.380e-003				

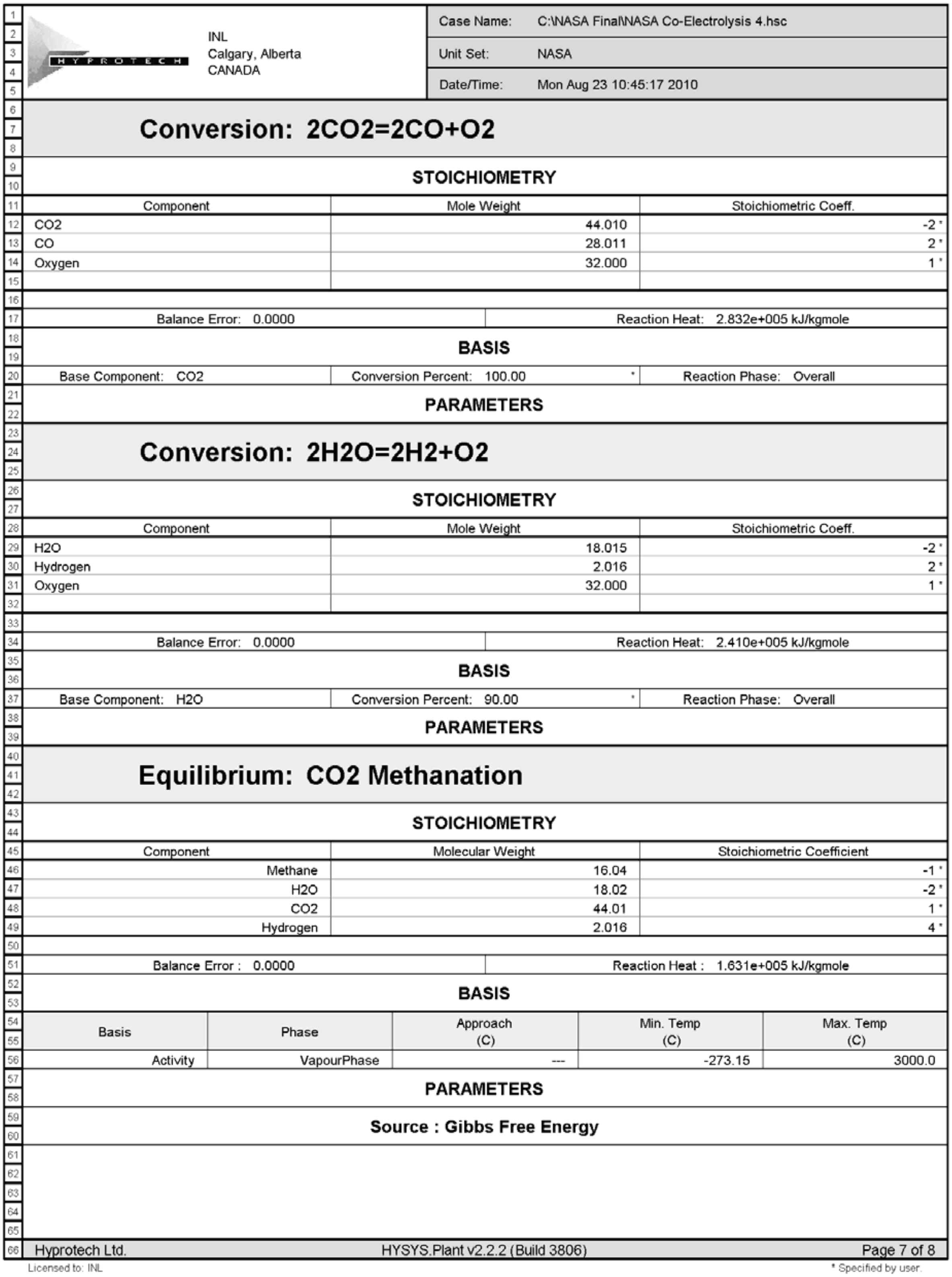
Component Splitters

Name	Electrodes @TPL2				
Overhead Stream Pressure (kPa)	104.1				
Overhead Stream Vapour Fraction	1.000				
Bottoms Stream Pressure (kPa)	104.1				
Bottoms Stream Vapour Fraction	1.000				
Overhead Fraction(1)	1.00000 *				
Overhead Fraction(2)	1.00000 *				
Overhead Fraction(3)	0.00000 *				
Overhead Fraction(4)	1.00000 *				
Overhead Fraction(5)	1.00000 *				
Overhead Fraction(6)	1.00000 *				
Overhead Fraction(7)	1.00000 *				
Overhead Fraction(8)	1.00000 *				
Overhead Fraction(9)	0.00000 *				

Unit Ops

Operation Name	Operation Type	Feeds	Products	Ignored	Calc. Level
Temp Average ASR @TPL2	Spreadsheet			Yes	500.0 *
Electrolysis Spreadsheet @	Spreadsheet			No	500.0 *
Steam Electrolysis @TPL2	Spreadsheet			No	500.0 *
CO2 Electrolysis @TPL2	Spreadsheet			No	500.0 *
Sweep Gas/O2 Mixer @TPL	Mixer	Anode @TPL2 Sweep Gas In @TPL2	O2 Out @TPL2	No	500.0 *
Isothermal Electrolysis @TP	Conversion Reactor	CO2, Water In @TPL2 Electrolysis Heatiing @TPL2	Liquid @TPL2 Gas Products @TPL2 Electrolysis Heatiing @TPL2	No	500.0 *
Electrodes @TPL2	Component Splitter	Gas Products @TPL2	Cathode @TPL2 Anode @TPL2	No	500.0 *
ADJ-1 @TPL2	Adjust			Yes	3500 *
Water gas Shift @TPL2	Gibbs Reactor	Cathode @TPL2 Shift Reactor 2 Heat @TPL2	2 @TPL2 H2,CO,H2O Out @TPL2 Shift Reactor 2 Heat @TPL2	No	500.0 *
SET-1 @TPL2	Set			No	500.0 *
SET-3 @TPL2	Set			No	500.0 *
SET-2 @TPL2	Set			No	500.0 *

* Specified by user.



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CANADA

Case Name: C:\NASA Final\NASA Co-Electrolysis 4.hsc
Unit Set: NASA
Date/Time: Mon Aug 23 10:45:17 2010

Conversion: 2CO2=2CO+O2

STOICHIOMETRY

Component	Mole Weight	Stoichiometric Coeff.
CO2	44.010	-2 *
CO	28.011	2 *
Oxygen	32.000	1 *

Balance Error: 0.0000 | Reaction Heat: 2.832e+005 kJ/kgmole

BASIS

Base Component: CO2 | Conversion Percent: 100.00 * | Reaction Phase: Overall

PARAMETERS

Conversion: 2H2O=2H2+O2

STOICHIOMETRY

Component	Mole Weight	Stoichiometric Coeff.
H2O	18.015	-2 *
Hydrogen	2.016	2 *
Oxygen	32.000	1 *

Balance Error: 0.0000 | Reaction Heat: 2.410e+005 kJ/kgmole

BASIS

Base Component: H2O | Conversion Percent: 90.00 * | Reaction Phase: Overall

PARAMETERS

Equilibrium: CO2 Methanation

STOICHIOMETRY

Component	Molecular Weight	Stoichiometric Coefficient
Methane	16.04	-1 *
H2O	18.02	-2 *
CO2	44.01	1 *
Hydrogen	2.016	4 *

Balance Error : 0.0000 | Reaction Heat : 1.631e+005 kJ/kgmole

BASIS

Basis	Phase	Approach (C)	Min. Temp (C)	Max. Temp (C)
Activity	VapourPhase	---	-273.15	3000.0

PARAMETERS

Source : Gibbs Free Energy

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Case Name:	C:\NASA Final\NASA Co-Electrolysis 4.hsc
Unit Set:	NASA
Date/Time:	Mon Aug 23 10:45:17 2010

Equilibrium: Methanation

STOICHIOMETRY

Component	Molecular Weight	Stoichiometric Coefficient
Methane	16.04	-1 *
H2O	18.02	-1 *
CO	28.01	1 *
Hydrogen	2.016	3 *

Balance Error : 0.0000

Reaction Heat : 2.053e+005 kJ/kgmole

BASIS

Basis	Phase	Approach (C)	Min. Temp (C)	Max. Temp (C)
Activity	VapourPhase	---	-273.15	3000.0

PARAMETERS

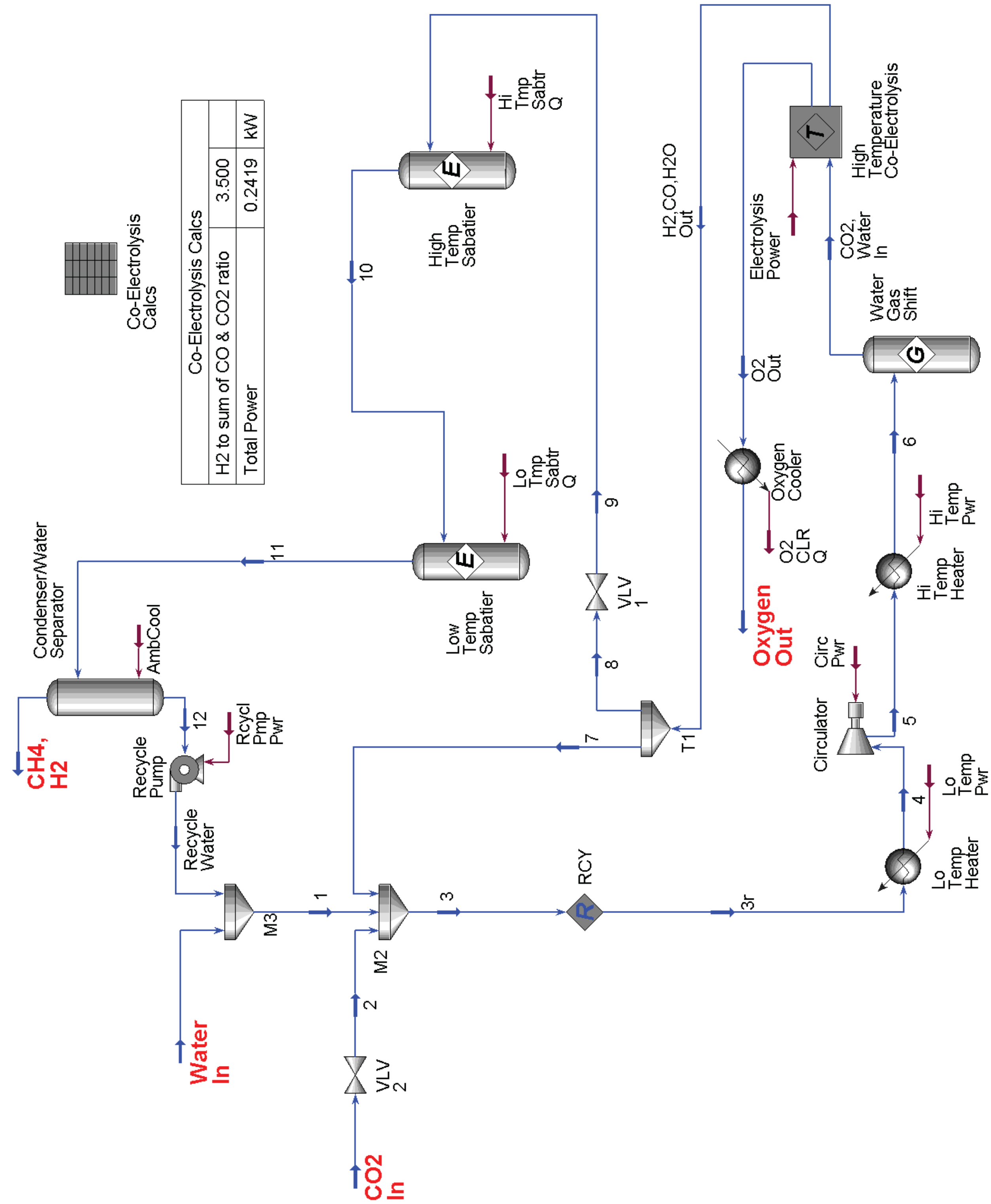
Source : K Vs. T Table

Coeff A	-20.55	R2	0.999961 *
Coeff B	-2.292e+004	T High	---
Coeff C	7.195	T Low	---
Coeff D	-2.949e-003		

Temperature (C)	Keq	KCalc	Percentage Error
93.333 *	7.813e-019 *	7.774e-019 *	0.5048 *
148.89 *	6.839e-015 *	6.854e-015 *	-0.2150 *
204.44 *	7.793e-012 *	7.849e-012 *	-0.7139 *
260.00 *	2.173e-009 *	2.184e-009 *	-0.5191 *
315.56 *	2.186e-007 *	2.187e-007 *	-3.464e-002 *
371.11 *	1.024e-005 *	1.020e-005 *	0.4196 *
426.67 *	2.659e-004 *	2.644e-004 *	0.5493 *
482.22 *	4.338e-003 *	4.325e-003 *	0.2956 *
537.78 *	4.900e-002 *	4.891e-002 *	0.1845 *
593.33 *	0.4098 *	0.4096 *	5.895e-002 *
648.89 *	2.679 *	2.676 *	0.1033 *
704.44 *	14.26 *	14.21 *	0.3276 *
760.00 *	63.43 *	63.35 *	0.1193 *
815.56 *	242.6 *	243.2 *	-0.2394 *
871.11 *	816.6 *	820.7 *	-0.5042 *
926.67 *	2464 *	2477 *	-0.5388 *
982.22 *	6755 *	6783 *	-0.4088 *
1037.8 *	1.701e+004 *	1.704e+004 *	-0.2007 *
1093.3 *	3.967e+004 *	3.970e+004 *	-8.074e-002 *
1148.9 *	8.664e+004 *	8.645e+004 *	0.2204 *
1204.4 *	1.784e+005 *	1.772e+005 *	0.6564 *

* Specified by user.

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



Co-Electrolysis Calcs

H2 to sum of CO & CO2 ratio	3.500	
Total Power	0.2419	kW

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

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CANADA

Case Name:	C:\NASA Final\NASA Co-Electrolysis wo Recup.hsc
Unit Set:	NASA2
Date/Time:	Mon Aug 23 11:24:48 2010

Workbook: Case (Main)

Streams

Name		1	2	3	3r	4
Vapour Fraction		0.0000	1.0000	0.3127	0.3127	1.0000 *
Temperature	(C)	19.698	20.781	50.841	50.876 *	90.860
Pressure	(kPa)	101.33	101.33	101.33	101.33 *	99.946
Molar Flow	(gmole/h)	2.5460	0.60416	3.5870	3.5879 *	3.5879
Mass Flow	(kg/d)	1.1008	0.63813	1.8419	1.8423	1.8423
Liquid Volume Flow	(m3/h)	4.596e-005	3.222e-005	9.094e-005	9.095e-005	9.095e-005
Heat Flow	(kW)	-0.2021	-6.612e-002	-0.2732	-0.2733	-0.2423
Molar Enthalpy	(kJ/kgmole)	-2.858e+005	-3.940e+005	-2.742e+005	-2.742e+005	-2.431e+005

Name		5	6	7	8	9
Vapour Fraction		1.0000	1.0000	1.0000	1.0000	1.0000
Temperature	(C)	100.22	800.00 *	800.00	800.00	800.01
Pressure	(kPa)	108.22	106.84	101.33	101.33	79.290 *
Molar Flow	(gmole/h)	3.5879	3.5879	0.43686	3.1367	3.1367
Mass Flow	(kg/d)	1.8423	1.8423	0.10297	0.73934	0.73934
Liquid Volume Flow	(m3/h)	9.095e-005	9.095e-005	1.276e-005	9.164e-005	9.164e-005
Heat Flow	(kW)	-0.2420	-0.2147	-4.948e-003	-3.553e-002	-3.553e-002
Molar Enthalpy	(kJ/kgmole)	-2.428e+005	-2.154e+005	-4.077e+004	-4.077e+004	-4.077e+004

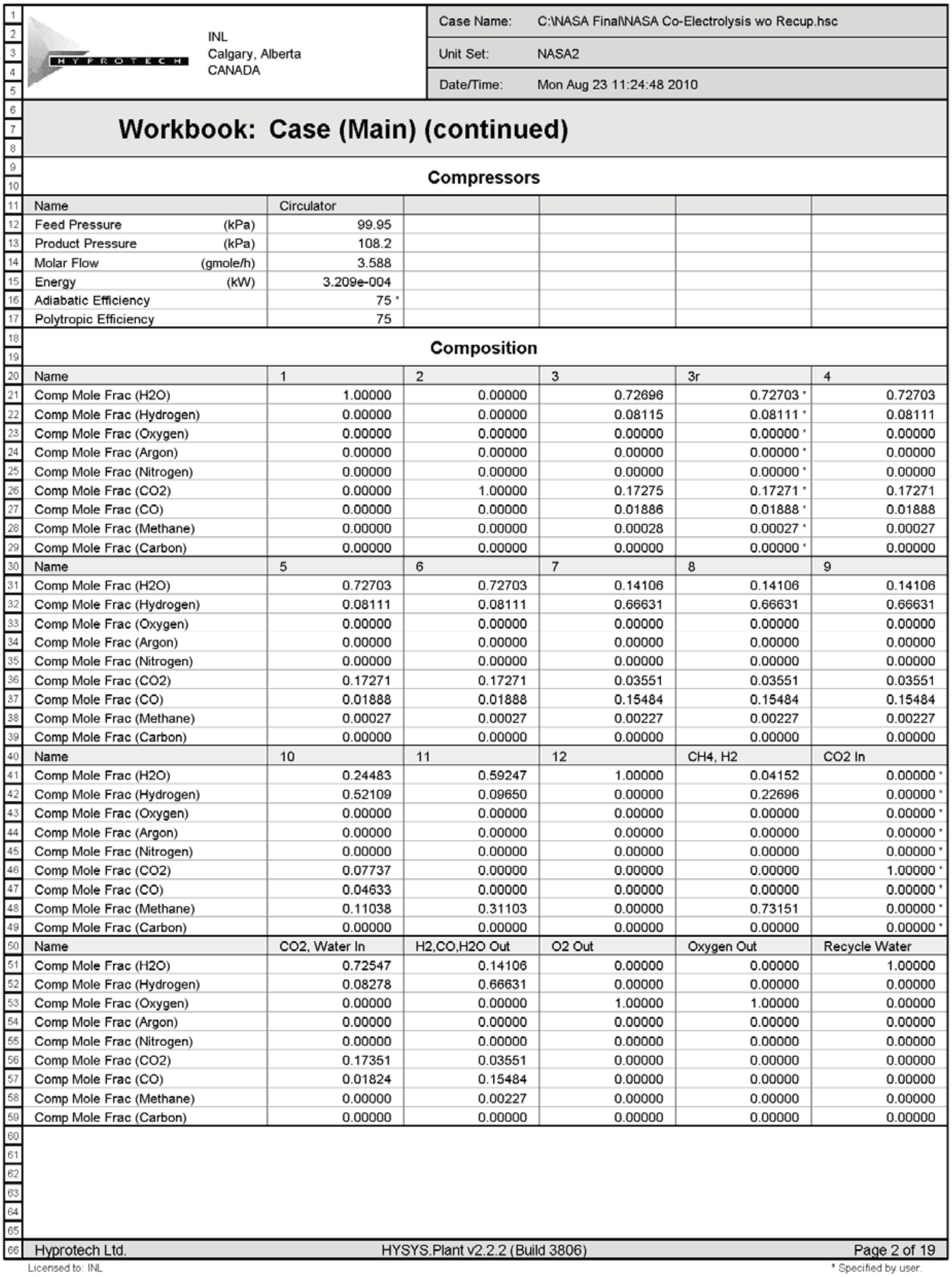
Name		10	11	12	AmbCool	CH4, H2
Vapour Fraction		1.0000	1.0000	0.0000	---	1.0000
Temperature	(C)	565.00 *	150.00 *	25.000	---	25.000 *
Pressure	(kPa)	77.911	76.532	75.153	---	75.153
Molar Flow	(gmole/h)	2.5811	1.9426	1.1166	---	0.82596
Mass Flow	(kg/d)	0.73933	0.73933	0.48279	---	0.25653
Liquid Volume Flow	(m3/h)	8.033e-005	5.856e-005	2.016e-005	---	3.840e-005
Heat Flow	(kW)	-6.038e-002	-8.727e-002	-8.853e-002	-1.612e-002	-1.487e-002
Molar Enthalpy	(kJ/kgmole)	-8.421e+004	-1.617e+005	-2.854e+005	---	-6.481e+004

Name		Circ Pwr	CO2 In	CO2, Water In	Electrolysis Power	H2,CO,H2O Out
Vapour Fraction		---	1.0000	1.0000	---	1.0000
Temperature	(C)	---	21.111 *	799.34	---	800.00
Pressure	(kPa)	---	131.00 *	105.46	---	101.33
Molar Flow	(gmole/h)	---	0.60416	3.5898	---	3.5736
Mass Flow	(kg/d)	---	0.63813 *	1.8423	---	0.84231
Liquid Volume Flow	(m3/h)	---	3.222e-005	9.109e-005	---	1.044e-004
Heat Flow	(kW)	3.209e-004	-6.612e-002	-0.2147	0.1834	-4.047e-002
Molar Enthalpy	(kJ/kgmole)	---	-3.940e+005	-2.153e+005	---	-4.077e+004

Name		Hi Temp Pwr	Hi Tmp Sabtr Q	Lo Temp Pwr	Lo Tmp Sabtr Q	O2 CLR Q
Vapour Fraction		---	---	---	---	---
Temperature	(C)	---	---	---	---	---
Pressure	(kPa)	---	---	---	---	---
Molar Flow	(gmole/h)	---	---	---	---	---
Mass Flow	(kg/d)	---	---	---	---	---
Liquid Volume Flow	(m3/h)	---	---	---	---	---
Heat Flow	(kW)	2.728e-002	-2.485e-002	3.096e-002	-2.690e-002	9.143e-003
Molar Enthalpy	(kJ/kgmole)	---	---	---	---	---

Name		O2 Out	Oxygen Out	Rcycl Pmp Pwr	Recycle Water	Water In
Vapour Fraction		1.0000	1.0000	---	0.0000	0.0000
Temperature	(C)	800.00	25.000 *	---	25.003	15.556 *
Pressure	(kPa)	102.70	101.33 *	---	101.33	101.33 *
Molar Flow	(gmole/h)	1.3021	1.3021	---	1.1166	1.4294
Mass Flow	(kg/d)	1.0000	1.0000	---	0.48279	0.61801
Liquid Volume Flow	(m3/h)	3.662e-005	3.662e-005	---	2.016e-005	2.580e-005
Heat Flow	(kW)	9.140e-003	-3.452e-006	1.936e-007	-8.853e-002	-0.1136
Molar Enthalpy	(kJ/kgmole)	2.527e+004	-9.543	---	-2.854e+005	-2.861e+005

* Specified by user.



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Calgary, Alberta
CANADA

Case Name:	C:\NASA Final\NASA Co-Electrolysis wo Recup.hsc
Unit Set:	NASA2
Date/Time:	Mon Aug 23 11:24:48 2010

Workbook: Case (Main) (continued)

Compressors

Name	Circulator				
Feed Pressure (kPa)	99.95				
Product Pressure (kPa)	108.2				
Molar Flow (gmole/h)	3.588				
Energy (kW)	3.209e-004				
Adiabatic Efficiency	75 *				
Polytropic Efficiency	75				

Composition

Name	1	2	3	3r	4
Comp Mole Frac (H2O)	1.00000	0.00000	0.72696	0.72703 *	0.72703
Comp Mole Frac (Hydrogen)	0.00000	0.00000	0.08115	0.08111 *	0.08111
Comp Mole Frac (Oxygen)	0.00000	0.00000	0.00000	0.00000 *	0.00000
Comp Mole Frac (Argon)	0.00000	0.00000	0.00000	0.00000 *	0.00000
Comp Mole Frac (Nitrogen)	0.00000	0.00000	0.00000	0.00000 *	0.00000
Comp Mole Frac (CO2)	0.00000	1.00000	0.17275	0.17271 *	0.17271
Comp Mole Frac (CO)	0.00000	0.00000	0.01886	0.01888 *	0.01888
Comp Mole Frac (Methane)	0.00000	0.00000	0.00028	0.00027 *	0.00027
Comp Mole Frac (Carbon)	0.00000	0.00000	0.00000	0.00000 *	0.00000
Name	**5**	**6**	**7**	**8**	**9**
Comp Mole Frac (H2O)	0.72703	0.72703	0.14106	0.14106	0.14106
Comp Mole Frac (Hydrogen)	0.08111	0.08111	0.66631	0.66631	0.66631
Comp Mole Frac (Oxygen)	0.00000	0.00000	0.00000	0.00000	0.00000
Comp Mole Frac (Argon)	0.00000	0.00000	0.00000	0.00000	0.00000
Comp Mole Frac (Nitrogen)	0.00000	0.00000	0.00000	0.00000	0.00000
Comp Mole Frac (CO2)	0.17271	0.17271	0.03551	0.03551	0.03551
Comp Mole Frac (CO)	0.01888	0.01888	0.15484	0.15484	0.15484
Comp Mole Frac (Methane)	0.00027	0.00027	0.00227	0.00227	0.00227
Comp Mole Frac (Carbon)	0.00000	0.00000	0.00000	0.00000	0.00000
Name	**10**	**11**	**12**	**CH4, H2**	**CO2 In**
Comp Mole Frac (H2O)	0.24483	0.59247	1.00000	0.04152	0.00000 *
Comp Mole Frac (Hydrogen)	0.52109	0.09650	0.00000	0.22696	0.00000 *
Comp Mole Frac (Oxygen)	0.00000	0.00000	0.00000	0.00000	0.00000 *
Comp Mole Frac (Argon)	0.00000	0.00000	0.00000	0.00000	0.00000 *
Comp Mole Frac (Nitrogen)	0.00000	0.00000	0.00000	0.00000	0.00000 *
Comp Mole Frac (CO2)	0.07737	0.00000	0.00000	0.00000	1.00000 *
Comp Mole Frac (CO)	0.04633	0.00000	0.00000	0.00000	0.00000 *
Comp Mole Frac (Methane)	0.11038	0.31103	0.00000	0.73151	0.00000 *
Comp Mole Frac (Carbon)	0.00000	0.00000	0.00000	0.00000	0.00000 *
Name	**CO2, Water In**	**H2,CO,H2O Out**	**O2 Out**	**Oxygen Out**	**Recycle Water**
Comp Mole Frac (H2O)	0.72547	0.14106	0.00000	0.00000	1.00000
Comp Mole Frac (Hydrogen)	0.08278	0.66631	0.00000	0.00000	0.00000
Comp Mole Frac (Oxygen)	0.00000	0.00000	1.00000	1.00000	0.00000
Comp Mole Frac (Argon)	0.00000	0.00000	0.00000	0.00000	0.00000
Comp Mole Frac (Nitrogen)	0.00000	0.00000	0.00000	0.00000	0.00000
Comp Mole Frac (CO2)	0.17351	0.03551	0.00000	0.00000	0.00000
Comp Mole Frac (CO)	0.01824	0.15484	0.00000	0.00000	0.00000
Comp Mole Frac (Methane)	0.00000	0.00227	0.00000	0.00000	0.00000
Comp Mole Frac (Carbon)	0.00000	0.00000	0.00000	0.00000	0.00000

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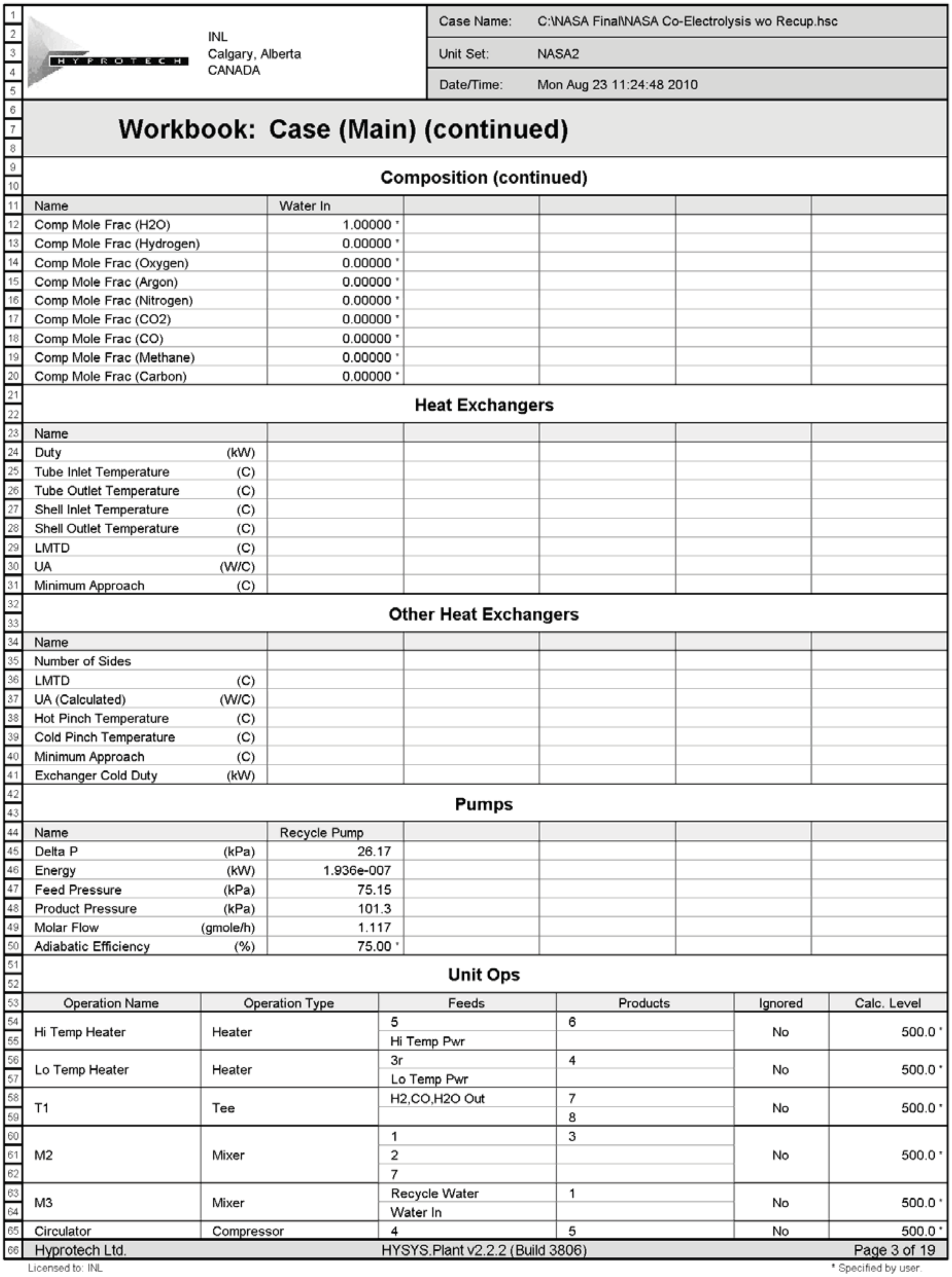

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CANADA

Case Name:	C:\NASA Final\NASA Co-Electrolysis wo Recup.hsc
Unit Set:	NASA2
Date/Time:	Mon Aug 23 11:24:48 2010

Workbook: Case (Main) (continued)

Composition (continued)

Name	Water In				
Comp Mole Frac (H2O)	1.00000 *				
Comp Mole Frac (Hydrogen)	0.00000 *				
Comp Mole Frac (Oxygen)	0.00000 *				
Comp Mole Frac (Argon)	0.00000 *				
Comp Mole Frac (Nitrogen)	0.00000 *				
Comp Mole Frac (CO2)	0.00000 *				
Comp Mole Frac (CO)	0.00000 *				
Comp Mole Frac (Methane)	0.00000 *				
Comp Mole Frac (Carbon)	0.00000 *				

Heat Exchangers

Name						
Duty	(kW)					
Tube Inlet Temperature	(C)					
Tube Outlet Temperature	(C)					
Shell Inlet Temperature	(C)					
Shell Outlet Temperature	(C)					
LMTD	(C)					
UA	(W/C)					
Minimum Approach	(C)					

Other Heat Exchangers

Name						
Number of Sides						
LMTD	(C)					
UA (Calculated)	(W/C)					
Hot Pinch Temperature	(C)					
Cold Pinch Temperature	(C)					
Minimum Approach	(C)					
Exchanger Cold Duty	(kW)					

Pumps

Name		Recycle Pump				
Delta P	(kPa)	26.17				
Energy	(kW)	1.936e-007				
Feed Pressure	(kPa)	75.15				
Product Pressure	(kPa)	101.3				
Molar Flow	(gmole/h)	1.117				
Adiabatic Efficiency	(%)	75.00 *				

Unit Ops

Operation Name	Operation Type	Feeds	Products	Ignored	Calc. Level
Hi Temp Heater	Heater	5 Hi Temp Pwr	6	No	500.0 *
Lo Temp Heater	Heater	3r Lo Temp Pwr	4	No	500.0 *
T1	Tee	H2,CO,H2O Out	7 8	No	500.0 *
M2	Mixer	1 2 7	3	No	500.0 *
M3	Mixer	Recycle Water Water In	1	No	500.0 *
Circulator	Compressor	4	5	No	500.0 *

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Workbook: Case (Main) (continued)

Unit Ops (continued)

Operation Name	Operation Type	Feeds	Products	Ignored	Calc. Level
Circulator	Compressor	Circ Pwr		No	500.0 *
Oxygen Cooler	Cooler	O2 Out	Oxygen Out O2 CLR Q	No	500.0 *
High Temperature Co-Electr	Standard Sub-Flowsheet	Sweep Gas In CO2, Water In Process Heat Electrolysis Power	O2 Out H2,CO,H2O Out	No	2500 *
Electrolysis Input and Outpu	Spreadsheet			No	500.0 *
Co-Electrolysis Calcs	Spreadsheet			No	500.0 *
High Temp Sabatier	Equilibrium Reactor	9 Hi Tmp Sabtr Q	300 10 Hi Tmp Sabtr Q	No	500.0 *
Low Temp Sabatier	Equilibrium Reactor	10 Lo Tmp Sabtr Q	200 11 Lo Tmp Sabtr Q	No	500.0 *
Recycle Pump	Pump	12 Rcycl Pmp Pwr	Recycle Water	No	500.0 *
RCY	Recycle	3	3r	No	3500 *
Condenser/Water Separator	Separator	11 AmbCool	12 CH4, H2 AmbCool	No	500.0 *
Water Gas Shift	Gibbs Reactor	6	400 CO2, Water In	No	500.0 *
SET-2	Set			No	500.0 *
VLV 2	Valve	CO2 In	2	No	500.0 *
VLV 1	Valve	8	9	No	500.0 *

Spreadsheet: Co-Electrolysis Calcs

Units Set: NASA

CONNECTIONS

Imported Variables

Cell	Object	Variable Description	Value
B1	Material Stream: 9	Comp Mole Frac (Hydrogen)	0.66631
B2	Material Stream: 9	Comp Mole Frac (CO2)	0.03551
B3	Material Stream: 9	Comp Mole Frac (CO)	0.15484
D1	Energy Stream: Electrolysis Power	Power	0.1834 kW
D3	Energy Stream: Lo Temp Pwr	Power	3.096e-002 kW
D4	Energy Stream: Hi Temp Pwr	Power	2.728e-002 kW
D5	Energy Stream: Circ Pwr	Power	3.209e-004 kW
D6	Energy Stream: Rcycl Pmp Pwr	Power	1.936e-007 kW

Exported Variables' Formula Results

Cell	Object	Variable Description	Value

PARAMETERS

Exportable Variables

Cell	Visible Name	Variable Description	Variable Type	Value
B4	B4: H2 to sum of CO & CO2 ratio	H2 to sum of CO & CO2 ratio	---	3.500
B6	B6: Comp Molar Flow (Hydrogen)	Comp Molar Flow (Hydrogen)	Comp. Mole Flow	<empty>
B7	B7: Comp Molar Flow (Hydrogen)	Comp Molar Flow (Hydrogen)	Comp. Mole Flow	<empty>
D2	D2:		Power	0.0000 kW

Spreadsheet: Co-Electrolysis Calcs (continued)

Units Set: NASA

PARAMETERS

Exportable Variables

Cell	Visible Name	Variable Description	Variable Type	Value
D7	D7: Total Power	Total Power	Power	0.2419 kW

User Variables

FORMULAS

Cell	Formula	Result
B4	=B1/(B2+B3)	3.500
D7	=D1+D2+D3+D4+D5+D6	0.2419 kW

Spreadsheet

	A	B	C	D		
1	H2 @ 14 *	0.66631	Electrolysis Power *	0.1834 kW		
2	CO2 @ 14 *	0.03551		0.0000 kW *		
3	CO @ 14 *	0.15484	Lo Temp Pwr *	3.096e-002 kW		
4	sum of CO & CO2 ratio *	3.500	Hi Temp Pwr *	2.728e-002 kW		
5			Circ Pwr *	3.209e-004 kW		
6		<empty> *	Rcycl Pmp Pwr *	1.936e-007 kW		
7		<empty> *	Total Power *	0.2419 kW		
8						
9						
10						

Spreadsheet: Electrolysis Input and Output

Units Set: Electrolysis

CONNECTIONS

Imported Variables

Cell	Object	Variable Description	Value
B6	Conversion Reactor: Isothermal Electrolysis @	Spec % Conversion (Spec % Conversion_1)	100.00
B7	Conversion Reactor: Isothermal Electrolysis @	Act. % Conversion (Act. % Conversion_2)	0.0000
D1	Material Stream: 6	Comp Mole Frac (Hydrogen)	0.08111
D2	Material Stream: 6	Comp Mole Frac (CO)	0.01888

Exported Variables' Formula Results

Cell	Object	Variable Description	Value

PARAMETERS

Exportable Variables

Cell	Visible Name	Variable Description	Variable Type	Value
B2	B2: Number of Cells	Number of Cells	---	2.444
B3	B3: Cell Area	Cell Area	Small Area	64.00 cm2
B4	B4: Current Density (Amperes/cm2)	Current Density (Amperes/cm2)	Vapour Fraction	<empty>
B5	B5: ASR @ 1100 K (ohm*cm2)	ASR @ 1100 K (ohm*cm2)	---	0.4000
B8	B8: Comp Mole Frac (Hydrogen)	Comp Mole Frac (Hydrogen)	Vapour Fraction	<empty>
B9	B9: Comp Mole Frac (CO)	Comp Mole Frac (CO)	Vapour Fraction	<empty>
D3	D3:		Vapour Fraction	0.1000
D4	D4: Mass Flow	Mass Flow	Mass Flow	<empty>
D6	D6:		---	<empty>
D7	D7:		---	<empty>
D8	D8: Heat Flow	Heat Flow	Energy	<empty>

Spreadsheet: Electrolysis Input and Output (contin

Units Set: Electrolysis

PARAMETERS

Exportable Variables

Cell	Visible Name	Variable Description	Variable Type	Value
D9	D9:		---	<empty>

User Variables

FORMULAS

Cell	Formula	Result
D3	=D1+D2	0.1000

Spreadsheet

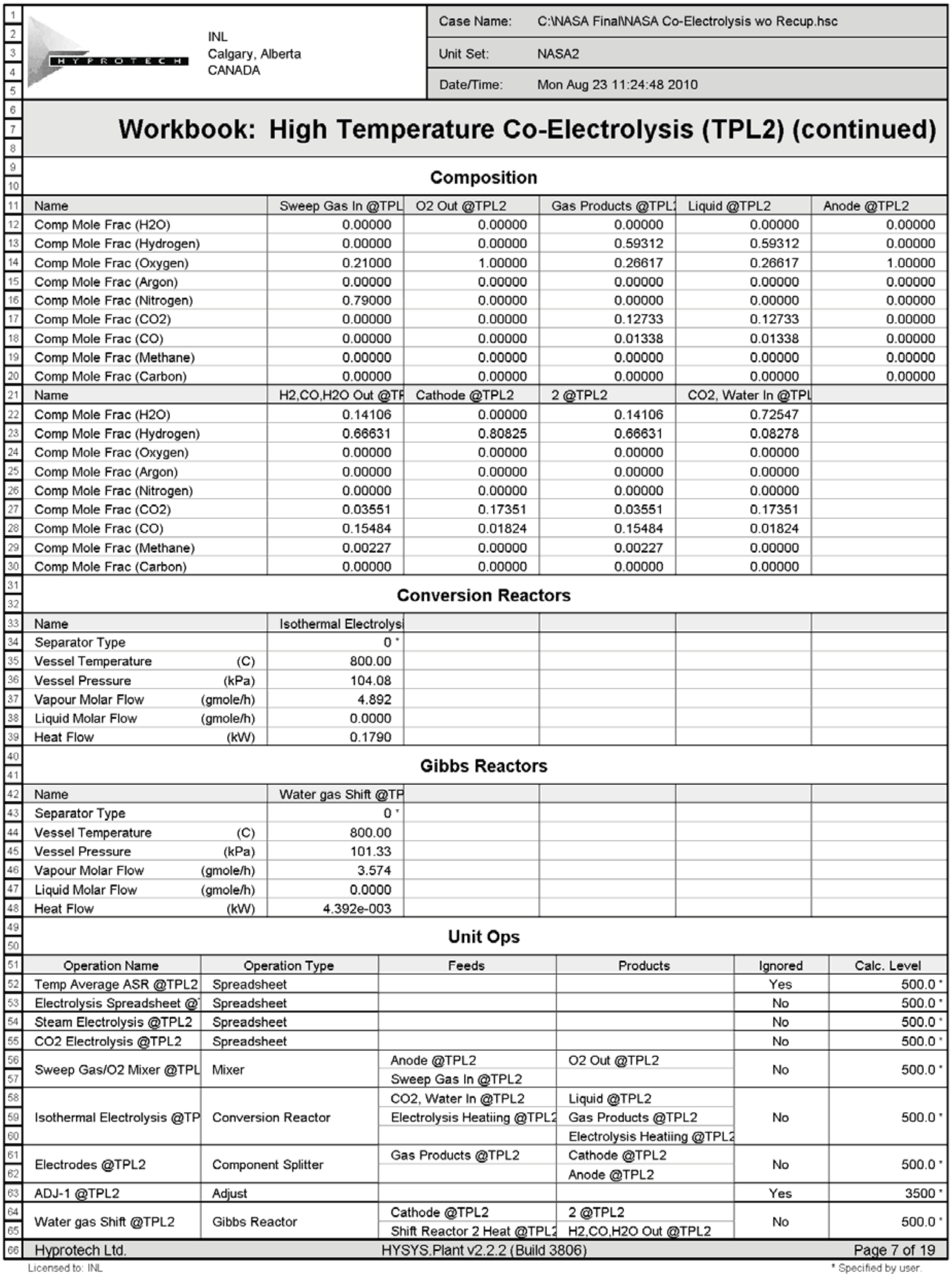
	A	B	C	D		
1	Input *	Input *	H2 @ 9 *	0.08111		
2	Number of Cells *	2.444 *	CO @ 9 *	0.01888		
3	Cell Area *	64.00 cm2 *		0.1000		
4		<empty> *		<empty> *		
5	@ 1100 K (ohms * cm2) *	0.4000 *				
6	% Water Conversion *	100.00 *		<empty> *		
7	% CO2 Conversion *	0.0000		<empty> *		
8		<empty> *		<empty> *		
9		<empty> *		<empty> *		
10						

Workbook: High Temperature Co-Electrolysis (TPL2)

Streams

Name		Sweep Gas In @TPL	O2 Out @TPL2	Gas Products @TPL	Liquid @TPL2	Anode @TPL2
Vapour Fraction		1.0000	1.0000	1.0000	0.0000	1.0000
Temperature	(C)	799.34	800.00	800.00 *	800.00	800.00
Pressure	(kPa)	102.70	102.70	104.08	104.08	102.70
Molar Flow	(gmole/h)	3.4662e-009	1.3021	4.8919	0.00000	1.3021
Mass Flow	(kg/d)	2.4000e-009	1.0000	1.8423	0.00000	1.0000
Liquid Volume Flow	(m3/h)	1.156e-013	3.662e-005	1.559e-004	0.0000	3.662e-005
Heat Flow	(kW)	2.342e-011	9.140e-003	-3.572e-002	0.0000	9.140e-003
Molar Enthalpy	(kJ/kgmole)	2.432e+004	2.527e+004	-2.629e+004	-2.629e+004	2.527e+004
Name		**H2,CO,H2O Out @TF**	**Cathode @TPL2**	**2 @TPL2**	**CO2, Water In @TPL**	**Electrolysis Heatiing**
Vapour Fraction		1.0000	1.0000	0.0000	1.0000	---
Temperature	(C)	800.00 *	800.00 *	800.00	799.34	---
Pressure	(kPa)	101.33	102.70	101.33	105.46	---
Molar Flow	(gmole/h)	3.5736	3.5898	0.00000	3.5898	---
Mass Flow	(kg/d)	0.84231	0.84230	0.00000	1.8423	---
Liquid Volume Flow	(m3/h)	1.044e-004	1.192e-004	0.0000	9.109e-005	---
Heat Flow	(kW)	-4.047e-002	-4.486e-002	0.0000	-0.2147	0.1790
Molar Enthalpy	(kJ/kgmole)	-4.077e+004	-4.499e+004	-4.077e+004	-2.153e+005	---
Name		**Process Heat @TPL**	**Shift Reactor 2 Heat**	**Electrolysis Power @**		
Vapour Fraction		---	---	---		
Temperature	(C)	---	---	---		
Pressure	(kPa)	---	---	---		
Molar Flow	(gmole/h)	---	---	---		
Mass Flow	(kg/d)	---	---	---		
Liquid Volume Flow	(m3/h)	---	---	---		
Heat Flow	(kW)	-3.162e-012	4.392e-003	0.1834		
Molar Enthalpy	(kJ/kgmole)	---	---	---		

* Specified by user.



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Calgary, Alberta
CANADA

Case Name:	C:\NASA Final\NASA Co-Electrolysis wo Recup.hsc
Unit Set:	NASA2
Date/Time:	Mon Aug 23 11:24:48 2010

Workbook: High Temperature Co-Electrolysis (TPL2) (continued)

Composition

Name	Sweep Gas In @TPL	O2 Out @TPL2	Gas Products @TPL	Liquid @TPL2	Anode @TPL2
Comp Mole Frac (H2O)	0.00000	0.00000	0.00000	0.00000	0.00000
Comp Mole Frac (Hydrogen)	0.00000	0.00000	0.59312	0.59312	0.00000
Comp Mole Frac (Oxygen)	0.21000	1.00000	0.26617	0.26617	1.00000
Comp Mole Frac (Argon)	0.00000	0.00000	0.00000	0.00000	0.00000
Comp Mole Frac (Nitrogen)	0.79000	0.00000	0.00000	0.00000	0.00000
Comp Mole Frac (CO2)	0.00000	0.00000	0.12733	0.12733	0.00000
Comp Mole Frac (CO)	0.00000	0.00000	0.01338	0.01338	0.00000
Comp Mole Frac (Methane)	0.00000	0.00000	0.00000	0.00000	0.00000
Comp Mole Frac (Carbon)	0.00000	0.00000	0.00000	0.00000	0.00000
Name	H2,CO,H2O Out @TF	Cathode @TPL2	2 @TPL2	CO2, Water In @TPL	
Comp Mole Frac (H2O)	0.14106	0.00000	0.14106	0.72547	
Comp Mole Frac (Hydrogen)	0.66631	0.80825	0.66631	0.08278	
Comp Mole Frac (Oxygen)	0.00000	0.00000	0.00000	0.00000	
Comp Mole Frac (Argon)	0.00000	0.00000	0.00000	0.00000	
Comp Mole Frac (Nitrogen)	0.00000	0.00000	0.00000	0.00000	
Comp Mole Frac (CO2)	0.03551	0.17351	0.03551	0.17351	
Comp Mole Frac (CO)	0.15484	0.01824	0.15484	0.01824	
Comp Mole Frac (Methane)	0.00227	0.00000	0.00227	0.00000	
Comp Mole Frac (Carbon)	0.00000	0.00000	0.00000	0.00000	

Conversion Reactors

Name		Isothermal Electrolysi
Separator Type		0 *
Vessel Temperature	(C)	800.00
Vessel Pressure	(kPa)	104.08
Vapour Molar Flow	(gmole/h)	4.892
Liquid Molar Flow	(gmole/h)	0.0000
Heat Flow	(kW)	0.1790

Gibbs Reactors

Name		Water gas Shift @TP
Separator Type		0 *
Vessel Temperature	(C)	800.00
Vessel Pressure	(kPa)	101.33
Vapour Molar Flow	(gmole/h)	3.574
Liquid Molar Flow	(gmole/h)	0.0000
Heat Flow	(kW)	4.392e-003

Unit Ops

Operation Name	Operation Type	Feeds	Products	Ignored	Calc. Level
Temp Average ASR @TPL2	Spreadsheet			Yes	500.0 *
Electrolysis Spreadsheet @	Spreadsheet			No	500.0 *
Steam Electrolysis @TPL2	Spreadsheet			No	500.0 *
CO2 Electrolysis @TPL2	Spreadsheet			No	500.0 *
Sweep Gas/O2 Mixer @TPL	Mixer	Anode @TPL2 Sweep Gas In @TPL2	O2 Out @TPL2	No	500.0 *
Isothermal Electrolysis @TP	Conversion Reactor	CO2, Water In @TPL2 Electrolysis Heatiing @TPL2	Liquid @TPL2 Gas Products @TPL2 Electrolysis Heatiing @TPL2	No	500.0 *
Electrodes @TPL2	Component Splitter	Gas Products @TPL2	Cathode @TPL2 Anode @TPL2	No	500.0 *
ADJ-1 @TPL2	Adjust			Yes	3500 *
Water gas Shift @TPL2	Gibbs Reactor	Cathode @TPL2 Shift Reactor 2 Heat @TPL2	2 @TPL2 H2,CO,H2O Out @TPL2	No	500.0 *

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Case Name:	C:\NASA Final\NASA Co-Electrolysis wo Recup.hsc
Unit Set:	NASA2
Date/Time:	Mon Aug 23 11:24:48 2010

Workbook: High Temperature Co-Electrolysis (TPL2) (continued)

Unit Ops (continued)

Operation Name	Operation Type	Feeds	Products	Ignored	Calc. Level
Water gas Shift @TPL2	Gibbs Reactor		Shift Reactor 2 Heat @TPL	No	500.0 *
SET-1 @TPL2	Set			No	500.0 *
SET-3 @TPL2	Set			No	500.0 *
SET-2 @TPL2	Set			No	500.0 *

Spreadsheet: CO2 Electrolysis @TPL2

Units Set: NewUser1

CONNECTIONS

Imported Variables

Cell	Object	Variable Description	Value
A8	Material Stream: CO2, Water In @TPL2	Pressure	0.10546 MPa
D2	Material Stream: CO2, Water In @TPL2	Temperature	1072.5 K
D3	Material Stream: H2,CO,H2O Out @TPL2	Temperature	1073.2 K
E2	Material Stream: CO2, Water In @TPL2	Comp Mole Frac (CO2)	0.17351
F2	Material Stream: CO2, Water In @TPL2	Comp Mole Frac (CO)	0.01824
G2	Material Stream: Sweep Gas In @TPL2	Comp Mole Frac (Oxygen)	0.21000
E3	Material Stream: H2,CO,H2O Out @TPL2	Comp Mole Frac (CO2)	0.03551
F3	Material Stream: H2,CO,H2O Out @TPL2	Comp Mole Frac (CO)	0.15484
G3	Material Stream: O2 Out @TPL2	Comp Mole Frac (Oxygen)	1.00000

Exported Variables' Formula Results

Cell	Object	Variable Description	Value

PARAMETERS

Exportable Variables

Cell	Visible Name	Variable Description	Variable Type	Value
A1	A1:		---	2.815e+005
A2	A2:		---	-37.53
A3	A3:		---	8.724e-003
A4	A4:		---	-8.470e-007
A5	A5:		---	-8.139
A6	A6:		---	9.649e+004
A7	A7:		---	8.314
A9	A9:		Pressure	0.10132 MPa
C1	C1:		---	<empty>
C7	C7:		---	<empty>
D4	D4:		Temperature	0.66058 K
D6	D6:		Temperature	1072.8 K
D8	D8:		---	4.613e-005
D9	D9:		---	6.984e-005
E4	E4:		Vapour Fraction	-0.1380
E5	E5:		Vapour Fraction	0.3234
F4	F4:		Vapour Fraction	0.1366
F5	F5:		Vapour Fraction	-0.3524
G4	G4:		Vapour Fraction	0.7900
G5	G5:		Vapour Fraction	-0.4623
H2	H2:		---	0.2186
H3	H3:		---	1.041
H4	H4:		---	0.8223
H5	H5:		---	-0.4482
I2	I2:		Molar Enthalpy	1.894e+005 J/gmole

* Specified by user.

Spreadsheet: CO2 Electrolysis @TPL2 (continued)

Units Set: NewUser1

PARAMETERS

Exportable Variables

Cell	Visible Name	Variable Description	Variable Type	Value
I3	I3:		Molar Enthalpy	1.893e+005 J/gmole
I6	I6:		Molar Enthalpy	1.893e+005 J/gmole
J2	J2:		---	2.533e+008
J3	J3:		---	2.535e+008
K2	K2:		---	0.8420
K3	K3:		---	1.050
K6	K6:		---	0.9587
K7	K7:		Vapour Fraction	0.9587

User Variables

FORMULAS

Cell	Formula	Result
D4	=D3-D2	0.66058 K
D6	=(D2+D3)/2	1072.8 K
D8	=1/(2*A6*H4*F4)	4.613e-005
D9	=1/(2*A6*H4*F4*D4)	6.984e-005
E4	=E3-E2	-0.1380
E5	=(E3*@LN(E3)-E3) - (E2*@LN(E2)-E2)	0.3234
F4	=F3-F2	0.1366
F5	=(F3*@LN(F3)-F3) - (F2*@LN(F2)-F2)	-0.3524
G4	=G3-G2	0.7900
G5	=(G3*@LN(G3)-G3) - (G2*@LN(G2)-G2)	-0.4623
H2	=G2*A8/A9	0.2186
H3	=G3*A8/A9	1.041
H4	=H3-H2	0.8223
H5	=(H3*@LN(H3)-H3) - (H2*@LN(H2)-H2)	-0.4482
I2	= A1 + A2*D2 + A3*D2^2 + A4*D2^3 + A5*D2*@LN(D2)	1.894e+005 J/gmole
I3	= A1 + A2*D3 + A3*D3^2 + A4*D3^3 + A5*D3*@LN(D3)	1.893e+005 J/gmole
I6	= A1 + A2*D6 + A3*D6^2 + A4*D6^3 + A5*D6*@LN(D6)	1.893e+005 J/gmole
J2	= A1*D2 + A2/2*D2^2 + A3/3*D2^3 + A4/4*D2^4 + A5/2*D2^2*(@LN(D2)-0.5)	2.533e+008
J3	= A1*D3 + A2/2*D3^2 + A3/3*D3^3 + A4/4*D3^4 + A5/2*D3^2*(@LN(D3)-0.5)	2.535e+008
K2	=1/(2*A6)*(I2-A7*D2*@LN(E2/(F2*H2^0.5)))	0.8420
K3	=1/(2*A6)*(I3-A7*D3*@LN(E3/(F3*H3^0.5)))	1.050
K6	=D8*(I6*F4*H4 + A7*D6*((E5+F5)*H4 + H5/2*F4))	0.9587
K7	=D9*(A7/2*(D3^2-D2^2)*((E5+F5)*H4 + H5/2*F4) + F4*H4*(J3-J2))	0.9587

Spreadsheet

	A	B	C	D	E	F
1	2.815e+005 *	A1 *	<empty> *	Temperature *	y CO2 *	y CO *
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> *			
8	0.10546 MPa	Pressure *	C isothermal *	4.613e-005		
9	0.10132 MPa *	Standard Pressure *	C *	6.984e-005		
10						

	G	H	I	J	K
1	y O2 *	y A *	Delta G *	Delta G dT (J-K/gmole) *	Nernst Voltage *
2	0.21000	0.2186	1.894e+005 J/gmole	2.533e+008	0.8420

* Specified by user.

Spreadsheet: CO2 Electrolysis @TPL2 (continued)

Units Set: NewUser1

Spreadsheet

3	1.00000	1.041	1.893e+005 J/gmole	2.535e+008	1.050	
4	0.7900	0.8223				
5	-0.4623	-0.4482				
6			1.893e+005 J/gmole	Isothermal *	0.9587	
7				Average *	0.9587	
8						
9						
10						

Spreadsheet: Electrolysis Spreadsheet @TPL2

Units Set: Electrolysis_

CONNECTIONS

Imported Variables

Cell	Object		Variable Description	Value
B8	SpreadSheetCell:	Electrolysis Input and Ou	B2: Number of Cells	2.444
B9	SpreadSheetCell:	Electrolysis Input and Ou	B3: Cell Area	64.00 cm2
D5	Material Stream:	CO2, Water In @TPL2	Comp Mole Frac (Hydrogen)	0.08278
D6	Material Stream:	H2,CO,H2O Out @TPL2	Comp Mole Frac (Hydrogen)	0.66631
D9	Material Stream:	CO2, Water In @TPL2	Pressure	0.10546 MPa
D1	Material Stream:	CO2, Water In @TPL2	Temperature	1072.5 K
D2	Material Stream:	H2,CO,H2O Out @TPL2	Temperature	1073.2 K
D3	Material Stream:	CO2, Water In @TPL2	Comp Mole Frac (H2O)	0.72547
D4	Material Stream:	H2,CO,H2O Out @TPL2	Comp Mole Frac (H2O)	0.14106
D7	Material Stream:	Sweep Gas In @TPL2	Comp Mole Frac (Oxygen)	0.21000
D8	Material Stream:	O2 Out @TPL2	Comp Mole Frac (Oxygen)	1.00000
B16	SpreadSheetCell:	Electrolysis Input and Ou	B5: ASR @ 1100 K (ohm*cm2)	0.4000
D14	Energy Stream:	Electrolysis Heatiing @T	Heat Flow	0.1790 kW
D17	Energy Stream:	Shift Reactor 2 Heat @T	Heat Flow	4.392e-003 kW
B18	Material Stream:	CO2, Water In @TPL2	Comp Molar Flow (H2O)	0.0007 gmole/s
B20	Material Stream:	CO2, Water In @TPL2	Comp Molar Flow (CO2)	0.0002 gmole/s
D19	Conversion Reactor:	Isothermal Electrolysis @	Act. % Conversion (Act. % Conversion_1)	100.0
D20	Material Stream:	Anode @TPL2	Comp Molar Flow (Oxygen)	0.0004 gmole/s
B19	Conversion Reactor:	Isothermal Electrolysis @	Act. % Conversion (Act. % Conversion_2)	0.0000

Exported Variables' Formula Results

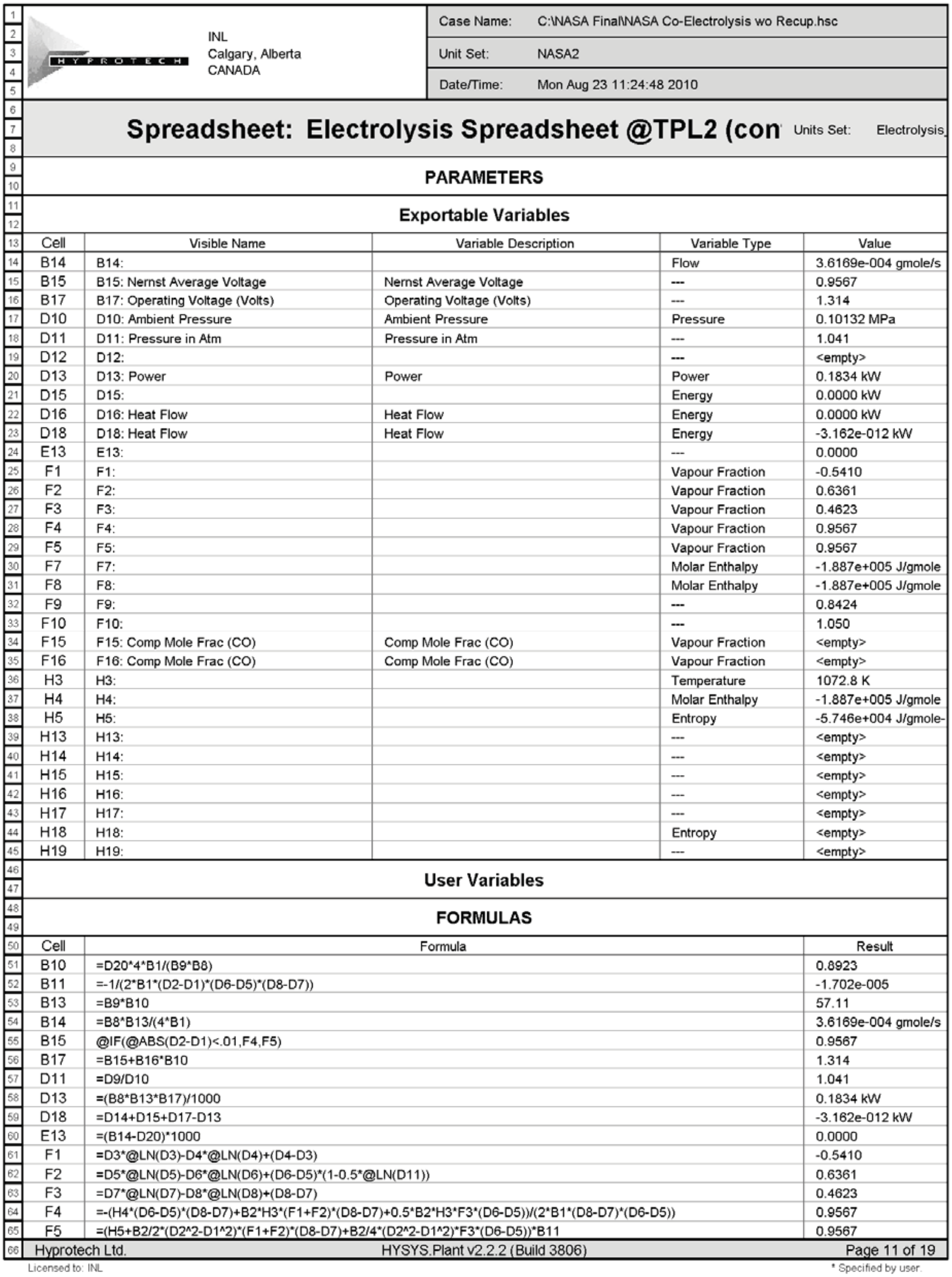
Cell	Object	Variable Description	Value
D13	Electrolysis Power @TPL2	Power	0.1834 kW
D18	Process Heat @TPL2	Heat Flow	-3.162e-012 kW

PARAMETERS

Exportable Variables

Cell	Visible Name	Variable Description	Variable Type	Value
B1	B1: Faraday Constant	Faraday Constant	---	9.649e+004
B2	B2: Universal Constant	Universal Constant	Entropy	8.314 J/gmole-K
B3	B3: A1 (J/gmol)	A1 (J/gmol)	---	-2.382e+005
B4	B4: A2 (J/gmol-K)	A2 (J/gmol-K)	---	-39.95
B5	B5: A3 (J/gmol-K^2)	A3 (J/gmol-K^2)	---	-3.319e-003
B6	B6: A4 (J/gmol-K^3)	A4 (J/gmol-K^3)	---	3.532e-008
B7	B7: A5 (J/gmol-K)	A5 (J/gmol-K)	---	12.85
B10	B10: B4: Current Density (Amperes/cm2)	B4: Current Density (Amperes/cm2)	---	0.8923
B11	B11: C (J-K/(volt-gmole))	C (J-K/(volt-gmole))	---	-1.702e-005
B13	B13: Current (amperes)	Current (amperes)	---	57.11

* Specified by user.



INL
Calgary, Alberta
CANADA

Case Name:	C:\NASA Final\NASA Co-Electrolysis wo Recup.hsc
Unit Set:	NASA2
Date/Time:	Mon Aug 23 11:24:48 2010

Spreadsheet: Electrolysis Spreadsheet @TPL2 (con

Units Set: Electrolysis

PARAMETERS

Exportable Variables

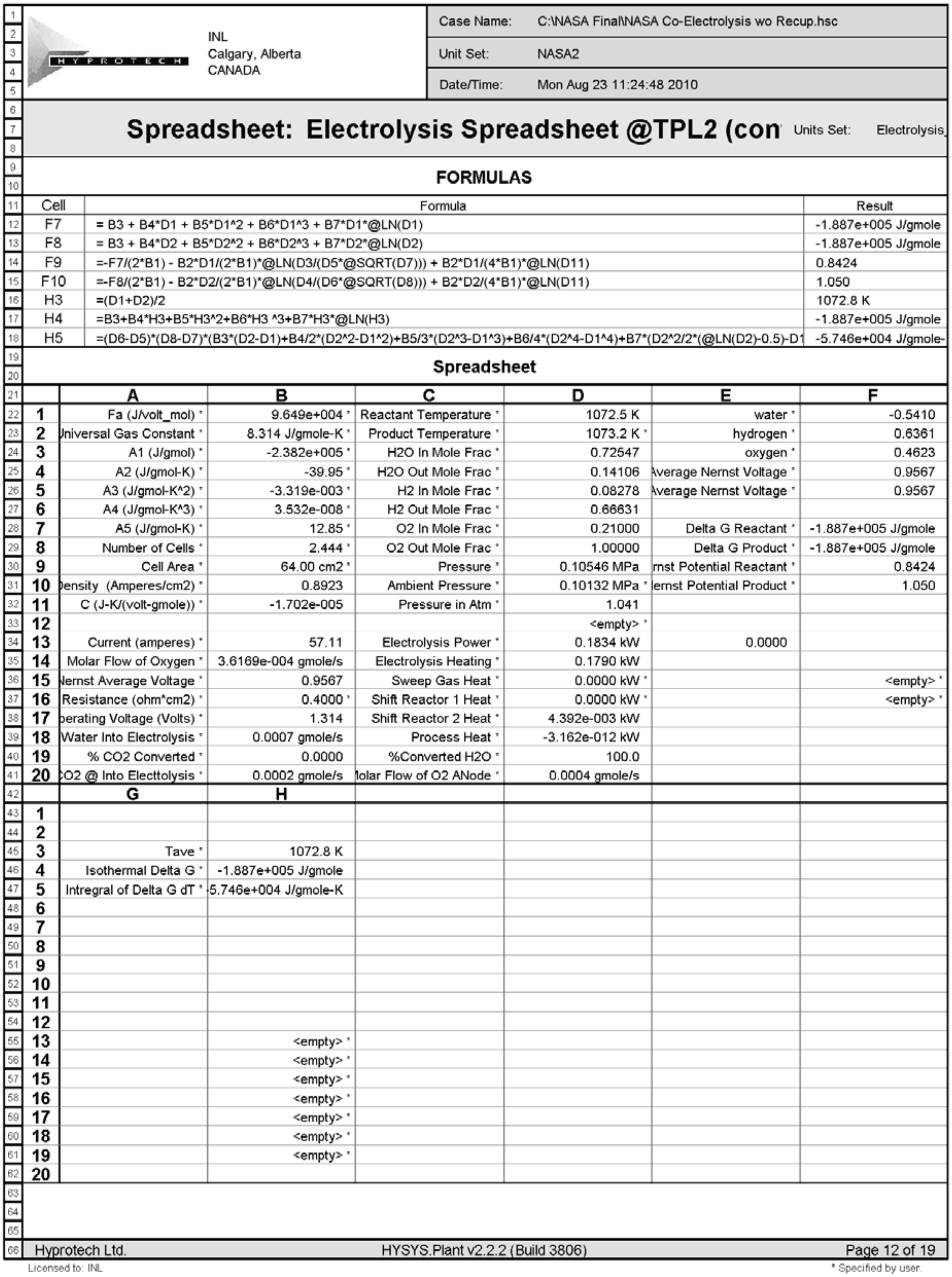
Cell	Visible Name	Variable Description	Variable Type	Value
B14	B14:		Flow	3.6169e-004 gmole/s
B15	B15: Nernst Average Voltage	Nernst Average Voltage	---	0.9567
B17	B17: Operating Voltage (Volts)	Operating Voltage (Volts)	---	1.314
D10	D10: Ambient Pressure	Ambient Pressure	Pressure	0.10132 MPa
D11	D11: Pressure in Atm	Pressure in Atm	---	1.041
D12	D12:		---	<empty>
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/gmole
F8	F8:		Molar Enthalpy	-1.887e+005 J/gmole
F9	F9:		---	0.8424
F10	F10:		---	1.050
F15	F15: Comp Mole Frac (CO)	Comp Mole Frac (CO)	Vapour Fraction	<empty>
F16	F16: Comp Mole Frac (CO)	Comp Mole Frac (CO)	Vapour Fraction	<empty>
H3	H3:		Temperature	1072.8 K
H4	H4:		Molar Enthalpy	-1.887e+005 J/gmole
H5	H5:		Entropy	-5.746e+004 J/gmole-
H13	H13:		---	<empty>
H14	H14:		---	<empty>
H15	H15:		---	<empty>
H16	H16:		---	<empty>
H17	H17:		---	<empty>
H18	H18:		Entropy	<empty>
H19	H19:		---	<empty>

User Variables

FORMULAS

Cell	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/s
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)*(D8-D7)+0.5*B2*H3*F3*(D6-D5))/(2*B1*(D8-D7)*(D6-D5))	0.9567
F5	=(H5+B2/2*(D2^2-D1^2)*(F1+F2)*(D8-D7)+B2/4*(D2^2-D1^2)*F3*(D6-D5))*B11	0.9567

* Specified by user.



INL
Calgary, Alberta
CANADA

Case Name:	C:\NASA Final\NASA Co-Electrolysis wo Recup.hsc
Unit Set:	NASA2
Date/Time:	Mon Aug 23 11:24:48 2010

Spreadsheet: Electrolysis Spreadsheet @TPL2 (con

Units Set: Electrolysis_

FORMULAS

Cell	Formula	Result
F7	= B3 + B4*D1 + B5*D1^2 + B6*D1^3 + B7*D1*@LN(D1)	-1.887e+005 J/gmole
F8	= B3 + B4*D2 + B5*D2^2 + B6*D2^3 + B7*D2*@LN(D2)	-1.887e+005 J/gmole
F9	=-F7/(2*B1) - B2*D1/(2*B1)*@LN(D3/(D5*@SQRT(D7))) + B2*D1/(4*B1)*@LN(D11)	0.8424
F10	=-F8/(2*B1) - B2*D2/(2*B1)*@LN(D4/(D6*@SQRT(D8))) + B2*D2/(4*B1)*@LN(D11)	1.050
H3	=(D1+D2)/2	1072.8 K
H4	=B3+B4*H3+B5*H3^2+B6*H3 ^3+B7*H3*@LN(H3)	-1.887e+005 J/gmole
H5	=(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)-D1	-5.746e+004 J/gmole-

Spreadsheet

	A	B	C	D	E	F
1	Fa (J/volt_mol) *	9.649e+004 *	Reactant Temperature *	1072.5 K	water *	-0.5410
2	Jniversal Gas Constant *	8.314 J/gmole-K *	Product Temperature *	1073.2 K *	hydrogen *	0.6361
3	A1 (J/gmol) *	-2.382e+005 *	H2O In Mole Frac *	0.72547	oxygen *	0.4623
4	A2 (J/gmol-K) *	-39.95 *	H2O Out Mole Frac *	0.14106	\verage Nernst Voltage *	0.9567
5	A3 (J/gmol-K^2) *	-3.319e-003 *	H2 In Mole Frac *	0.08278	\verage Nernst Voltage *	0.9567
6	A4 (J/gmol-K^3) *	3.532e-008 *	H2 Out Mole Frac *	0.66631		
7	A5 (J/gmol-K) *	12.85 *	O2 In Mole Frac *	0.21000	Delta G Reactant *	-1.887e+005 J/gmole
8	Number of Cells *	2.444 *	O2 Out Mole Frac *	1.00000	Delta G Product *	-1.887e+005 J/gmole
9	Cell Area *	64.00 cm2 *	Pressure *	0.10546 MPa	rnst Potential Reactant *	0.8424
10	)ensity (Amperes/cm2) *	0.8923	Ambient Pressure *	0.10132 MPa *	lernst Potential Product *	1.050
11	C (J-K/(volt-gmole)) *	-1.702e-005	Pressure in Atm *	1.041		
12				<empty> *		
13	Current (amperes) *	57.11	Electrolysis Power *	0.1834 kW	0.0000	
14	Molar Flow of Oxygen *	3.6169e-004 gmole/s	Electrolysis Heating *	0.1790 kW		
15	lernst Average Voltage *	0.9567	Sweep Gas Heat *	0.0000 kW *		<empty> *
16	Resistance (ohm*cm2) *	0.4000 *	Shift Reactor 1 Heat *	0.0000 kW *		<empty> *
17	)erating Voltage (Volts) *	1.314	Shift Reactor 2 Heat *	4.392e-003 kW		
18	Water Into Electrolysis *	0.0007 gmole/s	Process Heat *	-3.162e-012 kW		
19	% CO2 Converted *	0.0000	%Converted H2O *	100.0		
20	:O2 @ Into Electtolysis *	0.0002 gmole/s	lolar Flow of O2 ANode *	0.0004 gmole/s		

	G	H
1		
2		
3	Tave *	1072.8 K
4	Isothermal Delta G *	-1.887e+005 J/gmole
5	Intregral of Delta G dT *	5.746e+004 J/gmole-K
6		
7		
8		
9		
10		
11		
12		
13		<empty> *
14		<empty> *
15		<empty> *
16		<empty> *
17		<empty> *
18		<empty> *
19		<empty> *
20		

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* Specified by user.

Spreadsheet: Steam Electrolysis @TPL2

Units Set: NewUser1

CONNECTIONS

Imported Variables

Cell	Object	Variable Description	Value
D2	Material Stream: CO2, Water In @TPL2	Temperature	1072.5 K
D3	Material Stream: H2,CO,H2O Out @TPL2	Temperature	1073.2 K
E2	Material Stream: CO2, Water In @TPL2	Comp Mole Frac (H2O)	0.72547
E3	Material Stream: H2,CO,H2O Out @TPL2	Comp Mole Frac (H2O)	0.14106
F2	Material Stream: CO2, Water In @TPL2	Comp Mole Frac (Hydrogen)	0.08278
F3	Material Stream: H2,CO,H2O Out @TPL2	Comp Mole Frac (Hydrogen)	0.66631
G2	Material Stream: Sweep Gas In @TPL2	Comp Mole Frac (Oxygen)	0.21000
G3	Material Stream: O2 Out @TPL2	Comp Mole Frac (Oxygen)	1.00000
A8	Material Stream: CO2, Water In @TPL2	Pressure	0.10546 MPa

Exported Variables' Formula Results

Cell	Object	Variable Description	Value

PARAMETERS

Exportable Variables

Cell	Visible Name	Variable Description	Variable Type	Value
A1	A1: A1 for Gibbs Formation Energy	A1 for Gibbs Formation Energy	Molar Enthalpy	2.382e+005 J/gmole
A2	A2: A2 for Gibbs Formation Energy	A2 for Gibbs Formation Energy	Entropy	39.95 J/gmole-K
A3	A3: A3 for Gibbs Formation Energy	A3 for Gibbs Formation Energy	Gibbs. Coeff. CC	3.319e-003 kJ/kgmol-
A4	A4: A4 for Gibbs Formation Energy	A4 for Gibbs Formation Energy	---	-3.532e-008
A5	A5: A5 for Gibbs Formation Energy	A5 for Gibbs Formation Energy	Entropy	-12.85 J/gmole-K
A6	A6: Fa (J/Volt-gmole)	Fa (J/Volt-gmole)	---	9.649e+004
A7	A7: Universal Gas Contant	Universal Gas Contant	Entropy	8.314 J/gmole-K
A9	A9: Standard Pressure	Standard Pressure	Pressure	0.10132 MPa
D4	D4:		Temperature	0.66058 K
D6	D6:		Temperature	1072.8 K
D8	D8:		---	1.080e-005
D9	D9:		---	1.635e-005
E4	E4:		Vapour Fraction	-0.5844
E5	E5:		Vapour Fraction	0.5410
F4	F4:		Vapour Fraction	0.5835
F5	F5:		Vapour Fraction	-0.6478
G4	G4:		Vapour Fraction	0.7900
G5	G5:		Vapour Fraction	-0.4623
H2	H2:		---	0.2186
H3	H3:		---	1.041
H4	H4:		---	0.8223
H5	H5:		---	-0.4482
I2	I2:		Molar Enthalpy	1.887e+005 J/gmole
I3	I3:		Molar Enthalpy	1.887e+005 J/gmole
I6	I6:		Molar Enthalpy	1.887e+005 J/gmole
J2	J2:		---	2.320e+008
J3	J3:		---	2.321e+008
K2	K2:		---	0.8424
K3	K3:		---	1.050
K6	K6:		Vapour Fraction	0.9567
K7	K7:		---	0.9567

User Variables

* Specified by user.

Spreadsheet: Steam Electrolysis @TPL2 (continued

Units Set: NewUser1

FORMULAS

Cell	Formula	Result
D4	=D3-D2	0.66058 K
D6	= (D2+D3)/2	1072.8 K
D8	=1/(2*A6*H4*F4)	1.080e-005
D9	=1/(2*A6*H4*F4*D4)	1.635e-005
E4	=E3-E2	-0.5844
E5	= (E3*@LN(E3)-E3) - (E2*@LN(E2)-E2)	0.5410
F4	=F3-F2	0.5835
F5	= (F3*@LN(F3)-F3) - (F2*@LN(F2)-F2)	-0.6478
G4	=G3-G2	0.7900
G5	= (G3*@LN(G3)-G3) - (G2*@LN(G2)-G2)	-0.4623
H2	=G2*A8/A9	0.2186
H3	=G3*A8/A9	1.041
H4	=H3-H2	0.8223
H5	= (H3*@LN(H3)-H3) - (H2*@LN(H2)-H2)	-0.4482
I2	= A1 + A2*D2 + A3*D2^2 + A4*D2^3 + A5*D2*@LN(D2)	1.887e+005 J/gmole
I3	= A1 + A2*D3 + A3*D3^2 + A4*D3^3 + A5*D3*@LN(D3)	1.887e+005 J/gmole
I6	= A1 + A2*D6 + A3*D6^2 + A4*D6^3 + A5*D6*@LN(D6)	1.887e+005 J/gmole
J2	= A1*D2 + A2/2*D2^2 + A3/3*D2^3 + A4/4*D2^4 + A5/2*D2^2*(@LN(D2)-0.5)	2.320e+008
J3	= A1*D3 + A2/2*D3^2 + A3/3*D3^3 + A4/4*D3^4 + A5/2*D3^2*(@LN(D3)-0.5)	2.321e+008
K2	=1/(2*A6)*(I2-A7*D2*@LN(E2/(F2*H2^0.5)))	0.8424
K3	=1/(2*A6)*(I3-A7*D3*@LN(E3/(F3*H3^0.5)))	1.050
K6	=D8*(I6*F4*H4 + A7*D6*((E5+F5)*H4 + H5/2*F4))	0.9567
K7	=D9*(A7/2*(D3^2-D2^2)*((E5+F5)*H4 + H5/2*F4) + F4*H4*(J3-J2))	0.9567

Spreadsheet

	A	B	C	D	E	F
1	2.382e+005 J/gmole *	A1 *		Temperature *	y H2O *	y H2 *
2	39.95 J/gmole-K *	A2 *	in *	1072.5 K	0.72547	0.08278
3	319e-003 kJ/kgmol-K^2 *	A3 *	out *	1073.2 K *	0.14106	0.66631
4	-3.532e-008 *	A4 (J/gmole-K^3) *	Delta *	0.66058 K	-0.5844	0.5835
5	-12.85 J/gmole-K *	A5 *	Integration Coeff *		0.5410	-0.6478
6	9.649e+004 *	Fa (J/Volt-gmole) *	Average *	1072.8 K		
7	8.314 J/gmole-K *	Ru *				
8	0.10546 MPa	Pressure *	C isothermal *	1.080e-005		
9	0.10132 MPa *	Standard Pressure *	C *	1.635e-005		
10						

	G	H	I	J	K	
1	y O2 *	y A *	Delta G *	Delta G dT (J-K/gmole) *	Nernst Voltage *	
2	0.21000	0.2186	1.887e+005 J/gmole	2.320e+008	0.8424	
3	1.00000	1.041	1.887e+005 J/gmole	2.321e+008	1.050	
4	0.7900	0.8223				
5	-0.4623	-0.4482				
6			1.887e+005 J/gmole	Isothermal *	0.9567	
7				Average *	0.9567	
8						
9						
10						

* Specified by user.

Spreadsheet: Temp Average ASR @TPL2

(Ignored) Units Set: Electrolys

CONNECTIONS

Imported Variables

Cell	Object	Variable Description	Value
B1	SpreadSheetCell: Electrolysis Input and Ou	F14: ASR @ 1100 K	<empty>
E15	Material Stream: H2,CO,H2O Out @TPL2	Temperature	<empty>

Exported Variables' Formula Results

Cell	Object	Variable Description	Value

PARAMETERS

Exportable Variables

Cell	Visible Name	Variable Description	Variable Type	Value
A3	A3:		Temperature	<empty>
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A7	A7:		---	<empty>
A8	A8:		---	<empty>
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A10	A10:		---	<empty>
A11	A11:		---	<empty>
A12	A12:		---	<empty>
A13	A13:		---	<empty>
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A16	A16:		---	<empty>
A17	A17:		---	<empty>
A18	A18:		---	<empty>
A19	A19:		---	<empty>
A20	A20:		---	<empty>
B2	B2: Temp Aver ASR	Temp Aver ASR	---	<empty>
B3	B3:		---	<empty>
B4	B4:		---	<empty>
B5	B5:		---	<empty>
B6	B6:		---	<empty>
B7	B7:		---	<empty>
B8	B8:		---	<empty>
B9	B9:		---	<empty>
B10	B10:		---	<empty>
B11	B11:		---	<empty>
B12	B12:		---	<empty>
B13	B13:		---	<empty>
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B15	B15:		---	<empty>
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B19	B19:		---	<empty>
B20	B20:		---	<empty>
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C3	C3:		---	<empty>
C4	C4:		---	<empty>
C5	C5:		---	<empty>

* Specified by user.

Spreadsheet: Temp Average ASR @TPL2 (

(Ignored) Units Set: Electrolys

PARAMETERS

Exportable Variables

Cell	Visible Name	Variable Description	Variable Type	Value
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D2	D2:		---	<empty>
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D10	D10:		---	<empty>
D11	D11:		---	<empty>
D12	D12:		---	<empty>
D13	D13:		---	<empty>
D14	D14:		---	<empty>
D15	D15:		---	<empty>
D16	D16:		---	<empty>
D17	D17:		---	<empty>
D18	D18:		---	<empty>
D19	D19:		---	<empty>
E1	E1:		---	<empty>
E2	E2:		---	<empty>
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E5	E5:		---	<empty>
E6	E6:		---	<empty>
E7	E7:		---	<empty>
E8	E8:		---	<empty>
E9	E9:		---	<empty>
E10	E10:		---	<empty>
E11	E11:		---	<empty>
E12	E12:		---	<empty>
E13	E13:		---	<empty>
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F1	F1:		---	<empty>
F2	F2:		---	<empty>
F3	F3:		---	<empty>
F4	F4:		---	<empty>
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Spreadsheet: Temp Average ASR @TPL2 (

(Ignored) Units Set: Electrolys

PARAMETERS

Exportable Variables

Cell	Visible Name	Variable Description	Variable Type	Value
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F10	F10:		---	<empty>
F11	F11:		---	<empty>
F12	F12:		---	<empty>
F13	F13:		---	<empty>
F14	F14:		---	<empty>
F15	F15:		---	<empty>
F16	F16:		---	<empty>

User Variables

FORMULAS

Cell	Formula	Result
A4	=A3+F16	<empty>
A5	=A4+F16	<empty>
A6	=A5+F16	<empty>
A7	=A6+F16	<empty>
A8	=A7+F16	<empty>
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A11	=A10+F16	<empty>
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A13	=A12+F16	<empty>
A14	=A13+F16	<empty>
A15	=A14+F16	<empty>
A16	=A15+F16	<empty>
A17	=A16+F16	<empty>
A18	=A17+F16	<empty>
A19	=A18+F16	<empty>
A20	=4*(B4+B6+B8+B10+B12+B14+B16+B18+D1+D3+D5+D7+D9+D11+D13+D15+D17+D19+F2+F4+F6+F8+F10+F12+F1	<empty>
B2	@if(E15==A3,F15,(1/3*F16*(B3+A20+B20+F15))/(E15-A3))	<empty>
B3	@EXP(10300/A3)*0.00003973+(B1-0.463)	<empty>
B4	@EXP(10300/A4)*0.00003973+(B1-0.463)	<empty>
B5	@EXP(10300/A5)*0.00003973+(B1-0.463)	<empty>
B6	@EXP(10300/A6)*0.00003973+(B1-0.463)	<empty>
B7	@EXP(10300/A7)*0.00003973+(B1-0.463)	<empty>
B8	@EXP(10300/A8)*0.00003973+(B1-0.463)	<empty>
B9	@EXP(10300/A9)*0.00003973+(B1-0.463)	<empty>
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B11	@EXP(10300/A11)*0.00003973+(B1-0.463)	<empty>
B12	@EXP(10300/A12)*0.00003973+(B1-0.463)	<empty>
B13	@EXP(10300/A13)*0.00003973+(B1-0.463)	<empty>
B14	@EXP(10300/A14)*0.00003973+(B1-0.463)	<empty>
B15	@EXP(10300/A15)*0.00003973+(B1-0.463)	<empty>
B16	@EXP(10300/A16)*0.00003973+(B1-0.463)	<empty>
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B18	@EXP(10300/A18)*0.00003973+(B1-0.463)	<empty>
B19	@EXP(10300/A19)*0.00003973+(B1-0.463)	<empty>
B20	=2*(B5+B7+B9+B11+B13+B15+B17+B19+D2+D4+D6+D8+D10+D12+D14+D16+D18+F1+F3+F5+F7+F9+F11+F13)	<empty>

* Specified by user.

Spreadsheet: Temp Average ASR @TPL2 (

(Ignored) Units Set: Electrolys

FORMULAS

Cell	Formula	Result
C1	=A19+F16	<empty>
C2	=C1+F16	<empty>
C3	=C2+F16	<empty>
C4	=C3+F16	<empty>
C5	=C4+F16	<empty>
C6	=C5+F16	<empty>
C7	=C6+F16	<empty>
C8	=C7+F16	<empty>
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C10	=C9+F16	<empty>
C11	=C10+F16	<empty>
C12	=C11+F16	<empty>
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C17	=C16+F16	<empty>
C18	=C17+F16	<empty>
C19	=C18+F16	<empty>
D1	@EXP(10300/C1)*0.00003973+(B1-0.463)	<empty>
D2	@EXP(10300/C2)*0.00003973+(B1-0.463)	<empty>
D3	@EXP(10300/C3)*0.00003973+(B1-0.463)	<empty>
D4	@EXP(10300/C4)*0.00003973+(B1-0.463)	<empty>
D5	@EXP(10300/C5)*0.00003973+(B1-0.463)	<empty>
D6	@EXP(10300/C6)*0.00003973+(B1-0.463)	<empty>
D7	@EXP(10300/C7)*0.00003973+(B1-0.463)	<empty>
D8	@EXP(10300/C8)*0.00003973+(B1-0.463)	<empty>
D9	@EXP(10300/C9)*0.00003973+(B1-0.463)	<empty>
D10	@EXP(10300/C10)*0.00003973+(B1-0.463)	<empty>
D11	@EXP(10300/C11)*0.00003973+(B1-0.463)	<empty>
D12	@EXP(10300/C12)*0.00003973+(B1-0.463)	<empty>
D13	@EXP(10300/C13)*0.00003973+(B1-0.463)	<empty>
D14	@EXP(10300/C14)*0.00003973+(B1-0.463)	<empty>
D15	@EXP(10300/C15)*0.00003973+(B1-0.463)	<empty>
D16	@EXP(10300/C16)*0.00003973+(B1-0.463)	<empty>
D17	@EXP(10300/C17)*0.00003973+(B1-0.463)	<empty>
D18	@EXP(10300/C18)*0.00003973+(B1-0.463)	<empty>
D19	@EXP(10300/C19)*0.00003973+(B1-0.463)	<empty>
E1	=C19+F16	<empty>
E2	=E1+F16	<empty>
E3	=E2+F16	<empty>
E4	=E3+F16	<empty>
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E12	=E11+F16	<empty>
E13	=E12+F16	<empty>
E14	=E13+F16	<empty>
F1	@EXP(10300/E1)*0.00003973+(B1-0.463)	<empty>
F2	@EXP(10300/E2)*0.00003973+(B1-0.463)	<empty>

* Specified by user.

Spreadsheet: Temp Average ASR @TPL2 (

(Ignored) Units Set: Electrolys

FORMULAS

Cell	Formula	Result
F3	@EXP(10300/E3)*0.00003973+(B1-0.463)	<empty>
F4	@EXP(10300/E4)*0.00003973+(B1-0.463)	<empty>
F5	@EXP(10300/E5)*0.00003973+(B1-0.463)	<empty>
F6	@EXP(10300/E6)*0.00003973+(B1-0.463)	<empty>
F7	@EXP(10300/E7)*0.00003973+(B1-0.463)	<empty>
F8	@EXP(10300/E8)*0.00003973+(B1-0.463)	<empty>
F9	@EXP(10300/E9)*0.00003973+(B1-0.463)	<empty>
F10	@EXP(10300/E10)*0.00003973+(B1-0.463)	<empty>
F11	@EXP(10300/E11)*0.00003973+(B1-0.463)	<empty>
F12	@EXP(10300/E12)*0.00003973+(B1-0.463)	<empty>
F13	@EXP(10300/E13)*0.00003973+(B1-0.463)	<empty>
F14	@EXP(10300/E14)*0.00003973+(B1-0.463)	<empty>
F15	@EXP(10300/E15)*0.00003973+(B1-0.463)	<empty>
F16	=(E15-A3)/50	<empty>

Spreadsheet

	A	B	C	D	E	F
1	ASR @ 1100 K *	<empty> *	<empty>	<empty>	<empty>	<empty>
2	Temp Average ASR *	<empty>	<empty>	<empty>	<empty>	<empty>
3	<empty> *	<empty>	<empty>	<empty>	<empty>	<empty>
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16	<empty>	<empty>	<empty>	<empty>	delta T *	<empty>
17	<empty>	<empty>	<empty>	<empty>		
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20	<empty>	<empty>				

* Specified by user.

A.7 Boudouard Process with Co-electrolysis

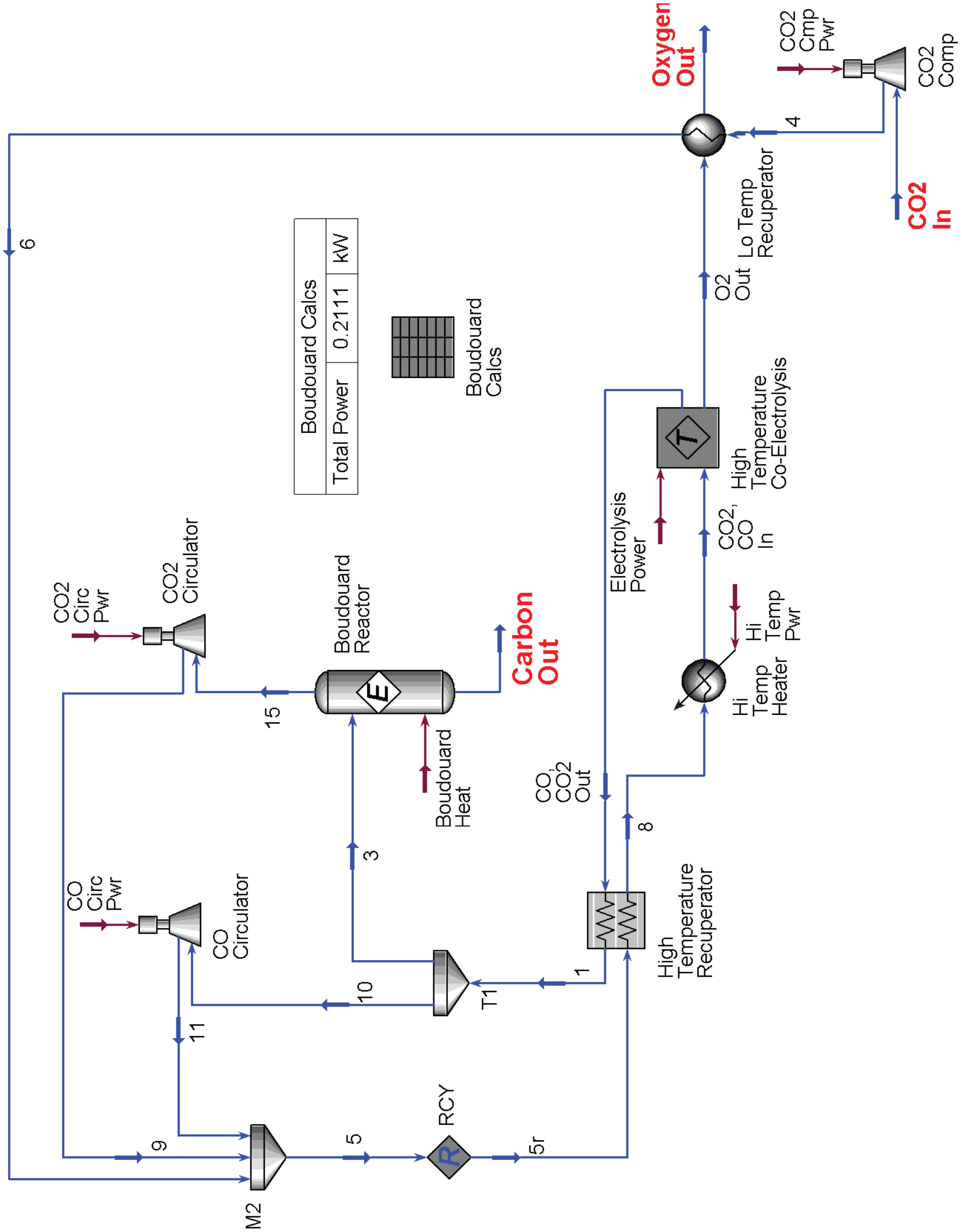


Figure A - 13   Process flow diagram of Boudouard process with co-electrolysis

Workbook: Case (Main)

Streams

Name	5	Sweep Gas In	CO, CO2 Out	5r	CO2, CO In
Vapour Fraction	1.0000	1.0000	1.0000	1.0000	1.0000
Temperature (C)	461.72	800.00	800.00	461.71 *	800.00 *
Pressure (kPa)	185.75	175.37	175.37	185.75 *	179.75
Molar Flow (gmole/h)	3.2553	3.4662e-009 *	3.2552	3.2553 *	3.2553
Mass Flow (kg/d)	3.3134	2.4000e-009	2.3133	3.3133	3.3133
Liquid Volume Flow (m3/h)	1.676e-004	1.156e-013	1.200e-004	1.676e-004	1.676e-004
Heat Flow (kW)	-0.3136	2.344e-011	-0.1026	-0.3136	-0.2982
Molar Enthalpy (kJ/kgmole)	-3.468e+005	2.434e+004	-1.135e+005	-3.468e+005	-3.297e+005

Name	CO2 Circ Pwr	CO2 Cmp Pwr	Electrolysis Power	CO Circ Pwr	Hi Temp Pwr
Vapour Fraction	---	---	---	---	---
Temperature (C)	---	---	---	---	---
Pressure (kPa)	---	---	---	---	---
Molar Flow (gmole/h)	---	---	---	---	---
Mass Flow (kg/d)	---	---	---	---	---
Liquid Volume Flow (m3/h)	---	---	---	---	---
Heat Flow (kW)	2.847e-004	4.450e-004	0.2047	6.332e-005	5.595e-003
Molar Enthalpy (kJ/kgmole)	---	---	---	---	---

Name	O2 Out	Boudouard Heat	8	4	6
Vapour Fraction	1.0000	---	1.0000	1.0000	1.0000
Temperature (C)	800.00	---	680.97	53.253	568.99
Pressure (kPa)	175.37	---	182.75	188.75 *	185.75
Molar Flow (gmole/h)	1.3021	---	3.2553	1.3022	1.3022
Mass Flow (kg/d)	1.0000	---	3.3133	1.3754	1.3754
Liquid Volume Flow (m3/h)	3.662e-005	---	1.676e-004	6.944e-005	6.944e-005
Heat Flow (kW)	9.140e-003	-6.638e-002	-0.3037	-0.1421	-0.1335
Molar Enthalpy (kJ/kgmole)	2.527e+004	---	-3.359e+005	-3.928e+005	-3.690e+005

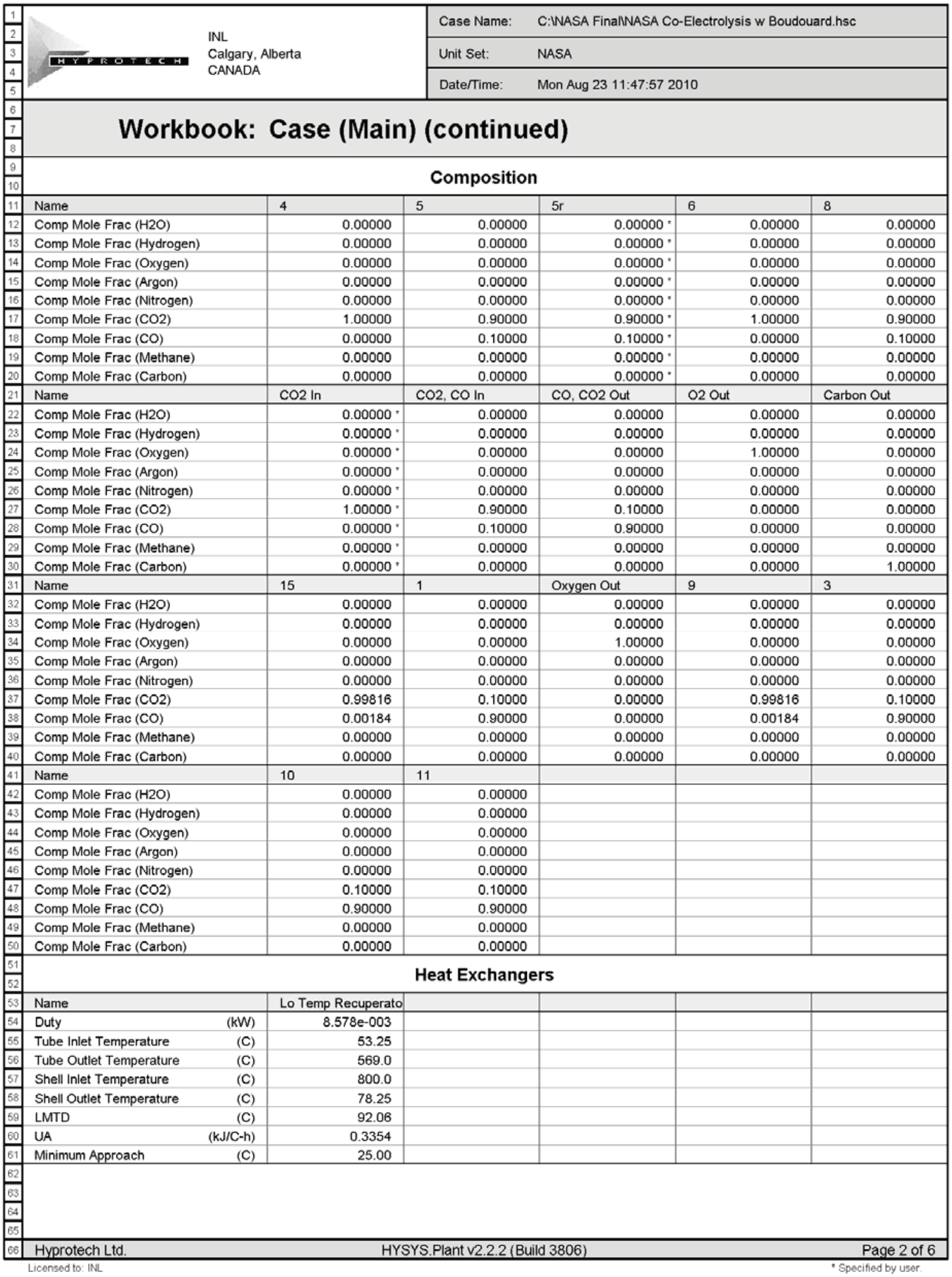
Name	Carbon Out	15	1	Oxygen Out	9
Vapour Fraction	0.0000	1.0000	1.0000	1.0000	1.0000
Temperature (C)	350.00	350.00 *	486.71	78.253	363.64
Pressure (kPa)	169.37	169.37	172.37	172.37	185.75
Molar Flow (gmole/h)	1.3021	1.5947	3.2552	1.3021	1.5947
Mass Flow (kg/d)	0.37534	1.6832	2.3133	1.0000	1.6832
Liquid Volume Flow (m3/h)	9.524e-006	8.498e-005	1.200e-004	3.662e-005	8.498e-005
Heat Flow (kW)	1.609e-003	-0.1680	-0.1124	5.633e-004	-0.1678
Molar Enthalpy (kJ/kgmole)	4450	-3.793e+005	-1.243e+005	1557	-3.787e+005

Name	3	10	11		
Vapour Fraction	1.0000	1.0000	1.0000		
Temperature (C)	486.71	486.71	505.70		
Pressure (kPa)	172.37	172.37	185.75		
Molar Flow (gmole/h)	2.8968	0.35844	0.35844		
Mass Flow (kg/d)	2.0586	0.25473	0.25473		
Liquid Volume Flow (m3/h)	1.068e-004	1.322e-005	1.322e-005		
Heat Flow (kW)	-0.1001	-1.238e-002	-1.232e-002		
Molar Enthalpy (kJ/kgmole)	-1.243e+005	-1.243e+005	-1.237e+005		

Compressors

Name	CO2 Circulator	CO2 Comp	CO Circulator		
Feed Pressure (kPa)	169.4	131.0 *	172.4		
Product Pressure (kPa)	185.7	188.7 *	185.7		
Molar Flow (gmole/h)	1.595	1.302	0.3584		
Energy (kW)	2.847e-004	4.450e-004	6.332e-005		
Adiabatic Efficiency	75 *	75 *	75 *		
Polytropic Efficiency	75	76	75		

* Specified by user.



INL
Calgary, Alberta
CANADA

Case Name:	C:\NASA Final\NASA Co-Electrolysis w Boudouard.hsc
Unit Set:	NASA
Date/Time:	Mon Aug 23 11:47:57 2010

Workbook: Case (Main) (continued)

Composition

Name	4	5	5r	6	8
Comp Mole Frac (H2O)	0.00000	0.00000	0.00000 *	0.00000	0.00000
Comp Mole Frac (Hydrogen)	0.00000	0.00000	0.00000 *	0.00000	0.00000
Comp Mole Frac (Oxygen)	0.00000	0.00000	0.00000 *	0.00000	0.00000
Comp Mole Frac (Argon)	0.00000	0.00000	0.00000 *	0.00000	0.00000
Comp Mole Frac (Nitrogen)	0.00000	0.00000	0.00000 *	0.00000	0.00000
Comp Mole Frac (CO2)	1.00000	0.90000	0.90000 *	1.00000	0.90000
Comp Mole Frac (CO)	0.00000	0.10000	0.10000 *	0.00000	0.10000
Comp Mole Frac (Methane)	0.00000	0.00000	0.00000 *	0.00000	0.00000
Comp Mole Frac (Carbon)	0.00000	0.00000	0.00000 *	0.00000	0.00000

Name	CO2 In	CO2, CO In	CO, CO2 Out	O2 Out	Carbon Out
Comp Mole Frac (H2O)	0.00000 *	0.00000	0.00000	0.00000	0.00000
Comp Mole Frac (Hydrogen)	0.00000 *	0.00000	0.00000	0.00000	0.00000
Comp Mole Frac (Oxygen)	0.00000 *	0.00000	0.00000	1.00000	0.00000
Comp Mole Frac (Argon)	0.00000 *	0.00000	0.00000	0.00000	0.00000
Comp Mole Frac (Nitrogen)	0.00000 *	0.00000	0.00000	0.00000	0.00000
Comp Mole Frac (CO2)	1.00000 *	0.90000	0.10000	0.00000	0.00000
Comp Mole Frac (CO)	0.00000 *	0.10000	0.90000	0.00000	0.00000
Comp Mole Frac (Methane)	0.00000 *	0.00000	0.00000	0.00000	0.00000
Comp Mole Frac (Carbon)	0.00000 *	0.00000	0.00000	0.00000	1.00000

Name	15	1	Oxygen Out	9	3
Comp Mole Frac (H2O)	0.00000	0.00000	0.00000	0.00000	0.00000
Comp Mole Frac (Hydrogen)	0.00000	0.00000	0.00000	0.00000	0.00000
Comp Mole Frac (Oxygen)	0.00000	0.00000	1.00000	0.00000	0.00000
Comp Mole Frac (Argon)	0.00000	0.00000	0.00000	0.00000	0.00000
Comp Mole Frac (Nitrogen)	0.00000	0.00000	0.00000	0.00000	0.00000
Comp Mole Frac (CO2)	0.99816	0.10000	0.00000	0.99816	0.10000
Comp Mole Frac (CO)	0.00184	0.90000	0.00000	0.00184	0.90000
Comp Mole Frac (Methane)	0.00000	0.00000	0.00000	0.00000	0.00000
Comp Mole Frac (Carbon)	0.00000	0.00000	0.00000	0.00000	0.00000

Name	10	11			
Comp Mole Frac (H2O)	0.00000	0.00000			
Comp Mole Frac (Hydrogen)	0.00000	0.00000			
Comp Mole Frac (Oxygen)	0.00000	0.00000			
Comp Mole Frac (Argon)	0.00000	0.00000			
Comp Mole Frac (Nitrogen)	0.00000	0.00000			
Comp Mole Frac (CO2)	0.10000	0.10000			
Comp Mole Frac (CO)	0.90000	0.90000			
Comp Mole Frac (Methane)	0.00000	0.00000			
Comp Mole Frac (Carbon)	0.00000	0.00000			

Heat Exchangers

Name		Lo Temp Recuperato				
Duty	(kW)	8.578e-003				
Tube Inlet Temperature	(C)	53.25				
Tube Outlet Temperature	(C)	569.0				
Shell Inlet Temperature	(C)	800.0				
Shell Outlet Temperature	(C)	78.25				
LMTD	(C)	92.06				
UA	(kJ/C-h)	0.3354				
Minimum Approach	(C)	25.00				

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Workbook: Case (Main) (continued)

Other Heat Exchangers

Name		High Temperature Re				
Number of Sides		2 *				
LMTD	(C)	60.71 *				
UA (Calculated)	(kJ/C-h)	0.5819				
Hot Pinch Temperature	(C)	486.7				
Cold Pinch Temperature	(C)	461.7				
Minimum Approach	(C)	25.00				
Exchanger Cold Duty	(kW)	9.813e-003				

Pumps

Name						
Delta P	(kPa)					
Energy	(kW)					
Feed Pressure	(kPa)					
Product Pressure	(kPa)					
Molar Flow	(gmole/h)					
Adiabatic Efficiency	(%)					

Unit Ops

Operation Name	Operation Type	Feeds	Products	Ignored	Calc. Level
Hi Temp Heater	Heater	8 Hi Temp Pwr	CO2, CO In	No	500.0 *
T1	Tee	1	3 10	No	500.0 *
Lo Temp Recuperator	Heat Exchanger	4 O2 Out	6 Oxygen Out	No	500.0 *
M2	Mixer	9 6 11	5	No	500.0 *
CO2 Circulator	Compressor	15 CO2 Circ Pwr	9	No	500.0 *
CO2 Comp	Compressor	CO2 In CO2 Cmp Pwr	4	No	500.0 *
CO Circulator	Compressor	10 CO Circ Pwr	11	No	500.0 *
High Temperature Recupera	LNG	5r CO, CO2 Out	8 1	No	500.0 *
High Temperature Co-Electr	Standard Sub-Flowsheet	Sweep Gas In CO2, CO In Process Heat Electrolysis Power	O2 Out CO, CO2 Out	No	2500 *
Electrolysis Input and Output	Spreadsheet			No	500.0 *
Boudouard Calcs	Spreadsheet			No	500.0 *
Boudouard Reactor	Equilibrium Reactor	3 Boudouard Heat	Carbon Out 15 Boudouard Heat	No	500.0 *
RCY	Recycle	5	5r	No	3500 *

* Specified by user.

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Calgary, Alberta
CANADA

Case Name:	C:\NASA Final\NASA Co-Electrolysis w Boudouard.hsc
Unit Set:	NASA
Date/Time:	Mon Aug 23 11:47:57 2010

Workbook: High Temperature Co-Electrolysis (TPL2)

Streams

Name		Sweep Gas In @TPL	O2 Out @TPL2	Gas Products @TPL	Liquid @TPL2	Anode @TPL2
Vapour Fraction		1.0000	1.0000	1.0000	0.0000	1.0000
Temperature	(C)	800.00	800.00	800.00 *	800.00	800.00
Pressure	(kPa)	175.37	175.37	176.75	176.75	175.37
Molar Flow	(gmole/h)	3.4662e-009	1.3021	4.5573	0.00000	1.3021
Mass Flow	(kg/d)	2.4000e-009	1.0000	3.3133	0.00000	1.0000
Liquid Volume Flow	(m3/h)	1.156e-013	3.662e-005	1.566e-004	0.0000	3.662e-005
Heat Flow	(kW)	2.344e-011	9.140e-003	-9.348e-002	0.0000	9.140e-003
Molar Enthalpy	(kJ/kgmole)	2.434e+004	2.527e+004	-7.384e+004	-7.384e+004	2.527e+004
Name		CO, CO2 Out @TPL2	CO2, Water In @TPL	Electrolysis Heatiing	Process Heat @TPL	Electrolysis Power @
Vapour Fraction		1.0000	1.0000	---	---	---
Temperature	(C)	800.00 *	800.00	---	---	---
Pressure	(kPa)	175.37	179.75	---	---	---
Molar Flow	(gmole/h)	3.2552	3.2553	---	---	---
Mass Flow	(kg/d)	2.3133	3.3133	---	---	---
Liquid Volume Flow	(m3/h)	1.200e-004	1.676e-004	---	---	---
Heat Flow	(kW)	-0.1026	-0.2982	0.2047	8.050e-009	0.2047
Molar Enthalpy	(kJ/kgmole)	-1.135e+005	-3.297e+005	---	---	---

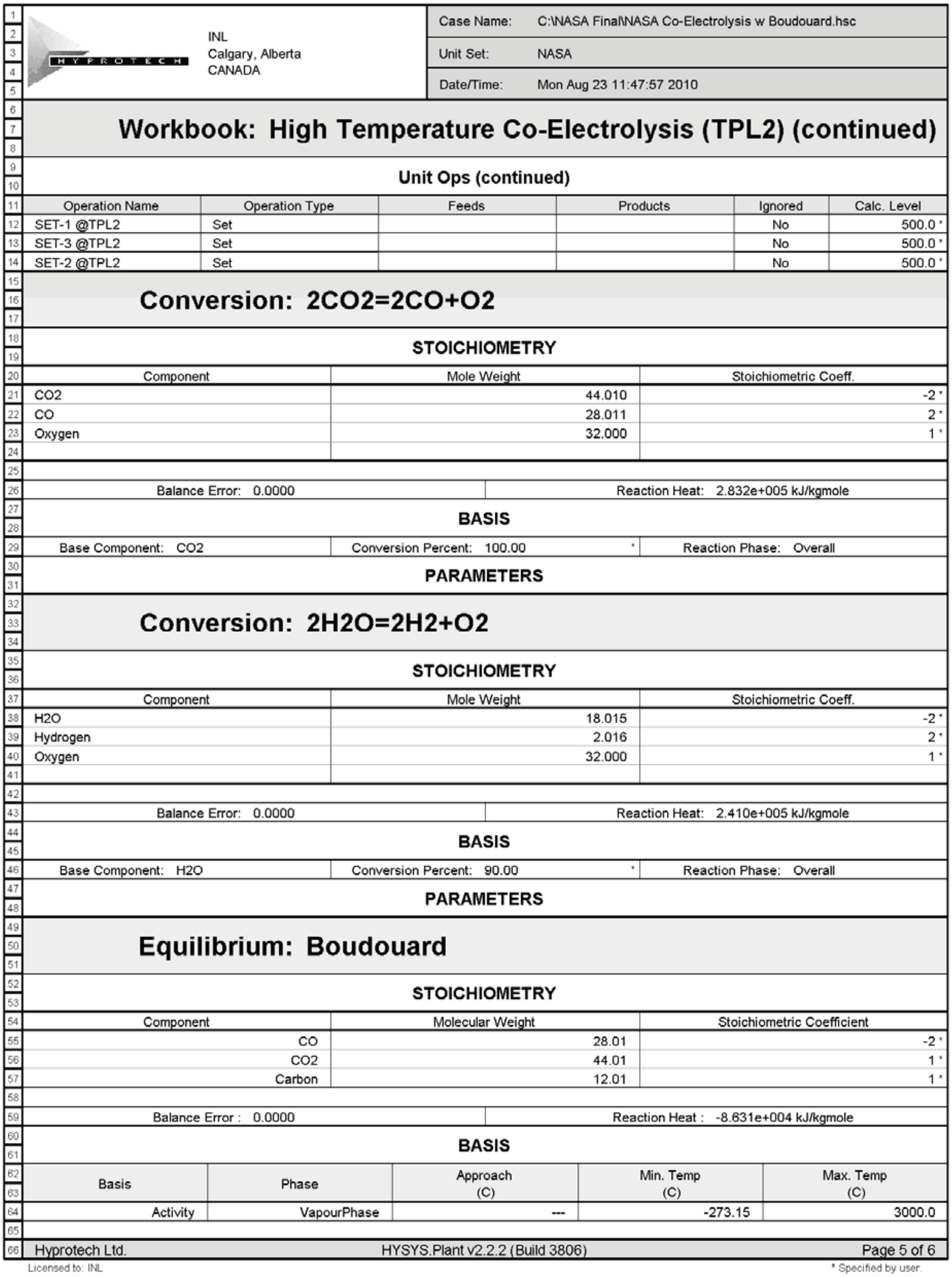
Material Streams

Name	Sweep Gas In @TPL	O2 Out @TPL2	Gas Products @TPL	Liquid @TPL2	Anode @TPL2
Comp Mole Frac (H2O)	0.00000	0.00000	0.00000	0.00000	0.00000
Comp Mole Frac (Hydrogen)	0.00000	0.00000	0.00000	0.00000	0.00000
Comp Mole Frac (Oxygen)	0.21000	1.00000	0.28571	0.28571	1.00000
Comp Mole Frac (Argon)	0.00000	0.00000	0.00000	0.00000	0.00000
Comp Mole Frac (Nitrogen)	0.79000	0.00000	0.00000	0.00000	0.00000
Comp Mole Frac (CO2)	0.00000	0.00000	0.07143	0.07143	0.00000
Comp Mole Frac (CO)	0.00000	0.00000	0.64286	0.64286	0.00000
Comp Mole Frac (Methane)	0.00000	0.00000	0.00000	0.00000	0.00000
Comp Mole Frac (Carbon)	0.00000	0.00000	0.00000	0.00000	0.00000
Name	CO, CO2 Out @TPL2	CO2, Water In @TPL			
Comp Mole Frac (H2O)	0.00000	0.00000			
Comp Mole Frac (Hydrogen)	0.00000	0.00000			
Comp Mole Frac (Oxygen)	0.00000	0.00000			
Comp Mole Frac (Argon)	0.00000	0.00000			
Comp Mole Frac (Nitrogen)	0.00000	0.00000			
Comp Mole Frac (CO2)	0.10000	0.90000			
Comp Mole Frac (CO)	0.90000	0.10000			
Comp Mole Frac (Methane)	0.00000	0.00000			
Comp Mole Frac (Carbon)	0.00000	0.00000			

Unit Ops

Operation Name	Operation Type	Feeds	Products	Ignored	Calc. Level
Temp Average ASR @TPL2	Spreadsheet			Yes	500.0 *
Electrolysis Spreadsheet @	Spreadsheet			No	500.0 *
Steam Electrolysis @TPL2	Spreadsheet			No	500.0 *
CO2 Electrolysis @TPL2	Spreadsheet			No	500.0 *
Sweep Gas/O2 Mixer @TPL	Mixer	Anode @TPL2 Sweep Gas In @TPL2	O2 Out @TPL2	No	500.0 *
Isothermal Electrolysis @TP	Conversion Reactor	CO2, Water In @TPL2 Electrolysis Heatiing @TPL2	Liquid @TPL2 Gas Products @TPL2 Electrolysis Heatiing @TPL2	No	500.0 *
Electrodes @TPL2	Component Splitter	Gas Products @TPL2	CO, CO2 Out @TPL2 Anode @TPL2	No	500.0 *
ADJ-1 @TPL2	Adjust			Yes	3500 *

* Specified by user.



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Case Name:	C:\NASA Final\NASA Co-Electrolysis w Boudouard.hsc
Unit Set:	NASA
Date/Time:	Mon Aug 23 11:47:57 2010

Workbook: High Temperature Co-Electrolysis (TPL2) (continued)

Unit Ops (continued)

Operation Name	Operation Type	Feeds	Products	Ignored	Calc. Level
SET-1 @TPL2	Set			No	500.0 *
SET-3 @TPL2	Set			No	500.0 *
SET-2 @TPL2	Set			No	500.0 *

Conversion: 2CO2=2CO+O2

STOICHIOMETRY

Component	Mole Weight	Stoichiometric Coeff.
CO2	44.010	-2 *
CO	28.011	2 *
Oxygen	32.000	1 *

Balance Error: 0.0000

Reaction Heat: 2.832e+005 kJ/kgmole

BASIS

Base Component: CO2

Conversion Percent: 100.00 *

Reaction Phase: Overall

PARAMETERS

Conversion: 2H2O=2H2+O2

STOICHIOMETRY

Component	Mole Weight	Stoichiometric Coeff.
H2O	18.015	-2 *
Hydrogen	2.016	2 *
Oxygen	32.000	1 *

Balance Error: 0.0000

Reaction Heat: 2.410e+005 kJ/kgmole

BASIS

Base Component: H2O

Conversion Percent: 90.00 *

Reaction Phase: Overall

PARAMETERS

Equilibrium: Boudouard

STOICHIOMETRY

Component	Molecular Weight	Stoichiometric Coefficient
CO	28.01	-2 *
CO2	44.01	1 *
Carbon	12.01	1 *

Balance Error : 0.0000

Reaction Heat : -8.631e+004 kJ/kgmole

BASIS

Basis	Phase	Approach (C)	Min. Temp (C)	Max. Temp (C)
Activity	VapourPhase	---	-273.15	3000.0

* Specified by user.

Equilibrium: Boudouard (continued)

PARAMETERS

Source : K Vs. T Table

Coeff A	-21.64	R2	1.000000 *
Coeff B	2.078e+004	T High	---
Coeff C	5.932e-002	T Low	---
Coeff D	-3.081e-005		

Temperature (C)	Keq	KCalc	Percentage Error
25.000 *	1.040e+021 *	1.040e+021 *	-9.850e-003 *
127.00 *	2.030e+013 *	2.028e+013 *	7.997e-002 *
227.00 *	6.330e+008 *	6.339e+008 *	-0.1356 *
327.00 *	6.290e+005 *	6.289e+005 *	1.221e-002 *
427.00 *	4500 *	4502 *	-3.523e-002 *
527.00 *	111.0 *	110.8 *	0.1967 *
627.00 *	6.210 *	6.210 *	-3.002e-003 *
727.00 *	0.6190 *	0.6194 *	-7.027e-002 *
827.00 *	9.390e-002 *	9.394e-002 *	-4.777e-002 *
927.00 *	1.950e-002 *	1.951e-002 *	-4.409e-002 *
1027.0 *	5.160e-003 *	5.159e-003 *	2.318e-002 *
1127.0 *	1.650e-003 *	1.649e-003 *	3.338e-002 *

A.8 Hydrogenation Process with Co-electrolysis

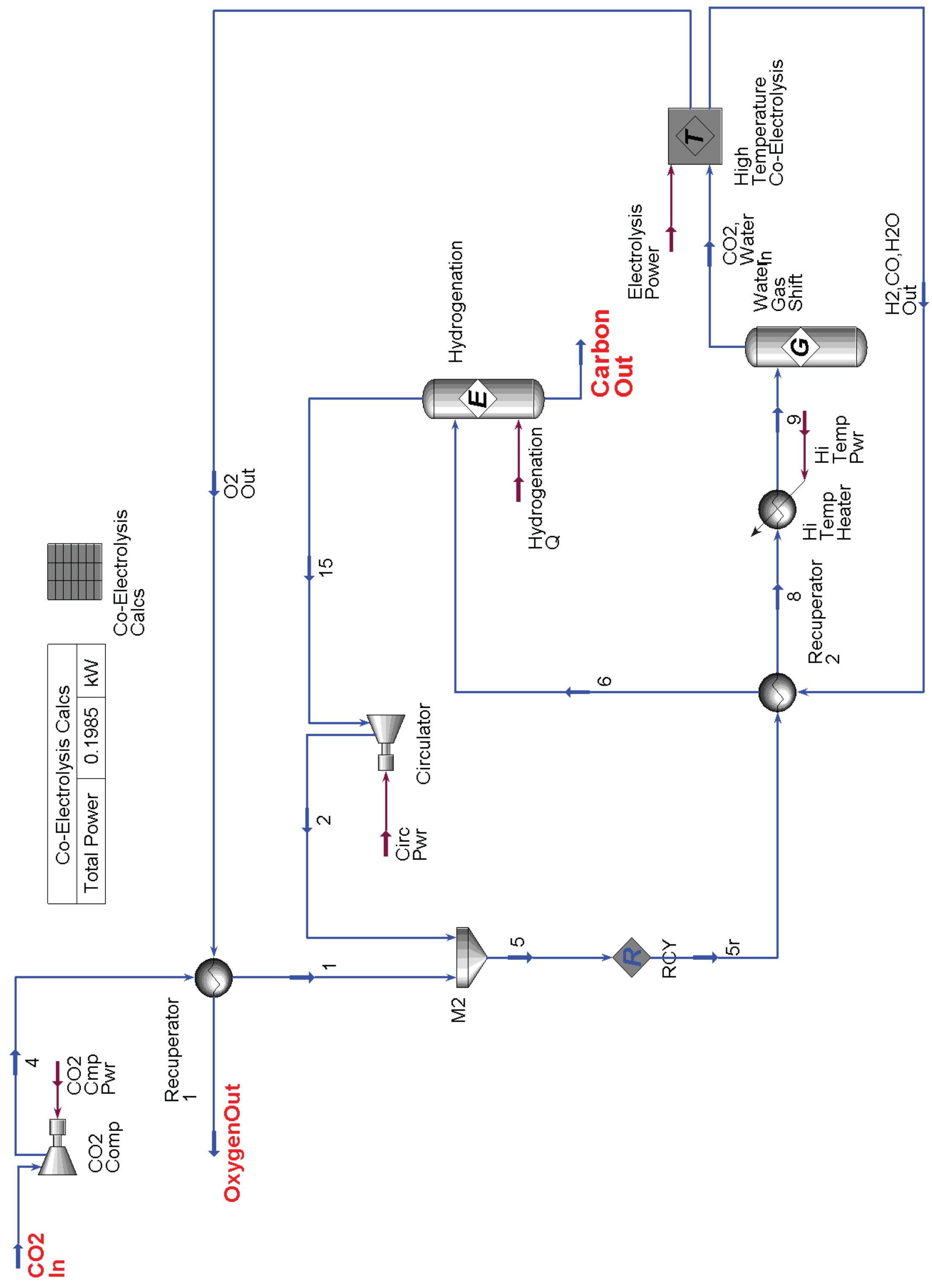
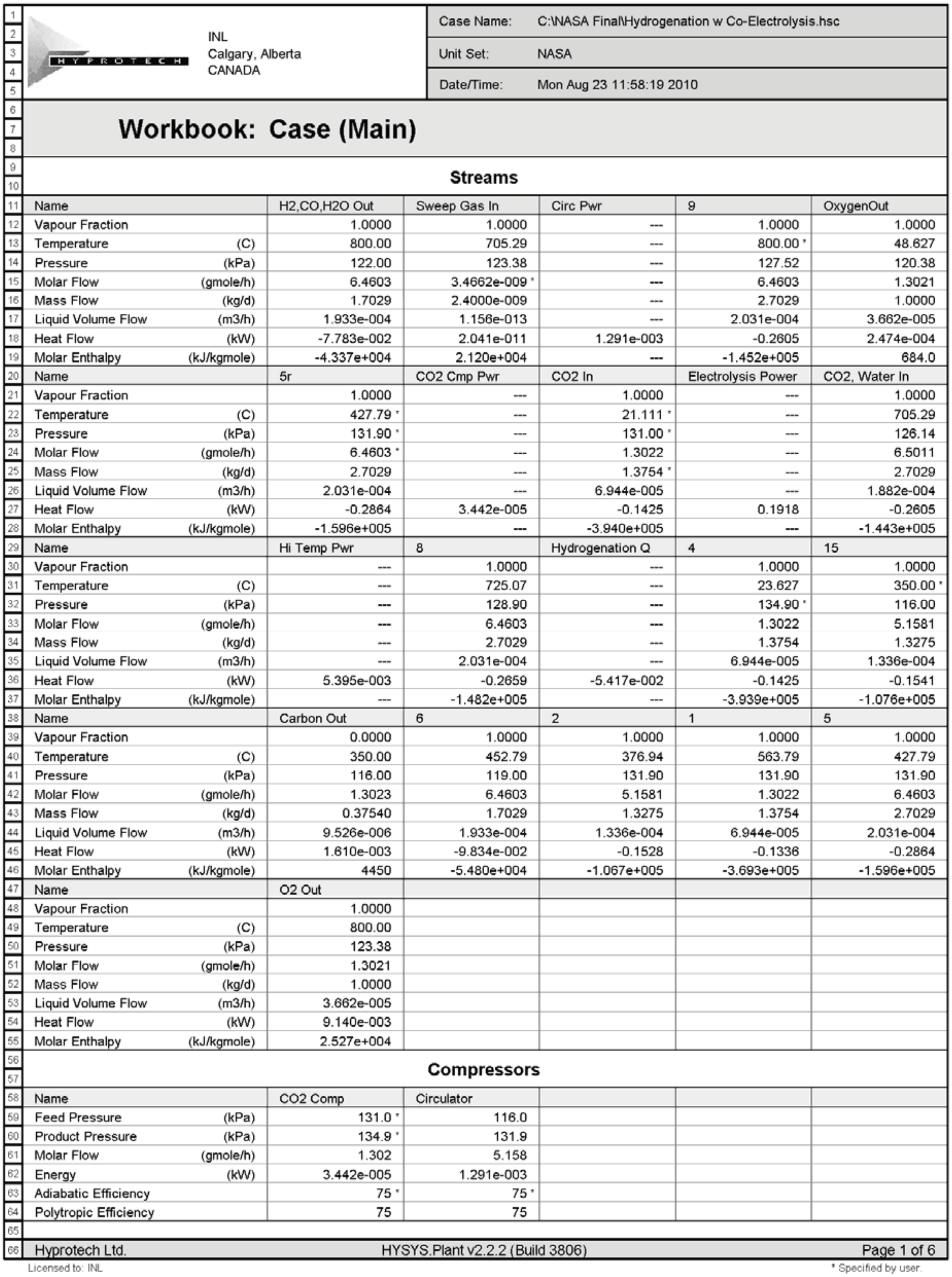


Figure A - 14 Process flow diagram of hydrogenation process with co-electrolysis



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CANADA

Case Name:	C:\NASA Final\Hydrogenation w Co-Electrolysis.hsc
Unit Set:	NASA
Date/Time:	Mon Aug 23 11:58:19 2010

Workbook: Case (Main)

Streams

Name	H2,CO,H2O Out	Sweep Gas In	Circ Pwr	9	OxygenOut
Vapour Fraction	1.0000	1.0000	---	1.0000	1.0000
Temperature (C)	800.00	705.29	---	800.00 *	48.627
Pressure (kPa)	122.00	123.38	---	127.52	120.38
Molar Flow (gmole/h)	6.4603	3.4662e-009 *	---	6.4603	1.3021
Mass Flow (kg/d)	1.7029	2.4000e-009	---	2.7029	1.0000
Liquid Volume Flow (m3/h)	1.933e-004	1.156e-013	---	2.031e-004	3.662e-005
Heat Flow (kW)	-7.783e-002	2.041e-011	1.291e-003	-0.2605	2.474e-004
Molar Enthalpy (kJ/kgmole)	-4.337e+004	2.120e+004	---	-1.452e+005	684.0

Name	5r	CO2 Cmp Pwr	CO2 In	Electrolysis Power	CO2, Water In
Vapour Fraction	1.0000	---	1.0000	---	1.0000
Temperature (C)	427.79 *	---	21.111 *	---	705.29
Pressure (kPa)	131.90 *	---	131.00 *	---	126.14
Molar Flow (gmole/h)	6.4603 *	---	1.3022	---	6.5011
Mass Flow (kg/d)	2.7029	---	1.3754 *	---	2.7029
Liquid Volume Flow (m3/h)	2.031e-004	---	6.944e-005	---	1.882e-004
Heat Flow (kW)	-0.2864	3.442e-005	-0.1425	0.1918	-0.2605
Molar Enthalpy (kJ/kgmole)	-1.596e+005	---	-3.940e+005	---	-1.443e+005

Name	Hi Temp Pwr	8	Hydrogenation Q	4	15
Vapour Fraction	---	1.0000	---	1.0000	1.0000
Temperature (C)	---	725.07	---	23.627	350.00 *
Pressure (kPa)	---	128.90	---	134.90 *	116.00
Molar Flow (gmole/h)	---	6.4603	---	1.3022	5.1581
Mass Flow (kg/d)	---	2.7029	---	1.3754	1.3275
Liquid Volume Flow (m3/h)	---	2.031e-004	---	6.944e-005	1.336e-004
Heat Flow (kW)	5.395e-003	-0.2659	-5.417e-002	-0.1425	-0.1541
Molar Enthalpy (kJ/kgmole)	---	-1.482e+005	---	-3.939e+005	-1.076e+005

Name	Carbon Out	6	2	1	5
Vapour Fraction	0.0000	1.0000	1.0000	1.0000	1.0000
Temperature (C)	350.00	452.79	376.94	563.79	427.79
Pressure (kPa)	116.00	119.00	131.90	131.90	131.90
Molar Flow (gmole/h)	1.3023	6.4603	5.1581	1.3022	6.4603
Mass Flow (kg/d)	0.37540	1.7029	1.3275	1.3754	2.7029
Liquid Volume Flow (m3/h)	9.526e-006	1.933e-004	1.336e-004	6.944e-005	2.031e-004
Heat Flow (kW)	1.610e-003	-9.834e-002	-0.1528	-0.1336	-0.2864
Molar Enthalpy (kJ/kgmole)	4450	-5.480e+004	-1.067e+005	-3.693e+005	-1.596e+005

Name	O2 Out
Vapour Fraction	1.0000
Temperature (C)	800.00
Pressure (kPa)	123.38
Molar Flow (gmole/h)	1.3021
Mass Flow (kg/d)	1.0000
Liquid Volume Flow (m3/h)	3.662e-005
Heat Flow (kW)	9.140e-003
Molar Enthalpy (kJ/kgmole)	2.527e+004

Compressors

Name	CO2 Comp	Circulator
Feed Pressure (kPa)	131.0 *	116.0
Product Pressure (kPa)	134.9 *	131.9
Molar Flow (gmole/h)	1.302	5.158
Energy (kW)	3.442e-005	1.291e-003
Adiabatic Efficiency	75 *	75 *
Polytropic Efficiency	75	75

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Workbook: Case (Main) (continued)

Composition

Name	4	5	5r	8	9
Comp Mole Frac (H2O)	0.00000	0.32176	0.32175 *	0.32175	0.32175
Comp Mole Frac (Hydrogen)	0.00000	0.43082	0.43082 *	0.43082	0.43082
Comp Mole Frac (Oxygen)	0.00000	0.00000	0.00000 *	0.00000	0.00000
Comp Mole Frac (Argon)	0.00000	0.00000	0.00000 *	0.00000	0.00000
Comp Mole Frac (Nitrogen)	0.00000	0.00000	0.00000 *	0.00000	0.00000
Comp Mole Frac (CO2)	1.00000	0.24307	0.24307 *	0.24307	0.24307
Comp Mole Frac (CO)	0.00000	0.00005	0.00005 *	0.00005	0.00005
Comp Mole Frac (Methane)	0.00000	0.00430	0.00430 *	0.00430	0.00430
Comp Mole Frac (Carbon)	0.00000	0.00000	0.00000 *	0.00000	0.00000
Name	**CO2 In**	**CO2, Water In**	**H2,CO,H2O Out**	**O2 Out**	**OxygenOut**
Comp Mole Frac (H2O)	0.00000 *	0.40060	0.12019	0.00000	0.00000
Comp Mole Frac (Hydrogen)	0.00000 *	0.35353	0.63239	0.00000	0.00000
Comp Mole Frac (Oxygen)	0.00000 *	0.00000	0.00000	1.00000	1.00000
Comp Mole Frac (Argon)	0.00000 *	0.00000	0.00000	0.00000	0.00000
Comp Mole Frac (Nitrogen)	0.00000 *	0.00000	0.00000	0.00000	0.00000
Comp Mole Frac (CO2)	1.00000 *	0.15754	0.04151	0.00000	0.00000
Comp Mole Frac (CO)	0.00000 *	0.08719	0.20162	0.00000	0.00000
Comp Mole Frac (Methane)	0.00000 *	0.00114	0.00430	0.00000	0.00000
Comp Mole Frac (Carbon)	0.00000 *	0.00000	0.00000	0.00000	0.00000
Name	**15**	**Carbon Out**	**6**	**2**	**1**
Comp Mole Frac (H2O)	0.40299	0.00000	0.12019	0.40299	0.00000
Comp Mole Frac (Hydrogen)	0.53958	0.00000	0.63239	0.53958	0.00000
Comp Mole Frac (Oxygen)	0.00000	0.00000	0.00000	0.00000	0.00000
Comp Mole Frac (Argon)	0.00000	0.00000	0.00000	0.00000	0.00000
Comp Mole Frac (Nitrogen)	0.00000	0.00000	0.00000	0.00000	0.00000
Comp Mole Frac (CO2)	0.05198	0.00000	0.04151	0.05198	1.00000
Comp Mole Frac (CO)	0.00006	0.00000	0.20162	0.00006	0.00000
Comp Mole Frac (Methane)	0.00539	0.00000	0.00430	0.00539	0.00000
Comp Mole Frac (Carbon)	0.00000	1.00000	0.00000	0.00000	0.00000

Heat Exchangers

Name		Recuperator 1	Recuperator 2			
Duty	(kW)	-8.893e-003	2.051e-002			
Tube Inlet Temperature	(C)	800.0	427.8 *			
Tube Outlet Temperature	(C)	48.63	725.1			
Shell Inlet Temperature	(C)	23.63	800.0			
Shell Outlet Temperature	(C)	563.8	452.8			
LMTD	(C)	92.86	45.38			
UA	(kJ/C-h)	0.3448	1.627			
Minimum Approach	(C)	25.00	25.00			

Other Heat Exchangers

Name						
Number of Sides						
LMTD	(C)					
UA (Calculated)	(kJ/C-h)					
Hot Pinch Temperature	(C)					
Cold Pinch Temperature	(C)					
Minimum Approach	(C)					
Exchanger Cold Duty	(kW)					

* Specified by user.

Workbook: Case (Main) (continued)

Pumps

Name					
Delta P (kPa)					
Energy (kW)					
Feed Pressure (kPa)					
Product Pressure (kPa)					
Molar Flow (gmole/h)					
Adiabatic Efficiency (%)					

Unit Ops

Operation Name	Operation Type	Feeds	Products	Ignored	Calc. Level
Hi Temp Heater	Heater	8 Hi Temp Pwr	9	No	500.0 *
Recuperator 1	Heat Exchanger	O2 Out 4	OxygenOut 1	No	500.0 *
Recuperator 2	Heat Exchanger	5r H2,CO,H2O Out	8 6	No	500.0 *
M2	Mixer	1 2	5	No	500.0 *
CO2 Comp	Compressor	CO2 In CO2 Cmp Pwr	4	No	500.0 *
Circulator	Compressor	15 Circ Pwr	2	No	500.0 *
High Temperature Co-Electr	Standard Sub-Flowsheet	Sweep Gas In CO2, Water In Process Heat Electrolysis Power	O2 Out H2,CO,H2O Out	No	2500 *
Electrolysis Input and Output	Spreadsheet			No	500.0 *
Co-Electrolysis Calcs	Spreadsheet			No	500.0 *
Hydrogenation	Equilibrium Reactor	6 Hydrogenation Q	Carbon Out 15 Hydrogenation Q	No	500.0 *
RCY	Recycle	5	5r	No	3500 *
Water Gas Shift	Gibbs Reactor	9	400 CO2, Water In	No	500.0 *

Workbook: High Temperature Co-Electrolysis (TPL2)

Streams

Name		Sweep Gas In @TPL	O2 Out @TPL2	Gas Products @TPL	Liquid @TPL2	Anode @TPL2
Vapour Fraction		1.0000	1.0000	1.0000	0.0000	1.0000
Temperature	(C)	705.29	800.00	800.00 *	800.00	800.00
Pressure	(kPa)	123.38	123.38	124.76	124.76	123.38
Molar Flow	(gmole/h)	3.4662e-009	1.3021	7.8032	0.00000	1.3021
Mass Flow	(kg/d)	2.4000e-009	1.0000	2.7029	0.00000	1.0000
Liquid Volume Flow	(m3/h)	1.156e-013	3.662e-005	2.530e-004	0.0000	3.662e-005
Heat Flow	(kW)	2.041e-011	9.140e-003	-7.488e-002	0.0000	9.140e-003
Molar Enthalpy	(kJ/kgmole)	2.120e+004	2.527e+004	-3.455e+004	-3.455e+004	2.527e+004

* Specified by user.

Workbook: High Temperature Co-Electrolysis (TPL2) (continued)

Streams (continued)

Name		H2,CO,H2O Out @TF	Cathode @TPL2	2 @TPL2	CO2, Water In @TPL	Electrolysis Heatiing
Vapour Fraction		1.0000	1.0000	0.0000	1.0000	---
Temperature	(C)	800.00 *	800.00 *	800.00	705.29	---
Pressure	(kPa)	122.00	123.38	122.00	126.14	---
Molar Flow	(gmole/h)	6.4603	6.5011	0.00000	6.5011	---
Mass Flow	(kg/d)	1.7029	1.7029	0.00000	2.7029	---
Liquid Volume Flow	(m3/h)	1.933e-004	2.164e-004	0.0000	1.882e-004	---
Heat Flow	(kW)	-7.783e-002	-8.402e-002	0.0000	-0.2605	0.1856
Molar Enthalpy	(kJ/kgmole)	-4.337e+004	-4.653e+004	-4.337e+004	-1.443e+005	---
Name		Process Heat @TPL	Shift Reactor 2 Heat	Electrolysis Power @		
Vapour Fraction		---	---	---		
Temperature	(C)	---	---	---		
Pressure	(kPa)	---	---	---		
Molar Flow	(gmole/h)	---	---	---		
Mass Flow	(kg/d)	---	---	---		
Liquid Volume Flow	(m3/h)	---	---	---		
Heat Flow	(kW)	-2.272e-007	6.193e-003	0.1918		
Molar Enthalpy	(kJ/kgmole)	---	---	---		

Composition

Name	Sweep Gas In @TPL	O2 Out @TPL2	Gas Products @TPL	Liquid @TPL2	Anode @TPL2
Comp Mole Frac (H2O)	0.00000	0.00000	0.00000	0.00000	0.00000
Comp Mole Frac (Hydrogen)	0.00000	0.00000	0.62829	0.62829	0.00000
Comp Mole Frac (Oxygen)	0.21000	1.00000	0.16687	0.16687	1.00000
Comp Mole Frac (Argon)	0.00000	0.00000	0.00000	0.00000	0.00000
Comp Mole Frac (Nitrogen)	0.79000	0.00000	0.00000	0.00000	0.00000
Comp Mole Frac (CO2)	0.00000	0.00000	0.13125	0.13126	0.00000
Comp Mole Frac (CO)	0.00000	0.00000	0.07264	0.07264	0.00000
Comp Mole Frac (Methane)	0.00000	0.00000	0.00095	0.00095	0.00000
Comp Mole Frac (Carbon)	0.00000	0.00000	0.00000	0.00000	0.00000
Name	H2,CO,H2O Out @TF	Cathode @TPL2	2 @TPL2	CO2, Water In @TPL	
Comp Mole Frac (H2O)	0.12019	0.00000	0.12019	0.40060	
Comp Mole Frac (Hydrogen)	0.63239	0.75413	0.63239	0.35353	
Comp Mole Frac (Oxygen)	0.00000	0.00000	0.00000	0.00000	
Comp Mole Frac (Argon)	0.00000	0.00000	0.00000	0.00000	
Comp Mole Frac (Nitrogen)	0.00000	0.00000	0.00000	0.00000	
Comp Mole Frac (CO2)	0.04151	0.15754	0.04151	0.15754	
Comp Mole Frac (CO)	0.20162	0.08719	0.20162	0.08719	
Comp Mole Frac (Methane)	0.00430	0.00114	0.00430	0.00114	
Comp Mole Frac (Carbon)	0.00000	0.00000	0.00000	0.00000	

Unit Ops

Operation Name	Operation Type	Feeds	Products	Ignored	Calc. Level
Temp Average ASR @TPL2	Spreadsheet			Yes	500.0 *
Electrolysis Spreadsheet @	Spreadsheet			No	500.0 *
Steam Electrolysis @TPL2	Spreadsheet			No	500.0 *
CO2 Electrolysis @TPL2	Spreadsheet			No	500.0 *
Sweep Gas/O2 Mixer @TPL	Mixer	Anode @TPL2 Sweep Gas In @TPL2	O2 Out @TPL2	No	500.0 *
Isothermal Electrolysis @TP	Conversion Reactor	CO2, Water In @TPL2 Electrolysis Heatiing @TPL2	Liquid @TPL2 Gas Products @TPL2 Electrolysis Heatiing @TPL2	No	500.0 *
Electrodes @TPL2	Component Splitter	Gas Products @TPL2	Cathode @TPL2 Anode @TPL2	No	500.0 *
ADJ-1 @TPL2	Adjust			Yes	3500 *

* Specified by user.

Workbook: High Temperature Co-Electrolysis (TPL2) (continued)

Unit Ops (continued)

Operation Name	Operation Type	Feeds	Products	Ignored	Calc. Level
Water gas Shift @TPL2	Gibbs Reactor	Cathode @TPL2 Shift Reactor 2 Heat @TPL	2 @TPL2 H2,CO,H2O Out @TPL2 Shift Reactor 2 Heat @TPL	No	500.0 *
SET-1 @TPL2	Set			No	500.0 *
SET-3 @TPL2	Set			No	500.0 *
SET-2 @TPL2	Set			No	500.0 *

Conversion: 2CO2=2CO+O2

STOICHIOMETRY

Component	Mole Weight	Stoichiometric Coeff.
CO2	44.010	-2 *
CO	28.011	2 *
Oxygen	32.000	1 *

Balance Error: 0.0000 | Reaction Heat: 2.832e+005 kJ/kgmole

BASIS

Base Component: CO2 | Conversion Percent: 100.00 * | Reaction Phase: Overall

PARAMETERS

Conversion: 2H2O=2H2+O2

STOICHIOMETRY

Component	Mole Weight	Stoichiometric Coeff.
H2O	18.015	-2 *
Hydrogen	2.016	2 *
Oxygen	32.000	1 *

Balance Error: 0.0000 | Reaction Heat: 2.410e+005 kJ/kgmole

BASIS

Base Component: H2O | Conversion Percent: 90.00 * | Reaction Phase: Overall

PARAMETERS

Equilibrium: Hydrogenation

STOICHIOMETRY

Component	Molecular Weight	Stoichiometric Coefficient
CO	28.01	-1 *
Hydrogen	2.016	-1 *
H2O	18.02	1 *
Carbon	12.01	1 *

Balance Error : 0.0000 | Reaction Heat : -1.304e+005 kJ/kgmole

* Specified by user.

Equilibrium: Hydrogenation (continued)

BASIS

Basis	Phase	Approach (C)	Min. Temp (C)	Max. Temp (C)
Activity	VapourPhase	---	-273.15	3000.0

PARAMETERS

Source : K Vs. T Table

Coeff A	-16.53	R2	1.000000 *
Coeff B	1.582e+004	T High	---
Coeff C	6.290e-002	T Low	---
Coeff D	-3.147e-005		

Temperature (C)	Keq	KCalc	Percentage Error
25.000 *	1.050e+016 *	1.050e+016 *	-1.546e-003 *
127.00 *	1.420e+010 *	1.420e+010 *	1.873e-002 *
227.00 *	5.280e+006 *	5.285e+006 *	-8.965e-002 *
327.00 *	2.740e+004 *	2.736e+004 *	0.1553 *
427.00 *	637.0 *	637.4 *	-5.515e-002 *
527.00 *	38.00 *	38.01 *	-3.314e-002 *
627.00 *	4.240 *	4.242 *	-5.571e-002 *
727.00 *	0.7340 *	0.7341 *	-1.337e-002 *
827.00 *	0.1750 *	0.1747 *	0.1466 *
927.00 *	5.280e-002 *	5.283e-002 *	-6.267e-002 *
1027.0 *	1.920e-002 *	1.920e-002 *	2.720e-003 *
1127.0 *	8.060e-003 *	8.062e-003 *	-2.036e-002 *
1227.0 *	3.800e-003 *	3.800e-003 *	7.913e-003 *

* Specified by user.