Final Technical Report

Cummins R-SOFC System Development

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Executive Summary

The overall purpose of this project was to reduce the Reversible-Solid Oxide Fuel Cell (R-SOFC) system cost by developing two technologies, an improved cell design and the incorporation of an ejector in the fuel recycle loop instead of a blower.

A Simulink model of the baseline SOFC system was developed and calibrated with experimental test data. The R-SOFC system model was built by integrating GT Suite developed models of the steam generation components into the baseline Simulink SOFC system model. The ability to run the stack in SOEC operating mode was also added to the model. The system model was used to explore the ability of the R-SOFC system to meet operational constraints on Steam/Carbon ratio and H_2 concentration on the fuel side electrode.

A CFD ejector model was developed and used to explore a range of ejector design parameters, leading to the final ejector design that was prototyped for testing. A prototype steam ejector was first tested in a laboratory environment using room temperature air. The steam ejector was subsequently tested using the full hot recycle loop with all relevant heat exchangers and steam generation components. The test conditions utilized temperatures, pressures, and flow rates expected in an R-SOFC application. Throughout the experimental testing work, ejector performance test data was used to improve and then validate the CFD ejector model.

A CFD cell model was developed and used to optimize thermal gradients, voltage, and cost of a new cell substrate design. A CFD comparison of co-flow and cross-flow cell designs informed the decision to use a co-flow design for the new cell substrate. Multiple rounds of CFD simulation were used to improve the cell design to minimize the variation in air and fuel distribution across cell channels and to minimize the variation in air and fuel distribution across different cells in the stack. A few prototypes of the new cell substrate design were produced and validated in a laboratory environment by thermally spraying and verifying that they met established manufacturing specifications. The cell manufacturing process was adjusted in order to bring these metrics within acceptable tolerances.

Cummins' internal calculations show that the new cell design reduces cost ~50% compared to the baseline cell, while the ejector + superheater/boiler concept reduces cost of the recycle loop by ~40%. The impact of these cost reductions on the cost of producing H_2 will depend on the specific system where they are applied. Therefore, a Techno-Economic Analysis was completed using system cost as a variable, and showing how the NREL Current and Future system costs translate into H_2 production cost.

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Project Accomplishments

Major Project Goals

The objective of this project is to design and develop two novel technologies that will enable \$2/kilogram (kg)-Hydrogen (H_2) production in a Reversible-Solid Oxide Fuel Cell (R-SOFC) plant capable of producing both electricity and hydrogen with a 30% overall product cost reduction from baseline.

The main goals of the proposed project are to: (i) determine the appropriate performance metrics so the cost targets for the R-SOFC system will be met, (ii) design a new cell substrate and fuel side steam ejector technology, (iii) build and test a cell substrate prototype and a prototype steam ejector component in a hot fuel loop test, (iv) complete a Techno-Economic Analysis (TEA) and analyze the system performance and cost using the technologies developed and the cost reduction goal to enable \$2/kg-H_2 production.

Project Activities

Task 1.0 – Project Management and Planning

The project work and milestones were managed using a MS Project document. The plan was regularly updated by the Cummins project team, and project status updates were provided to the DOE program manager via a monthly meeting. Additional updates to DOE were provided through the quarterly Research Performance Progress Reports (RPPRs), annual updates to DOE program managers, and the Annual Project Review meetings.

Task 2.0 – R-SOFC System Modeling

2.1 Baseline System Modeling

A Simulink model of the baseline SOFC system was developed, incorporating various components including fuel cell stack, 3 heat exchangers, burner, reformer, CPOx (catalytic partial oxidation), and CATOx (catalytic oxidation catalyst). Each component model solves mass transfer, heater transfer and chemical reactions mathematically. The full system model was calibrated with experimental test data of fuel cell stack and other BOP (balance of plant) components for 3 different operating conditions. The test data includes temperature and pressure measurements for various components, stack voltage and current measurements, and gas composition measurements taken at stack anode outlet. The model was able to predict stack performance and temperature variables within 5% of the experimental data, and absolute differences in pressure and anode out gas composition are reasonable.

2.2 R-SOFC System Modeling

The R-SOFC system model was built in Simulink using the baseline SOFC system model. Figure 2.3 shows a schematic of the baseline R-SOFC system architecture. Models of the boiler, condenser, and superheater in the fuel recycle loop were developed using GT Suite and integrated into the Simulink model via an S-function connection. Figure 2.4 shows the baseline R-SOFC system model. The individual steam generation components were assembled into a fuel recycle subsystem model in GT Suite and linked to Simulink input/output. The system includes a table-based ejector model that was created from performance curves generated from CFD simulations using high temperature steam for both primary and secondary flows. The ejector performance curves from CFD are shown in Figure 2.5.

The ability to run the stack in SOEC operating mode was also added to the model. One important parameter for the stack model is the Area Specific Resistance (ASR), and an ASR curve as a function of temperature was calibrated against stack temperature, voltage and outlet anode composition for two SOFC operating points. This stack calibration was validated by simulating the polarization curves for both SOFC

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and SOEC operation. The simulated stack data matched very well with testing data for both SOFC and SOEC operation.

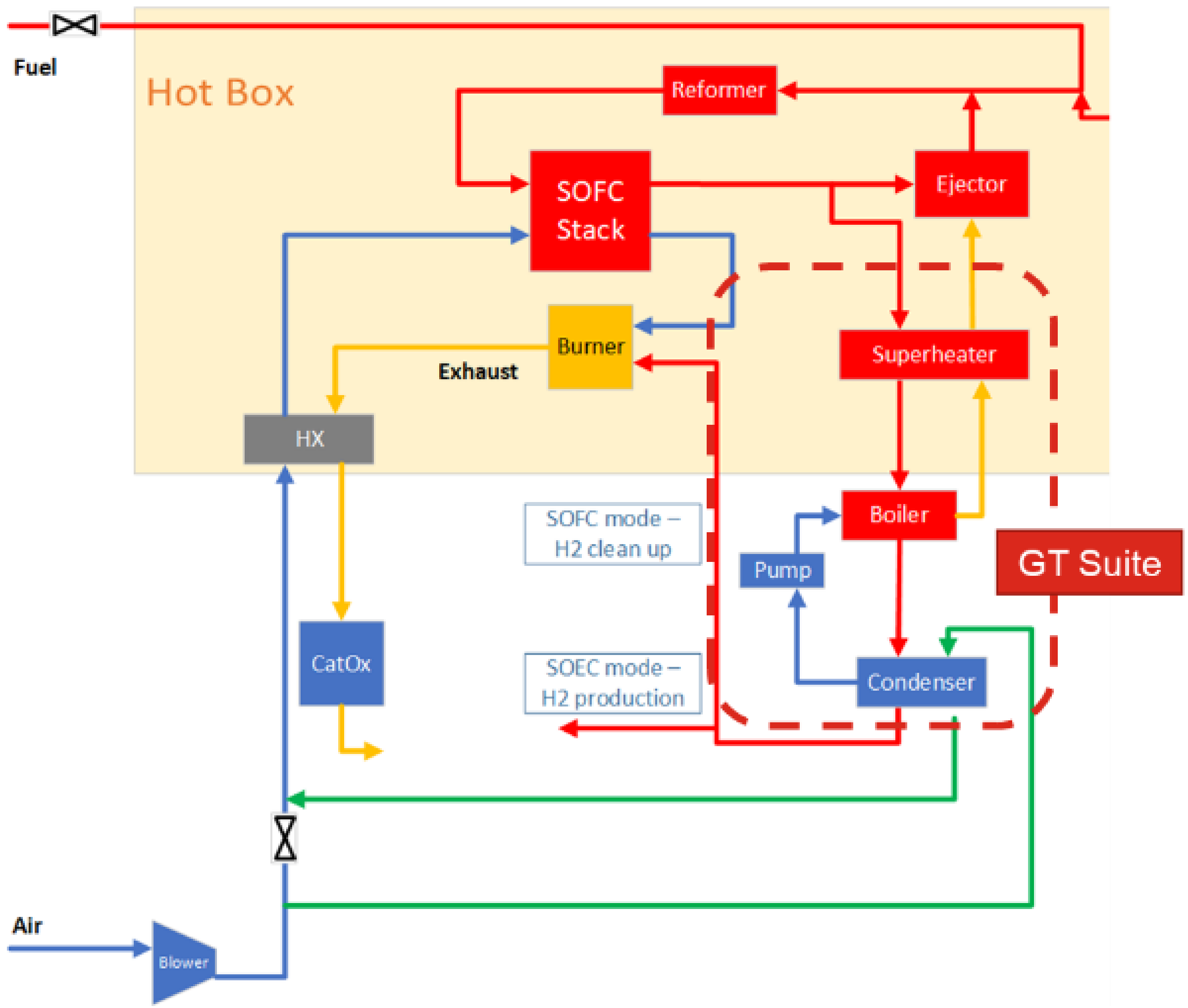

Figure 2.3: Schematic of baseline R-SOFC system model. The dashed box indicates the portion of the system being modeled in GT Suite, while the remainder is in Simulink.

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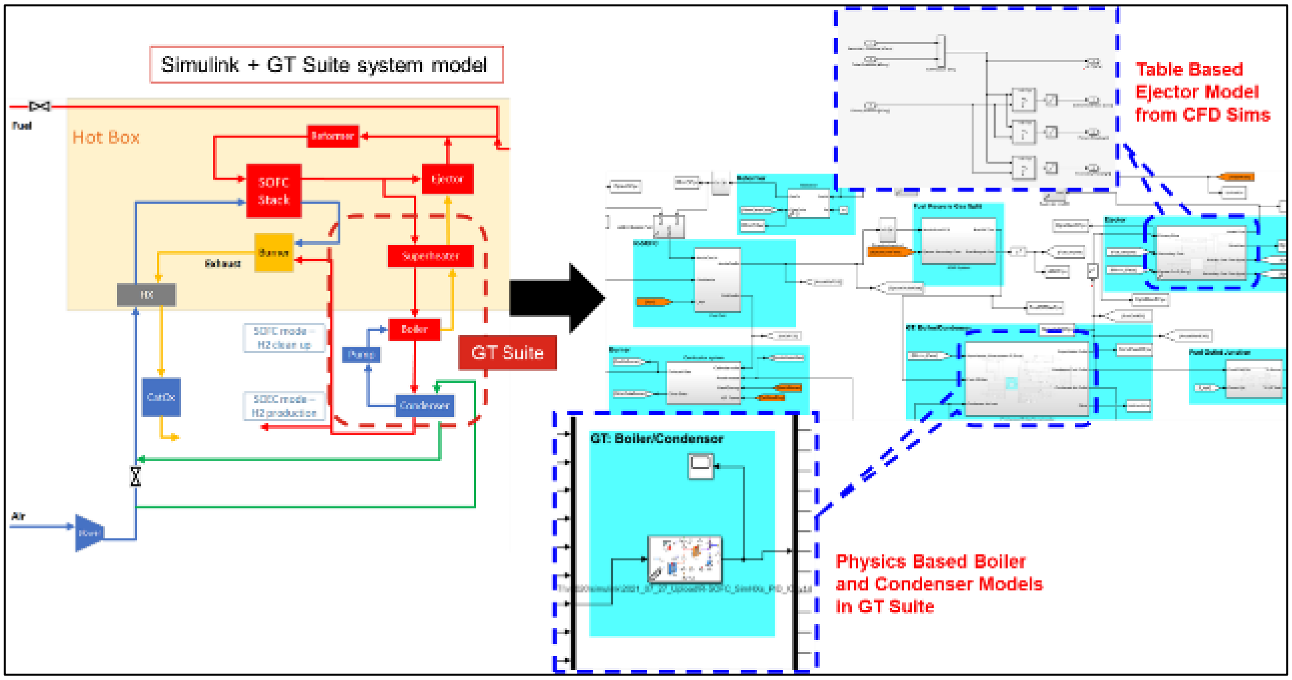

Figure 2.4: Baseline R-SOFC system model. The red dashed box in the schematic indicates the portion of the system being modeled in GT Suite, while the remainder is in Simulink.

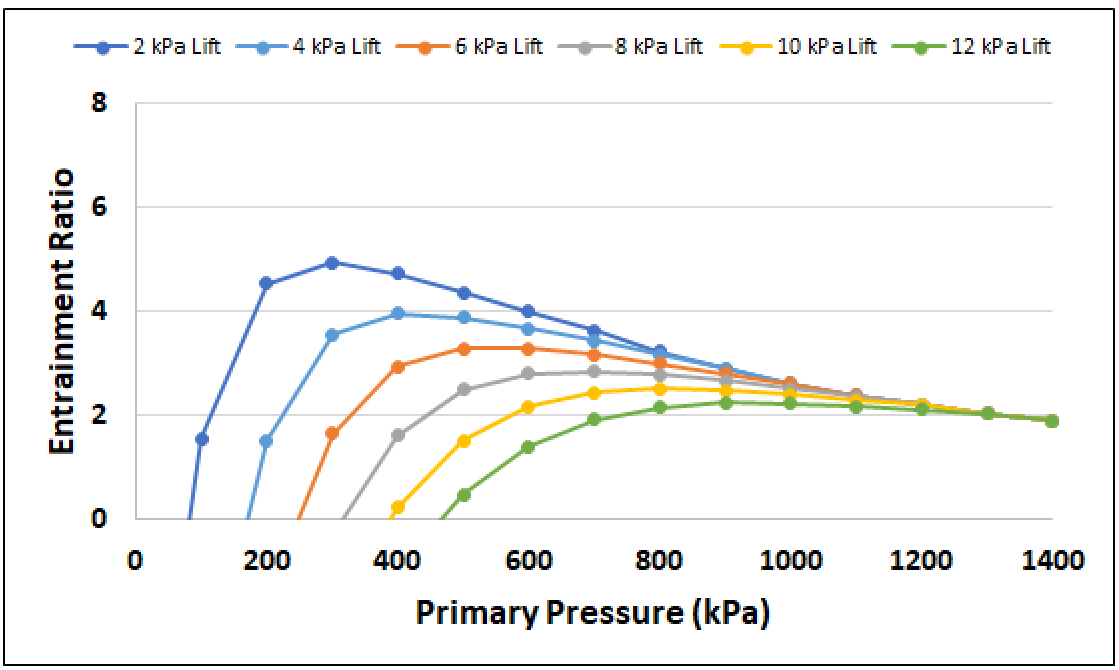

Figure 2.5: Performance curves generated by CFD model for concept steam ejector. Different curves correspond to different lift pressures.

The project objectives required that the Steam ejector operation maintained a steam-to-carbon ratio (S:C) ≥ 2.5. This requirement is to avoid operation in a regime that favors carbon formation and coking of the system. Simulations were therefore performed in SOFC mode at operating points representing the targeted SOFC operation range of 50 – 100% load. Figure 2.6 shows that the ejector is capable of sufficient

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recirculation to be above a Steam/Carbon (S/C) ratio of 2.5 for these loads, provided there is sufficient primary pressure.

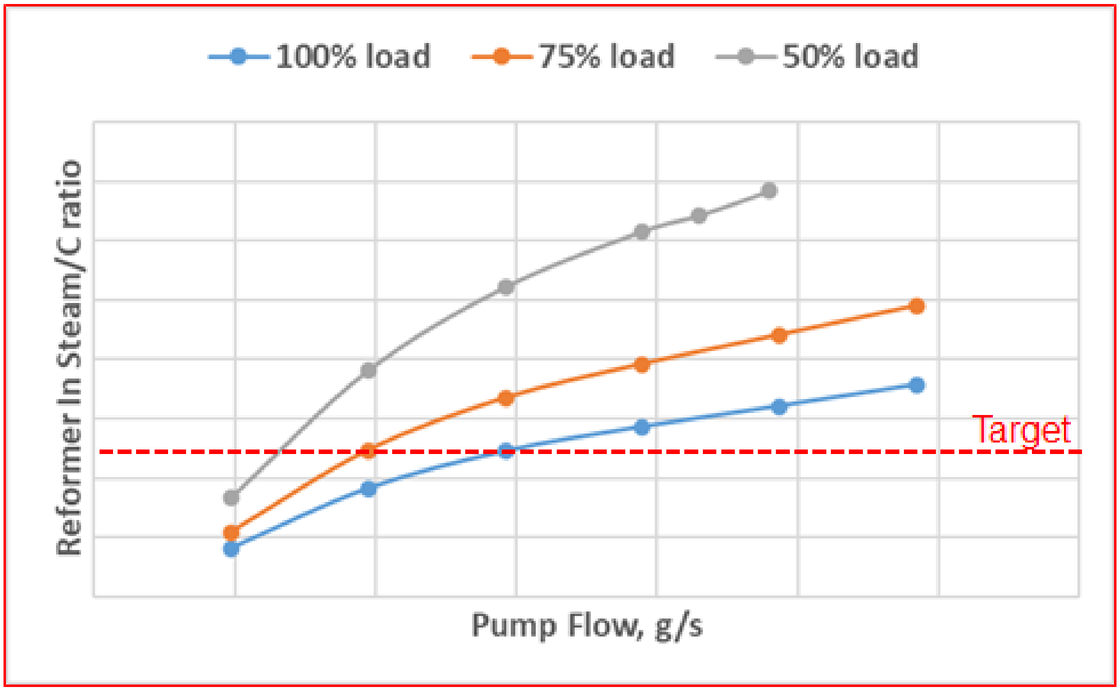

Figure 2.6: Ejector outlet Steam/Carbon ratio modeling results for SOFC operating points from 50 – 100% load

For SOEC mode there is no Carbon present in the anode gas feed so instead we use a criterion to maintain a rich environment in the stack fuel electrode via sufficient H_2 concentration. If the fuel side electrode is not kept rich, the Ni metal in the electrode will oxidize, leading to expansion, cracking, and failure of the electrode. Therefore, having an ejector that recycles enough of the H_2-rich fuel side outlet gas back to the fuel side inlet is essential. For the steam ejector the Lift Pressure is essentially equivalent to the stack backpressure, since in SOEC mode the Reformer would be bypassed. The R-SOFC system model is run in SOEC mode using the ejector performance curve for 12 kPa Lift pressure, which is the maximum stack back pressure expected when operating at 1 A/cm^2 current density. Figure 2.7 shows that the ejector can maintain an H_2 concentration which is sufficiently rich to preserve the Ni electrode, provided there is sufficient water pump flow.

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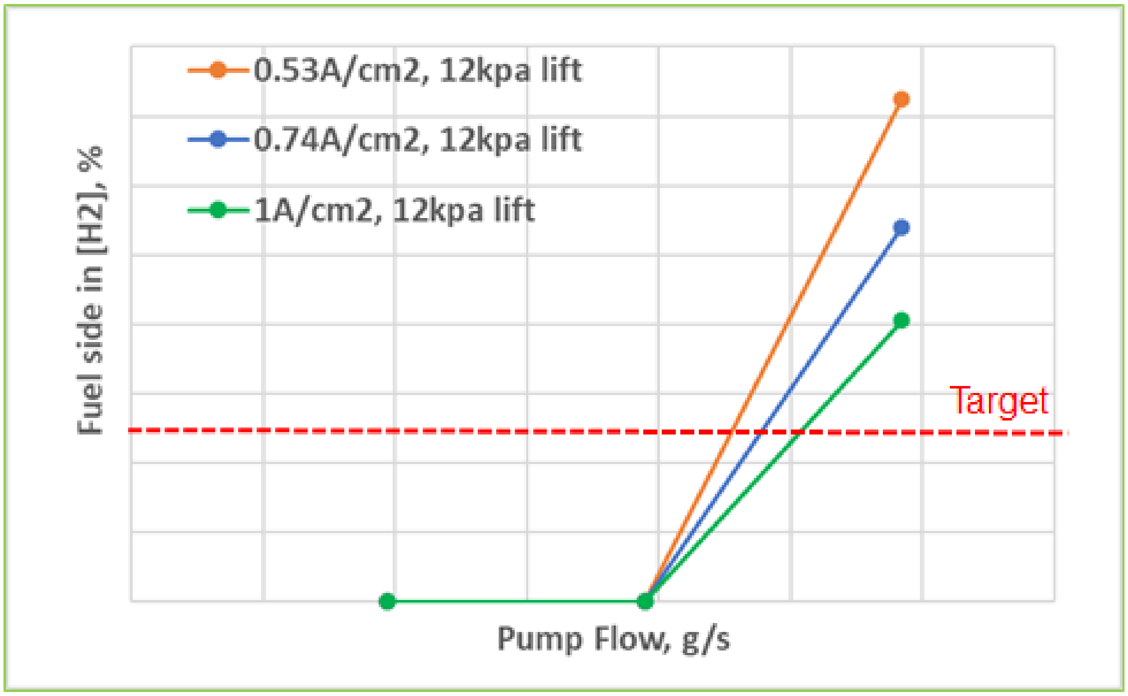

Figure 2.7: H_2 concentration at the fuel side electrode inlet versus water pump flow rate, for various current density cases.

Task 3.0 – R-SOFC Advanced Cell Design

An advanced R-SOFC cell has been designed and optimized using various CFD methodologies developed in Cummins. Ansys FLUENT has been used as a CFD tool in all these methodologies. These methodologies involve performing electrochemical analysis on SOFC reactive area as well as performing traditional CFD analysis (without any electrochemistry) on single cell or stack of a fuel cell design. Thermal and electrochemical performance of a fuel cell from the electrochemical CFD model was compared between cross-flow design and co-flow design. It was found that the cross-flow cell design has limitations in the performance due to a temperature hotspot (shown in Figure 3.1), which was experimentally verified. The co-flow design does not have as hot a hotspot which serves as an advantage for a cell durability and reliability.

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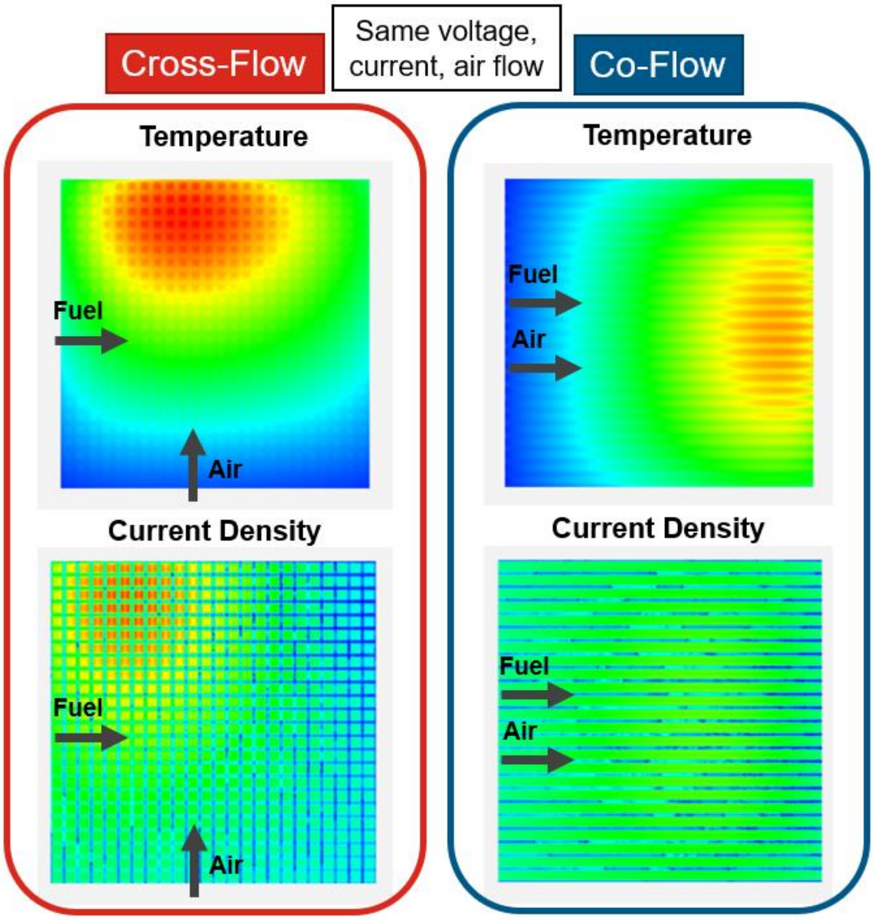

Figure 3.1: Performance comparison of cross-flow design vs. co-flow design

Non-reactive CFD analysis, which does not involve SOFC electrochemistry, was run on the fuel cell domain (both cathode and anode). The cell design was optimized to provide uniform flow distribution across all the channels for cathode and anode flow field. The flow distribution (for both air and fuel) across cell channels is shown in Figure 3.2.

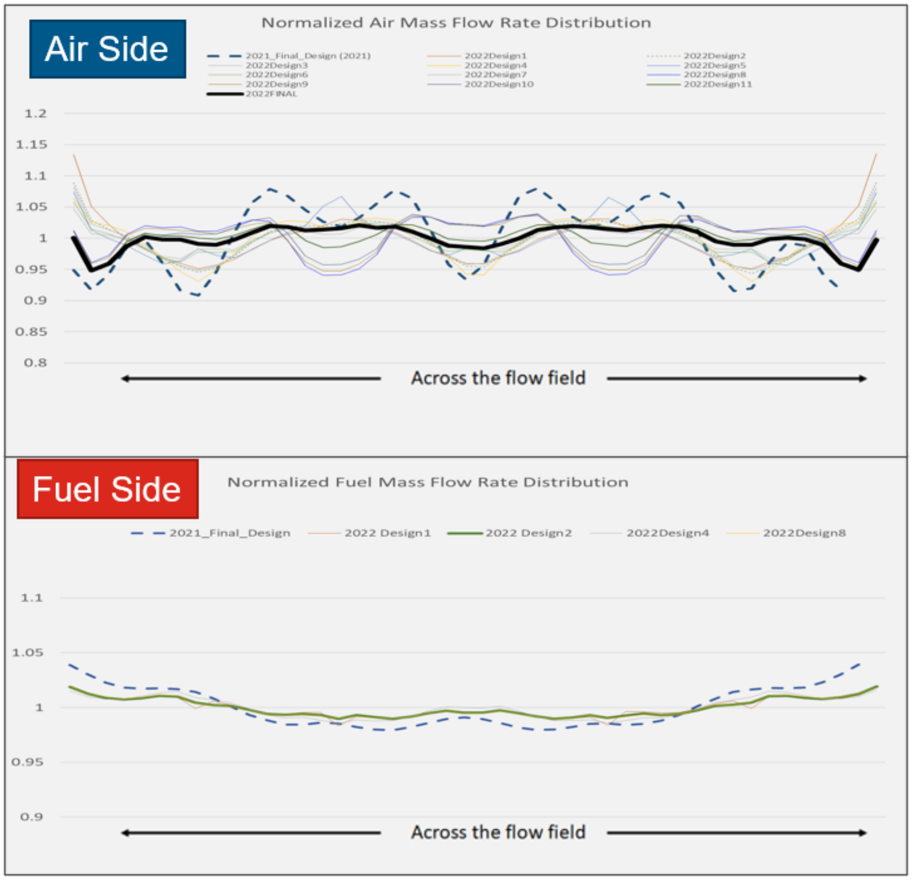

Figure 3.2: Flow distribution across cell channels

A stack CFD analysis was also performed to obtain close to even air and fuel distribution over the height of a 200-cell stack. It was determined through CFD analysis that increasing the outlet header flow area as well as decreasing the inlet header flow area provided a balanced flow between repeating units over the stack height – the variation in air flow is less than 7%, and the variation in fuel flow is less than 2%. The normalized cell to cell air flow distribution across the stack is shown in Figure 3.3, while Figure 3.4 shows higher pressure drop across the fuel domain that results in uniform fuel distribution across all the cells within the stack. The ratio of the outlet header area to the inlet header area is a critical factor in balancing the flow distribution.

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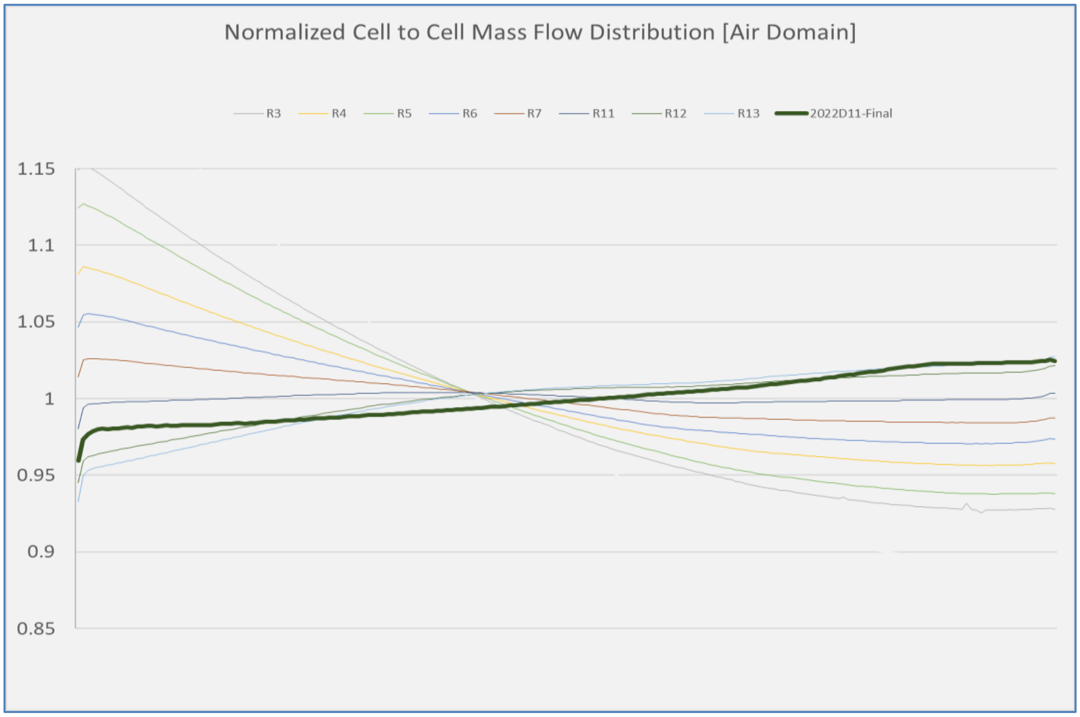

Figure 3.3: Cell to cell distribution (normalized) for air domain stack

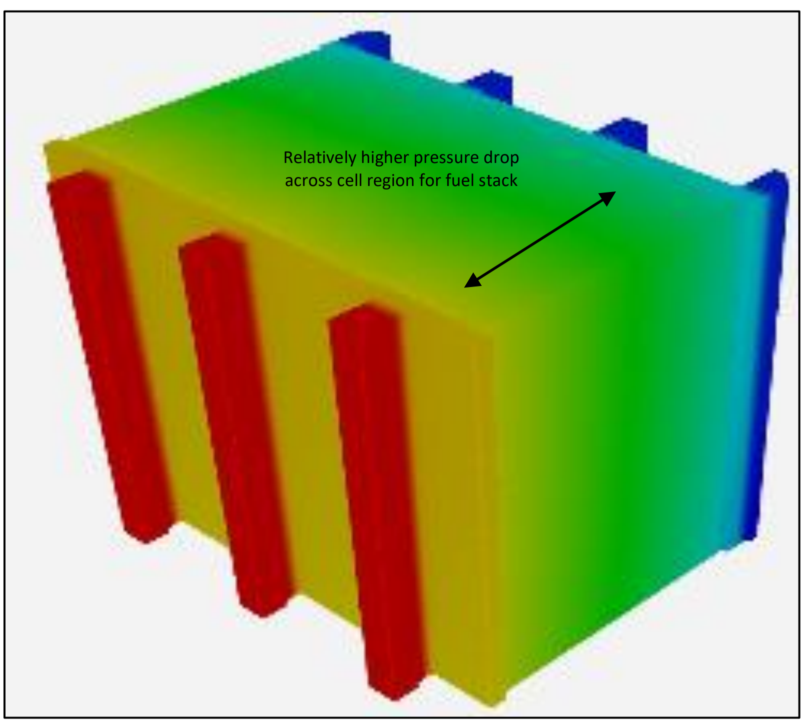

Figure 3.4: Reference concept design & dimensions for optimization

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Task 4.0 – Steam Ejector Development

Using extensive CFD analysis, the dimensions of the steam ejector design were determined and optimized. The reference concept and reference dimensions that were used for design optimization are shown in Figure 4.1. More than 3000 design variants were run on the reference concept to finalize the fully optimized ejector design/prototype, which is shown in Figure 4.2.

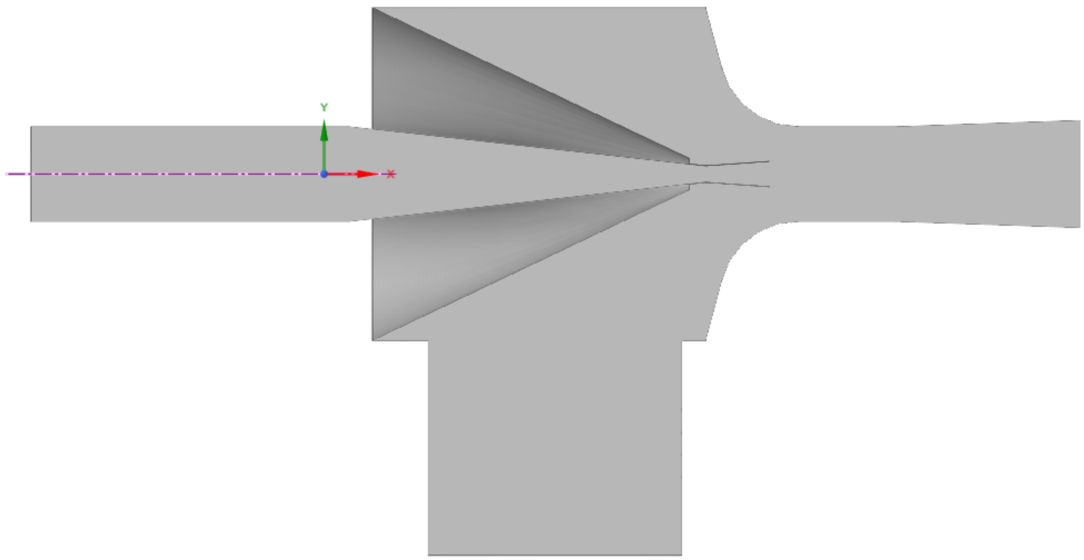

Figure 4.1: Reference concept design for optimization

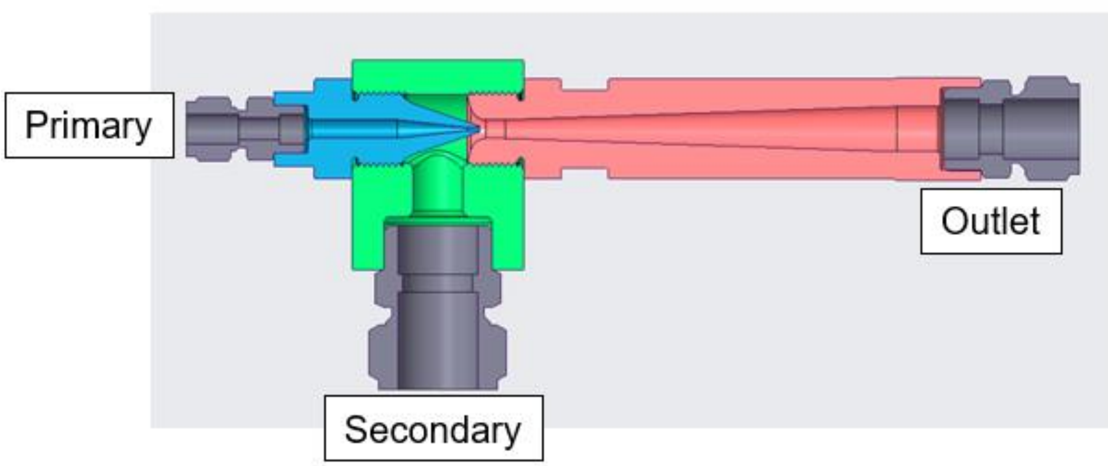

Figure 4.2: Steam ejector design

The CFD analysis that was performed to determine the steam ejector dimensions assumed high temperature, high pressure steam as the working fluid. Initially, air at room temperature was used to test the ejector design. In light of this, a CFD analysis was run to ensure that the ejector performance is not adversely affected by using low temperature air as the working fluid. The performance comparison between room temperature air and high temperature steam as the ejector working fluid is shown in Figure 4.3. The analysis results indicated no loss in the ejector performance when room temperature air is used as the working fluid. On the contrary, the ejector performance was improved when low temperature air was used as the working fluid. Due to the higher density of the air as compared to the steam, the primary mass flow rate was increased for the air as the working fluid as compared to the steam. Increased primary mass

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flow rate results in higher suction pressure through the ejector thereby increasing the entrainment of the secondary flow.

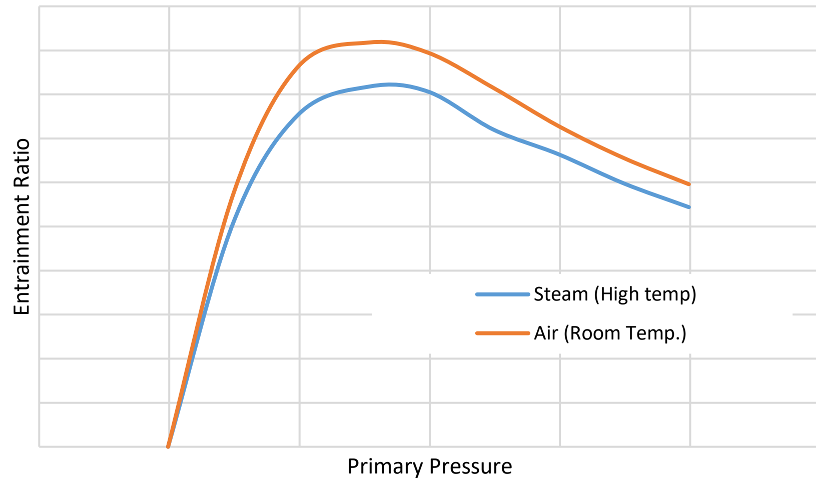

Figure 4.3: Effect of working fluid on entrainment ratio

Using the validated ejector model, entrainment ratio curves with high temperature steam as the working fluid were generated for a range of Lift pressures (Outlet Pressure – Secondary Pressure) as shown in Figure 4.4. This simulation data was used in the table-based ejector model used for Task 2.0 system simulations.

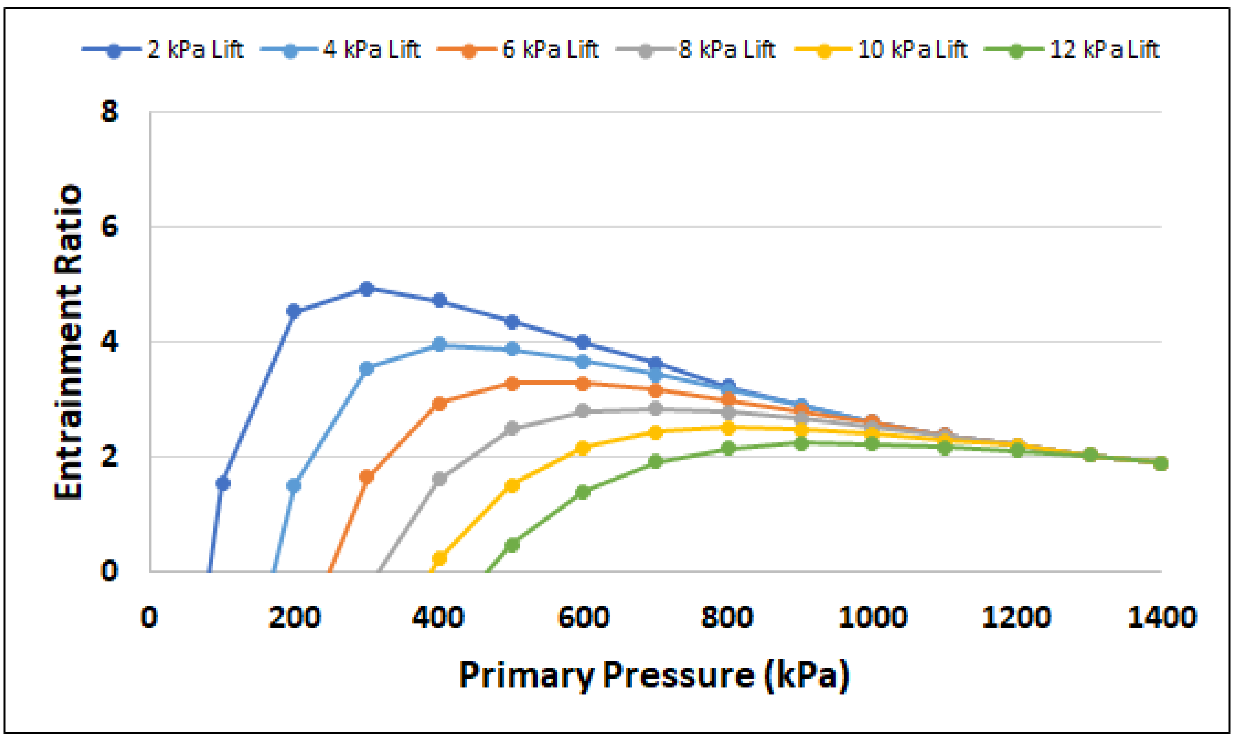

Figure 4.4: Entrainment ratio curves using high temperature steam for a range of Lift pressures (Outlet Pressure – Secondary Pressure).

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Task 5.0 – R-SOFC Substrate Fabrication

High volume manufacturers confirmed that the new cell substrate component designs are suitable for stamping in mass volume. Prototype parts were ordered and fabricated using prototype processes (laser cutting and photochemical machining, with stamping dies for localized forming) such that the parts accurately replicated parts from production tools.

Several prototype cells were manufactured using the new co-flow cell design. Anode and Electrolyte were deposited onto the substrate surface, resulting in a seal over the permeable membrane as shown in Figure 5.1. Recipes were developed to optimize the hermeticity and uniformity of the coatings. The braze process and fixturing required optimization for the co-flow cells. In general, brazing hermetic parts was successful by using past lessons learned on previous metal-supported substrates. Processing parameters were largely the same for time, temperature and atmosphere, and materials for brazing the metal were unchanged from historic recipes. However, fixturing and compression were tailored for the geometry of the part.

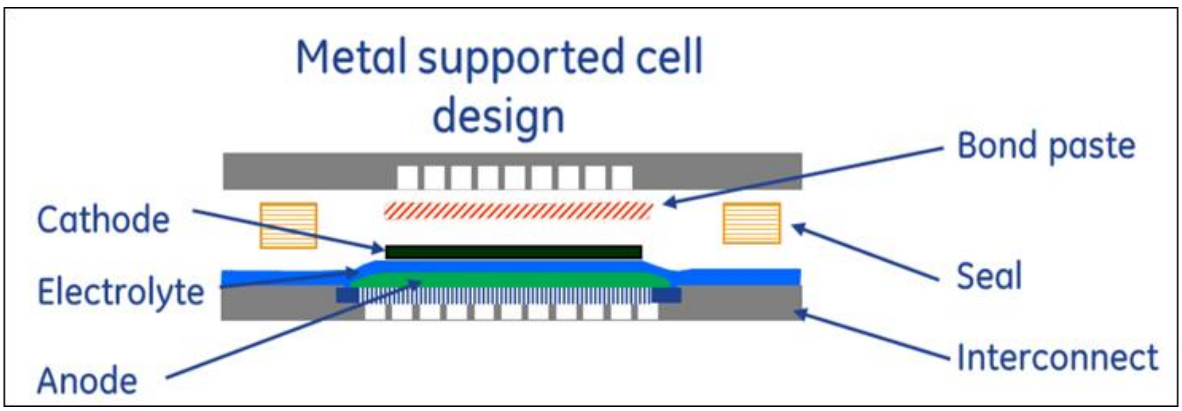

Figure 5.1: Schematic showing arrangement of various layers used in solid oxide cell.

Table 5.1 summarizes the measurements and criteria selected for quality control and diagnostics for development. Each cell was visually inspected and measured for leak tightness after brazing by gasket sealing the manifolds and permeable membrane. In addition, the pressure drop between the fuel inlet and outlet manifolds was measured using 15 LPM of air at room temperature. This measurement was used to determine the reproducibility of the metal forming and braze processes, namely, the ability to form to specification and align during joining.

The coating leak rate was measured to ensure that the co-flow designs could be sufficiently coated without any leakage in the anode flow field. Additionally, it was determined that the co-flow parts were sensitive to process parameters resulting in substantial curvature. As a result, the flatness of the parts was measured along the long and short axis of the rectangular part using a measurement gauge. Flat cells are desired for the subsequent cathode and glass printing operations and their uniformity.

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Table 5.1: A list of measurements performed on all groups of parts

Measurement	Primary Variable of Interest	Specification
Braze Leak Rate	Metal is braze joined hermetic	Upper spec limit (cm^3/s)
Pressure Drop (fuel inlet to outlet)	Metal is formed and aligned properly during braze	+/- 10% from median value (Pa @ 15 LPM air flow)
Visual Inspection	Permeable membrane does not have any defects	Pass / Fail
Surface Roughness	Roughness of textured surface prior to coating deposition	Lower spec limit (microns)
Coating Leak Rate	Electrolyte coating adequately seals membrane, does not have defects	Upper spec limit (cm^3/s)
Flatness	Stress state of metal substrate with ceramic coating is reproducible	Upper spec limit (mm)

Braze leak rates are shown in Figure 5.2 using box plots. Pressure drop across the fuel flow field was also measured using a pneumatic instrument and is shown in Figure 5.3. Both the braze leak rate and pressure drop were within specifications as shown.

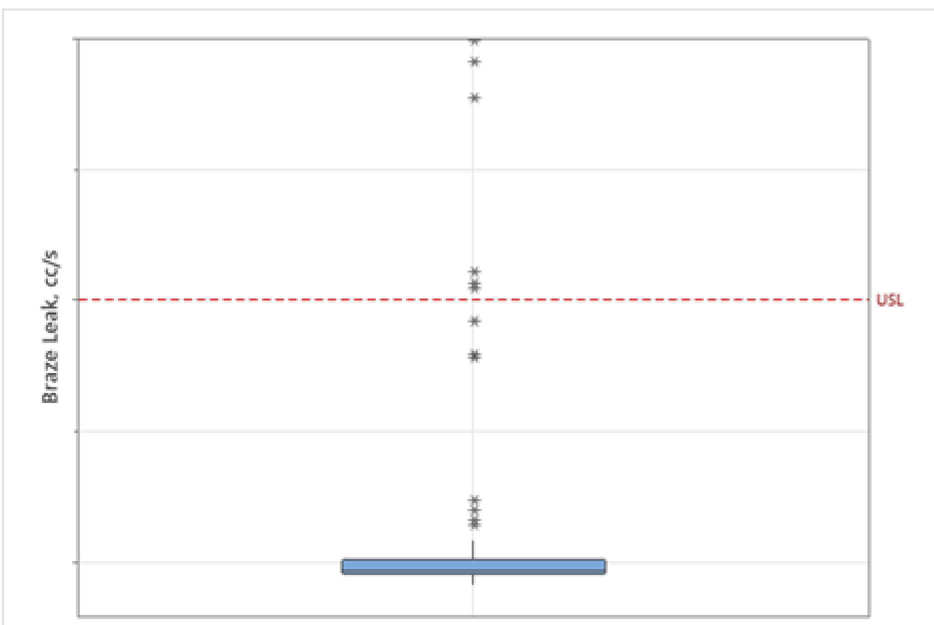

Figure 5.2: Boxplots of the leak rate measured after brazing. The upper specification limit (USL) is identified as reference.

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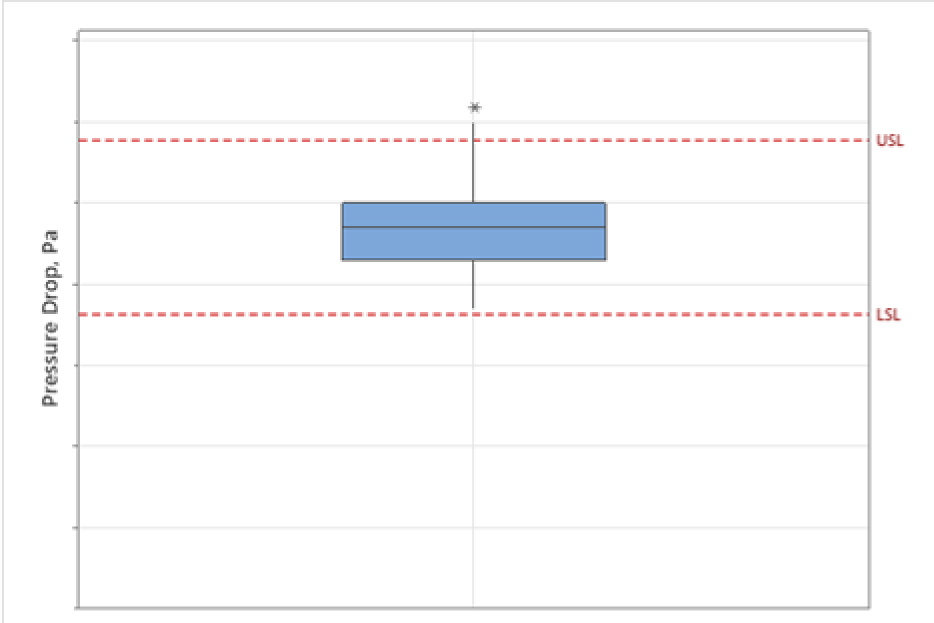

Figure 5.3: Boxplots of the fuel flow field pressure drop measured at 15 LPM using air at room temperature.

The new cell substrate has been determined to meet the required quality standards. The main goal of this project was to develop a new substrate design suitable for the Cummins SOFC thermal spray deposition process with a substantial reduction in $/kW. The new design uses the same sheet metal area with almost twice the active area which alone reduces the $/kW by almost half. There are further benefits to the total SOFC system cost from higher stack volumetric power density which yields a more compact system with substantially reduced cost for items such as the insulation package, framework, and enclosure.

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Task 6.0 – Steam Ejector Loop Demonstration

6.1 Demonstration Scope

For the steam ejector loop demonstration, below is a list of objectives and scope:

▪ **Objective**

- From SOPO: "advance the steam ejector TRL by testing in a relevant environment … using realistic gas compositions and temperatures"
- Advance to TRL 5

▪ **In Scope**

- Test ejector with steam generation components
- High temperature steam/H_2/CO_2/CO (SOFC) or steam/H_2 (SOEC)
- Relevant SOFC and SOEC operation environment
- Verify ejector performance and CFD model for high temperature steam operation

▪ **Out of Scope**

- Testing with full R-SOFC system – no stack, reformer, air side components
- Ejector durability – long range testing

Predictions from the prototype ejector were validated using two experimental setups. A first ejector design was tested with air as working fluid. Later during the program, the ejector design was tested with actual SOFC and SOEC compositions at high temperature.

6.2 Ejector performance with air as a working fluid:

The comparison between experimental measurements and CFD predictions is shown in Figure 6.1. Experiment and CFD Analysis was run using different lift pressures. Lift pressure is the difference between pressure at the secondary inlet to the ejector and ejector outlet. CFD predictions were found to be accurate (both qualitatively and quantitatively) for the range of lift pressures tested in the experimental setup.

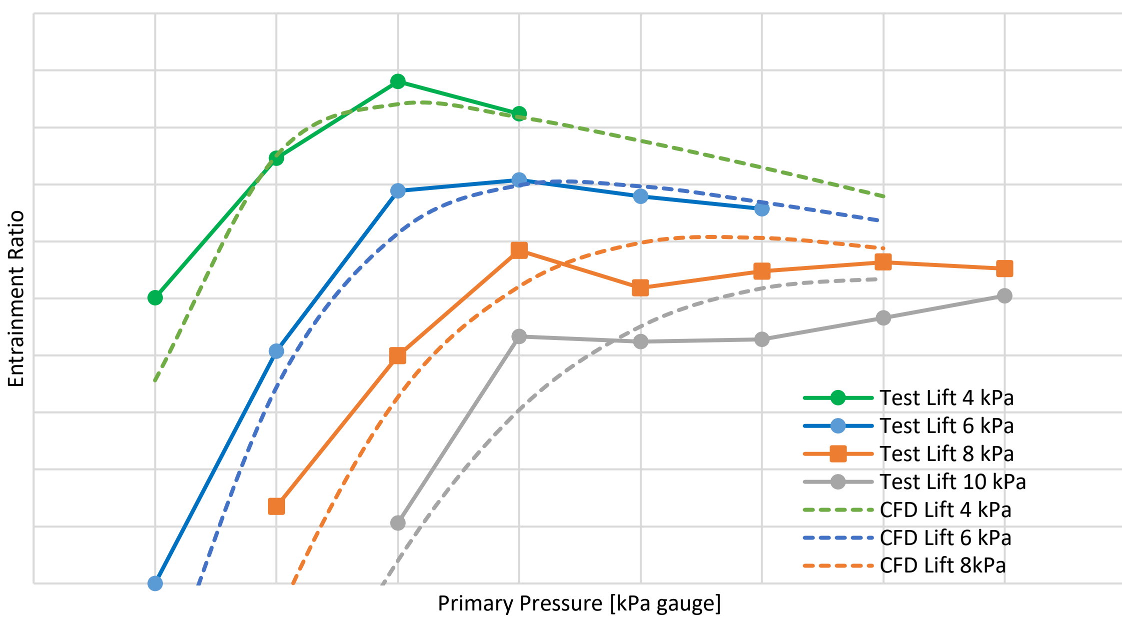

Figure 6.1: Comparison of entrainment ratio between CFD predictions and experimental measurements with air as a working fluid

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6.3 Ejector performance with actual SOFC and SOEC composition at high temperature:

The ejector was tested in the hot loop test setup with representative gases to mimic operation in an actual SOFC and SOEC and determine ejector entrainment ratio at a range of conditions as described above. The ejector hot loop test setup schematic is shown Figure 6.2. The image on the left shows the overall SOFC/SOEC configuration with a red box around the portion of the system that was tested. The right image shows the experimental components used for ejector hot loop testing to determine ejector performance.

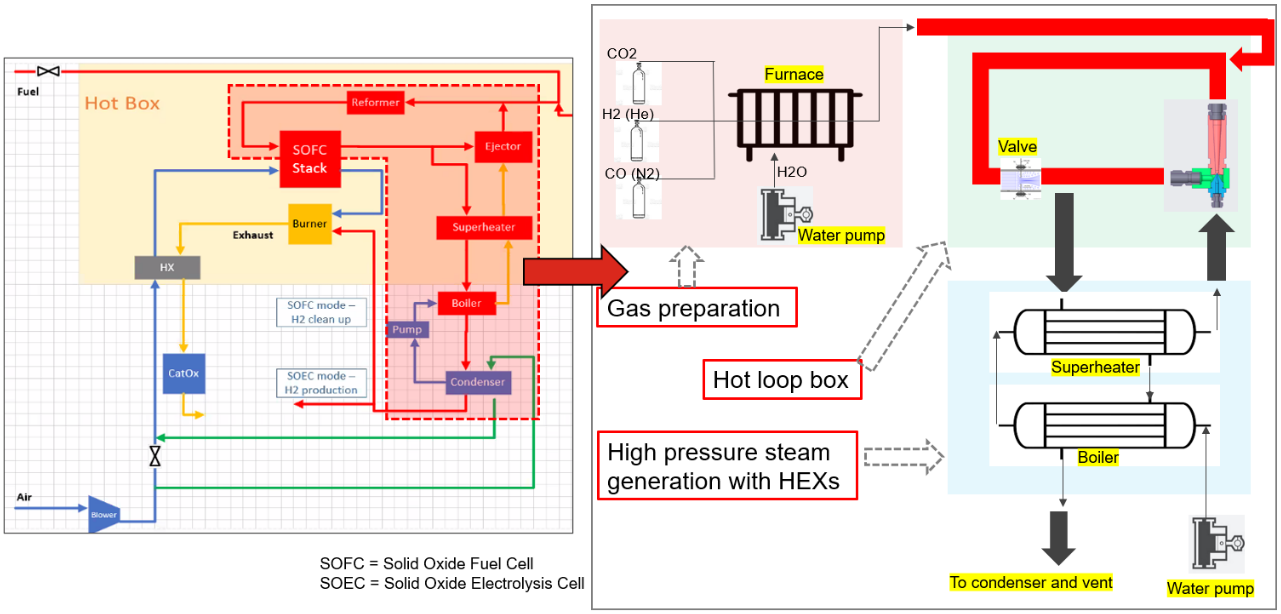

Figure 6.2: Overall SOFC/SOEC setup (left) and test setup for ejector hot-loop testing (right)

The ejector hot loop test setup hardware is shown in Figure 6.3. The image on the left shows the components prior to the full insulation of the hot loop. The major components and features include the ejector test article, the recirculation loop, the restriction valve to simulate the SOFC stack backpressure, the primary flow inlet which introduced superheated steam to the motive flow of the ejector, the secondary flow inlet which introduced the representative gases for SOFC or SOEC operation in the proper fractions, and the exhaust outlet. Sampling locations were located throughout the loop in key areas to measure concentration of gases, along with measured inlet flowrates to determine the entrainment ratio.

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Figure 6.3: Ejector hot loop test setup hardware: uninsulated (left) and insulated (right)

A comparison between CFD predictions and experimental measurements for an ejector working under SOFC anode composition is shown in Figure 6.4. The CFD methodology accurately captures the qualitative as well as quantitative aspects of ejector performance in fuel cell mode.

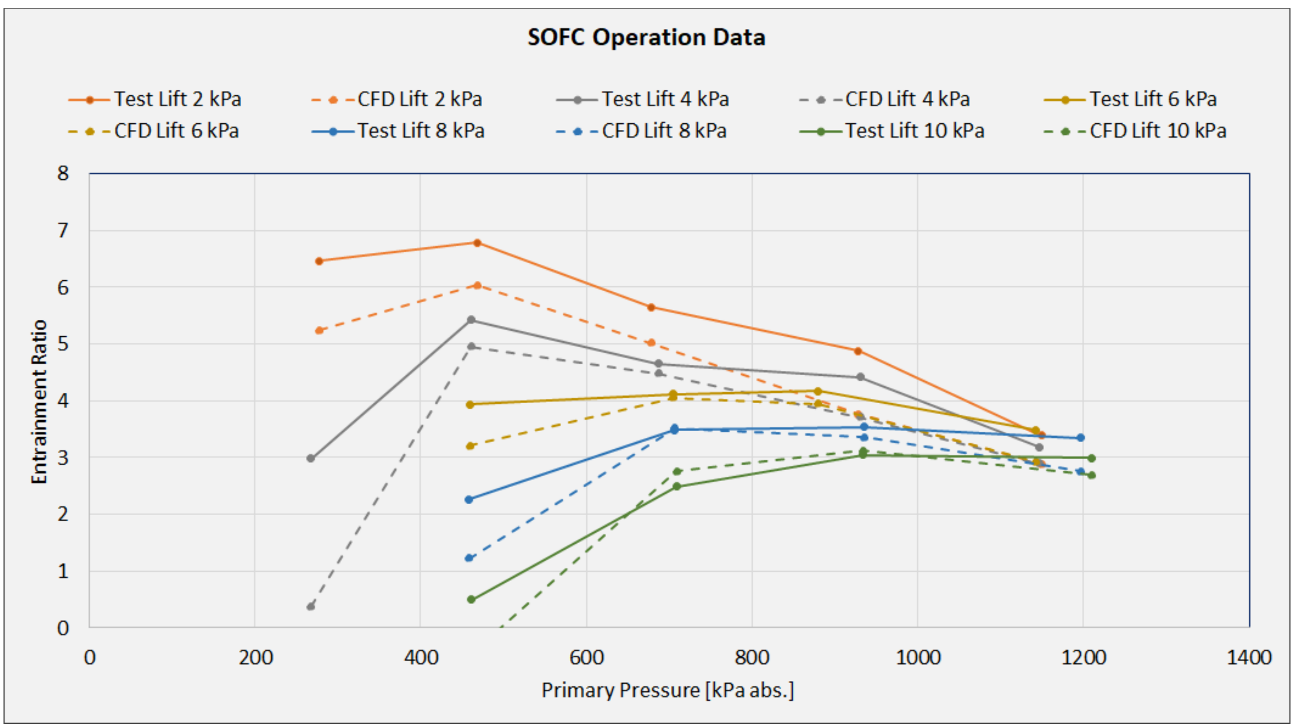

Figure 6.4: Ejector performance in fuel cell mode

A comparison between CFD predictions and experimental measurements for an ejector working under SOEC anode composition is shown in Figure 6.5. The CFD methodology accurately captures the qualitative as well as quantitative aspects of ejector performance in electrolyzer mode. The quantitative difference between experimental data and CFD predictions was observed to be higher when the ejector was tested in SOEC mode.

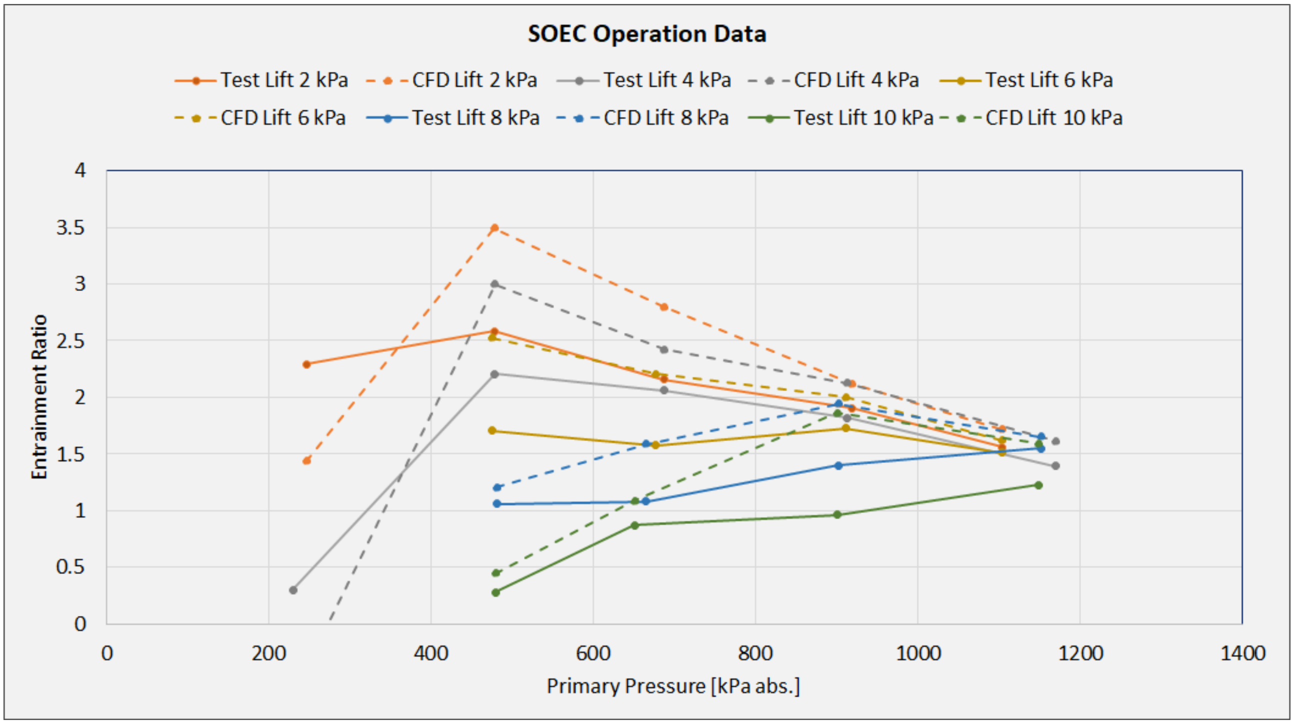

Figure 6.5: Ejector performance in electrolyzer cell mode

Task 7.0 – Techno-Economic Analysis (TEA)

The overall purpose of this project was to reduce R-SOFC system cost by developing two technologies, an improved cell design and the incorporation of an ejector in the fuel recycle loop instead of a blower. Cummins' internal calculations show that the new cell design reduces cost ~50% compared to the baseline cell, while the ejector + superheater/boiler concept reduces cost of the recycle loop by ~40%. The impact of these cost reductions on the cost of producing H_2 will depend on the specific system where they are applied. For this reason, we have completed the Techno-Economic Analysis using system cost as a variable, and then showing how the NREL Current and Future system costs translate into H_2 production cost.

The Techno-Economic Analysis (TEA) was performed for SOEC for two production size cases of 10,000 kg-H_2/day and 5,000 kg-H_2/day using the NREL H2A model future-central-solid-oxide-electrolysis-version-nov20. The basic premise in this calculation is that there will be smaller size electrolyzers which can be operated reversibly. They will produce hydrogen when the electricity price is low and produce electricity when its price is high. When the ejector based recycle loop is used, it replaces gas blowers and its related equipment on the anode gas side. This results in a cost reduction of 20% when the NREL future model assumption of $430/kW cell is taken as a baseline. Since the work in this project is future oriented, this assumption was considered reasonable. Aside from cost reduction from using ejector technology, we anticipate 50% cost reduction with our cell design improvements.

Since these are assumed to be small size plants, the base model was modified for a labor case of 3 FTE and a site size of 1 acre. Based on our cost analysis, the stack:BOP cost split came to 30:70 which was updated in the model. Based on our technology, we anticipate an electrical efficiency of 34.62 kWh/Kg-H_2 (96%) and this was used in the model. As mentioned in the proposal, we intend to run the system at thermoneutral voltage where the thermal energy requirement will be minimal and there is available waste heat to product input steam, and hence we removed the thermal energy requirement in the model. As per the project requirement, the cost of electricity was taken to be $30/MWh.

Under these assumptions, Figure 7.1 shows the analysis results where it can be deduced that the ejector has considerable advantage in meeting the DOE target of $2/kg-$H_2$. The scale of the plant**,** as expected**,** influences the cost as well. For the 10,000 kg/day case, i.e. without an ejector, the cost of the cell must be <$700/kW to meet DOE H_2 production target. However, with an ejector, this cell cost target can be increased to <$775/kW. For the 5000 kg/day case, these numbers are $575/kW and $650kW respectively. The ejector helps reduce the cost of producing H_2 independent of the system cost.

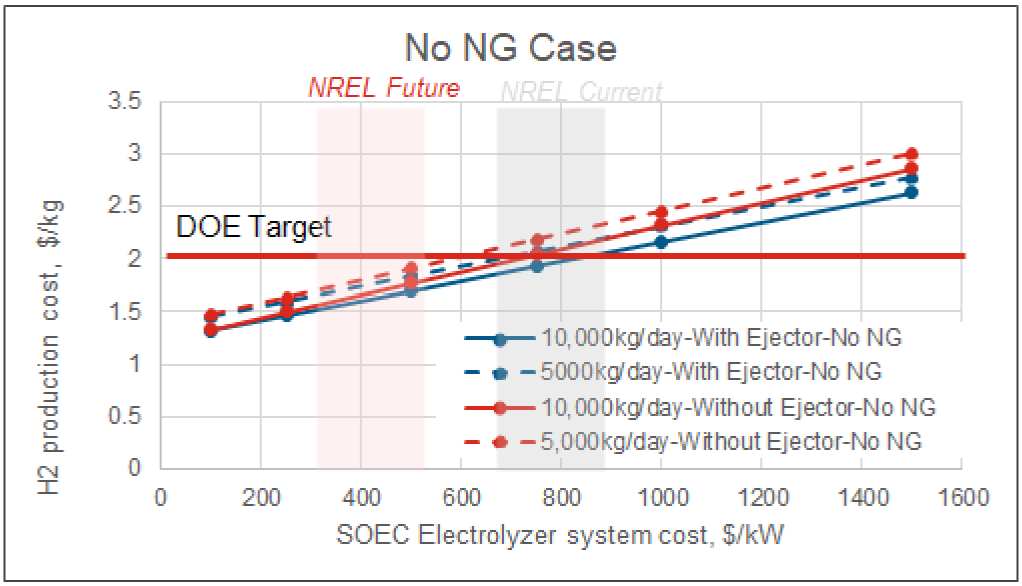

Figure 7.1: NREL H2A model analysis to study H_2 production cost as a function of Cell cost. The advantage of ejector on H_2 cost reduction can be seen for 2 different scale plants – 5000kg/day and 10,000kg/day. Note that this case involves no NG (natural gas) requirement as cell will operate at thermoneutral voltage and there will be available waste heat to produce input steam.

Another point to note is that the operation of the cell in reversible mode makes it possible to raise profits from the sale of electricity. Based on our calculations shown in the proposal, even if the electricity is sold at a modest $0.02/kWh, a profit of $0.24/kg-$H_2$ can be realized (assuming SOFC and SOEC operation for 12 hrs each). If this profit is accounted for, then the cost of the cell (see Figure 7.2) can be as high as $1050/kW for 10000kg/day case and $925/kW for 5000kg/day case when using an ejector. It can be clearly seen that even for NREL current case, it is possible to produce $2/kg-$H_2$ with the ejector technology.

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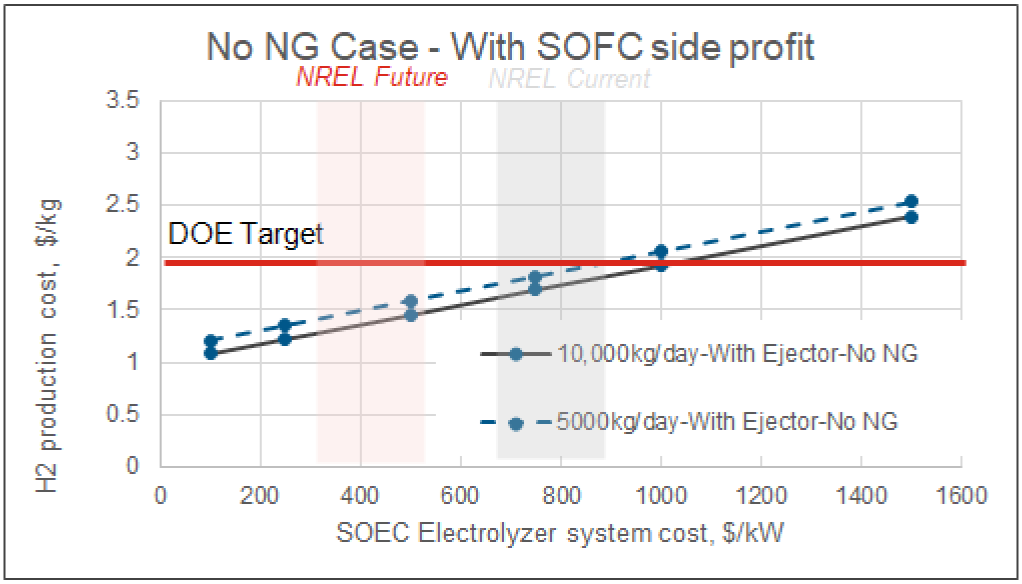

Figure 7.2: Same as Figure 7.1 but with profit made from SOFC side operation transferred to H_2 production. It is assumed that electricity from SOFC side operation is sold at $0.02/kW.

For comparison, we also ran the case with a natural gas requirement (Figure 7.3), that is, natural gas is needed produce input steam. The baseline natural gas consumption in the H2A model (0.04579 mmBTU/kg-H_2) was used. For the 10,000 kg/day case, for a system without an ejector the cost needs to be $425/kW but for system with an ejector the cost can as much as $500/kW. For the case of a much smaller plant producing 5,000 kg/day, the cost needs to be so low that the ejector has a minimal impact on the economics. The cost of the cell needs to be as low as $350/kW. Overall comparing to No NG (natural gas) case (Figure 7.1), the cell cost needs to be considerably lower if thermal energy is included. Hence, the best case for low cost H_2 production from reversible SOEC is to operate the cell such that no thermal energy is needed and transfer the profit from SOFC model to subsidize the H_2 production in SOEC mode.

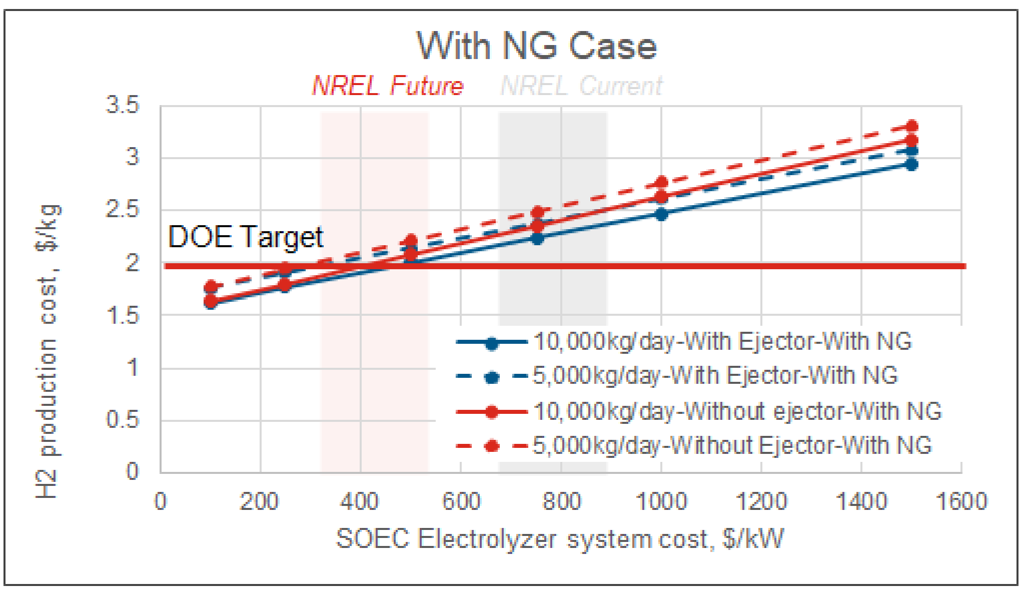

Figure 7.3: Same as Figure 7.1 but with thermal energy requirement via natural gas.