Liquid Tin Anode Direct Coal Fuel Cell

Final Program Report

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Significance, Background Information, and Technical Approach

Background

Coal plays a vital role in the power economies of major countries and biomass is a key fuel for sustainable power generation in the future. Improved generation efficiency can increase the economic viability and improve the environmental responsiveness of these fuels but efficient generation options are limited, particularly for applications where carbon capture and sequestration is desired. ElectroChemical Looping[1] (ECL) is a new concept for direct generation of power from a variety of fuels including coal and biomass. Direct conversion is more efficient. ECL combines multiple processes, reducing inefficiency and lowering capital cost compared to other advanced baseload technologies (Figure 1). For instance, there is no oxygen plant or gasifier required. The enabling technology for ECL is a new type of fuel cell that uses a liquid tin anode. The ECL concept has been evaluated by EPRI and DOE-NETL in several recent programs. Independent analyses by these organizations have predicted high efficiency (61% on coal) and low capital cost in configurations which also capture CO_2 for sequestration. The core fuel cell technology for ECL has been demonstrated in small scale and commercialization for small power applications provides an important link to commercialization of large scale generation technologies. A plan of action to accelerate ECL development includes further work on key risk items - durability, demonstration of a bench scale system and scale up of the enabling technology components. The commercialization path incorporates early revenue from markets such as portable power and distributed generation, providing near-term reliability improvement while reducing the time and risk associated with development of baseload applications.

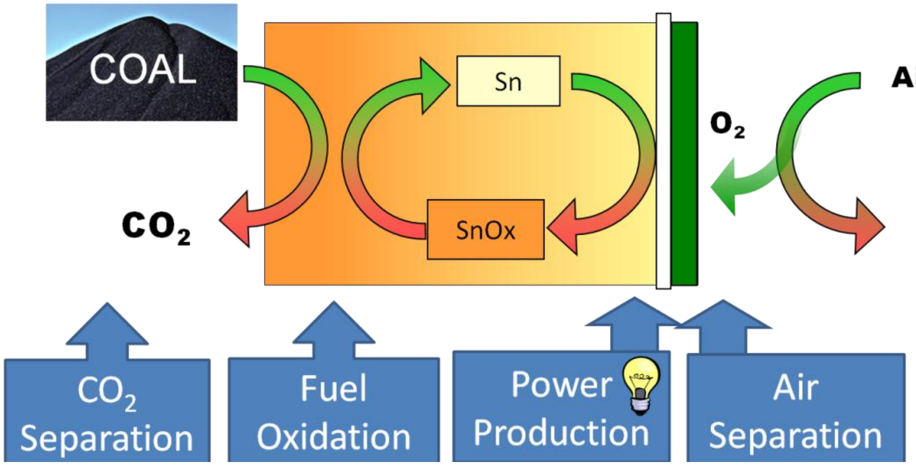

Figure 1 Electrochemical Looping utilizes the Liquid Tin Anode fuel cell to make power directly from coal. It eliminates multiple process steps and allows the capture of CO_2.

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[1] The electrochemical aspect refers to the highly efficient production of power without combustion while the looping concept refers to the shuttling or "looping" of oxygen by the liquid tin anode.

Solutions Needed for Coal and Biomass Power

A number of options are under development for addressing national energy needs consistent with environmental constraints. Figure 2 below compares several of the existing and proposed candidate technologies for coal power generation consistent with carbon capture. All of the advanced coal technologies require a feed of pure oxygen creating several disadvantages. First, production of oxygen from air requires a significant amount of energy; secondly, oxygen production plants tend to favor large scale, making most of these technologies unsuitable for distributed generation. Additionally, all of these technologies involve an additional step such as combustion or gasification prior to the power production step. These processes are inherently inefficient and add to capital costs.

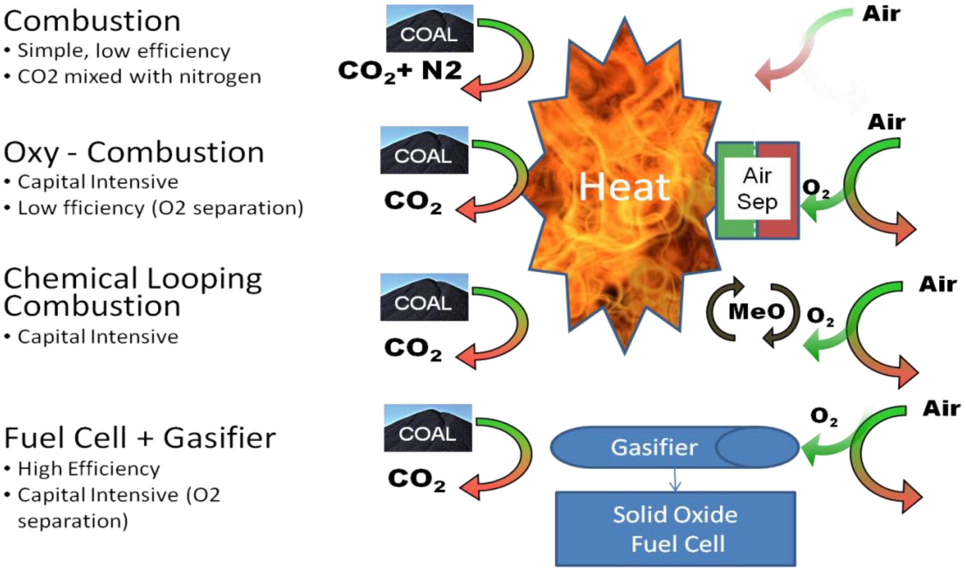


Figure 2 Other coal generation technologies require multiple process steps.

Electrochemical Looping Using Liquid Tin Anode Fuel Cell

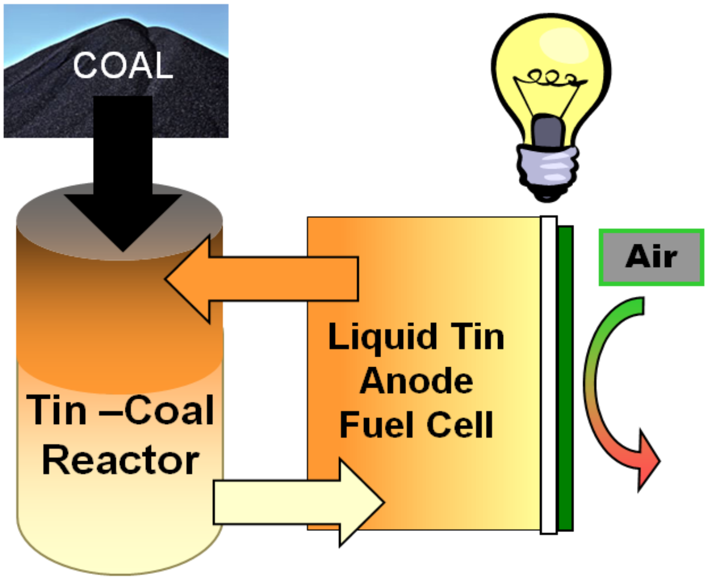


Figure 3 the two major elements of the ECL flowsheet are the Tin-Coal Reactor which processes the coal and the Liquid Tin Anode Fuel Cell which produces power

ElectroChemical Looping using the Liquid Tin Anode Fuel Cell produces DC electrical power in an electrochemical reaction powered by coal or many other fuels. For utility scale applications the fuel oxidation step is carried out in a separate tin reactor. The liquid tin "loops" between the fuel cell and the tin reactor, shuttling all of the oxygen used to convert the coal. The net effect is that power is produced directly and efficiently from coal or biomass without burning and with inherent separation/rejection of nitrogen. In Phase 1 of this SBIR, detailed flowsheets for this concept were created and analyzed to evaluate efficiency and cost as described below and in the review of Phase 1 activities. NOx is not formed because nitrogen does not participate in the reactions and sulfur emissions can be cleaned up using conventional technology. CO_2 can be captured in a pure stream from the ECL system. CO_2 emissions and ash production are lower than other alternatives because less coal is used per kWh produced. Coal can incorporate a number of elements which are potentially harmful to the fuel cell. Laboratory testing of tin/coal reactions has demonstrated that the tin coal reactor will act as a purifier, rejecting nearly all contaminants before they reach the fuel cell under certain conditions. This is a key positive finding for system longevity.

Specific Benefits of Phase II Activities

Commercialization of ElectroChemical Looping Direct Coal systems will require significantly more time and resources beyond this SBIR program. However, this program will make contributions in several important ways:

1. This SBIR program will result in improved LTA cell technology which is the fundamental building block of the Direct Coal ECL concept. As described below, ECL can make enormous efficiency and cost contributions to utility scale coal power.

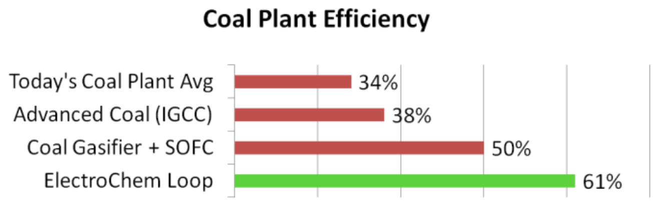
2. This program will improve LTA cells for small scale power generation. As described in the Commercialization section, there are important intermediate military and commercial markets for LTA generators that will provide an important bridge to the coal power application.

3. The specific technical information from this program relating to YSZ electrolyte durability will be broadly applicable SOFC developers working on coal based SOFC generally. This is an area about which very little is currently known and will be critical for successfully applying fuel cells to coal power generation.

Anticipated Public Benefits of ECL Technology

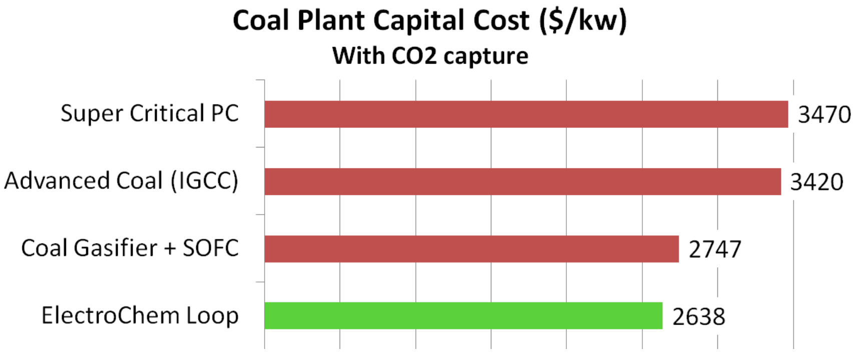
In the last several years, a number of organizations have joined CellTech Power in developing and evaluating the Electrochemical Looping concept for utility power production. DOE-NETL has begun lab based testing to evaluate the technical characteristics of tin. The Univ. of South Carolina is developing numerical models which will allow prediction and optimization of the fuel cell. And system level analyses have been conducted by EPRI (using Nexant, Inc) and DOE-NETL (using J.Thijssen LLC). These analyses utilized actual test data from laboratory testing of the core Liquid Tin Anode technology operating on coal and are summarized below.

High Efficiency



High generation efficiency contributes to lower electrical costs and reduces the emissions produced and the resources utilized for each kWh produced. Today coal plant efficiency is in the mid 30% range (without CO_2 capture penalties). IGCC coal plants can approach 40% efficiency and SOFC plants will approach 50% efficiency when catalytic gasifier technology is ready for deployment. In contrast, the ECL is predicted by DOE to have up to 61% efficiency *with CO_2 capture.* This higher efficiency comes from the efficiency of direct conversion of carbon to electricity and from the low parasitics of the simpler ECL system. This higher efficiency results in lower coal use/kW and lower production of waste products like ash.

Low Capital Cost



Low capital cost is key for the widespread adoption of ElectroChemical Looping technology. The capital cost and cost of electricity has been independently compared to alternatives, with favorable predictions for ECL. The lower capital cost is due to system simplicity and the use of tin a low cost commodity as a catalyst.

Scalability for Distributed Generation

The ECL will provide other unique advantages for utility scale applications. It is inherently multi-fuel, enabling the incorporation of biomass or other fuels as partial or complete substitutes for coal. Because the ECL does not have “lumpy” process units (like air separation), it can be scaled to smaller capacities for distributed generation or biomass utilization. Smaller scale generators can reduce biomass transport costs by deployment within an economic transport radius. The tin reservoir in the ECL is actually a media for the storage of chemical energy, allowing the ECL system to buffer instantaneous power surges or provide power even when fuel flow is disrupted.

Phase I Results

The Phase I program successfully focused on Liquid Tin Anode cell development for Direct Coal applications, within the context of a SYSTEM level analysis.

The objective of Phase I of this program was to evaluate the technical merit and feasibility of the Direct Coal powerplant incorporating a Liquid Tin Anode Fuel Cell. CellTech has successfully met this objective. The tasks in Phase I focused mainly on defining the characteristics of a Liquid Tin Anode cell which could be successfully incorporated into a Direct Coal powerplant. The SBIR Phase I program has been carried out in conjunction with DOE Cooperative Agreement Phase I (SECA). In Phase I CellTech successfully completed all 5 technical tasks as summarized in the Table 1 and described in the following sections:

Phase I Tasks	Key Accomplishments	Specific Results
1. Baseline System Conceptual Development	Developed a baseline power plant schematic which was used as the basis for deriving the required fuel cell specifications.	- Conceptual plant design with Tin-Coal Reactor separates coal oxidation from electrochemical reaction. Near 100% fuel utilization.
2. Direct Carbon Cell Performance Analysis and Preliminary Design	Evaluated the expected performance of the LTA-SOFC cell in the Direct Coal application. This work involved synthesis of available test data, preliminary design of a full scale (1kW) Direct Coal cell (Task 2a) and experimental evaluation of cell degradation (Task 2b).	- Developed 3 designs for 1 kW single cell that meet performance requirements. - Identified 10 elements that are detrimental to the LTA-SOFC: As, Se, V, Cr, Mo, Nb, Ta, W, Mn and U - Conducted chemical reactor testing of coal + tin and measured small levels of As, V, Cr, Nb and Mo impurities. -Conducted electrochemical testing of LTA cell with spiked impurities and measured degradation rate.
3. System Performance Analysis	Developed cell performance data and worked with consultants to analyze Direct Coal plant cost and performance.	Thermodynamic analysis projects 61% HHV efficiency for Direct Coal powerplant Cost analysis projects CAPEX of $1888/kw, slightly higher than IGFC.
4. Identification of Risk Areas	Identified the most significant technical risks to achieving a full scale Direct Coal fuel cell Identified actions to mitigate risks.	Cell development risk items identified. Major concern is for material longevity. Proposed mitigating action is durability testing/material development.
5. Development Plan	Developed a high-level Development Plan for the commercialization of the Direct Coal Liquid Tin Anode concept.	Development plan leverages early commercial markets for LTA to assist in development of Direct Coal technology.

Table 1- CellTech has successfully completed all 5 technical tasks in Phase I leading to a promising outlook for further development of the Direct Coal powerplant.

Task 1- Baseline System Development

CellTech Power developed the baseline system diagram for a Direct Coal LTA system in conjunction with Jan Thijssen, a consultant to the project. Attributes for this systems concept include:

- Provides a means for feeding coal directly into the tin anode by using a Tin-Coal Reactor (TCR). Introduction of a separate reactor also allowed for separation of ash, slag and contaminants.
- Maximization of fuel utilization by recirculating fuel to the TCR after stripping of CO$_2$.
- Use of conventional technology for cooling, cleaning and heat recovery.

The high-level PFD is shown in Figure 4. Results of the analysis of this system are described in Task 3.

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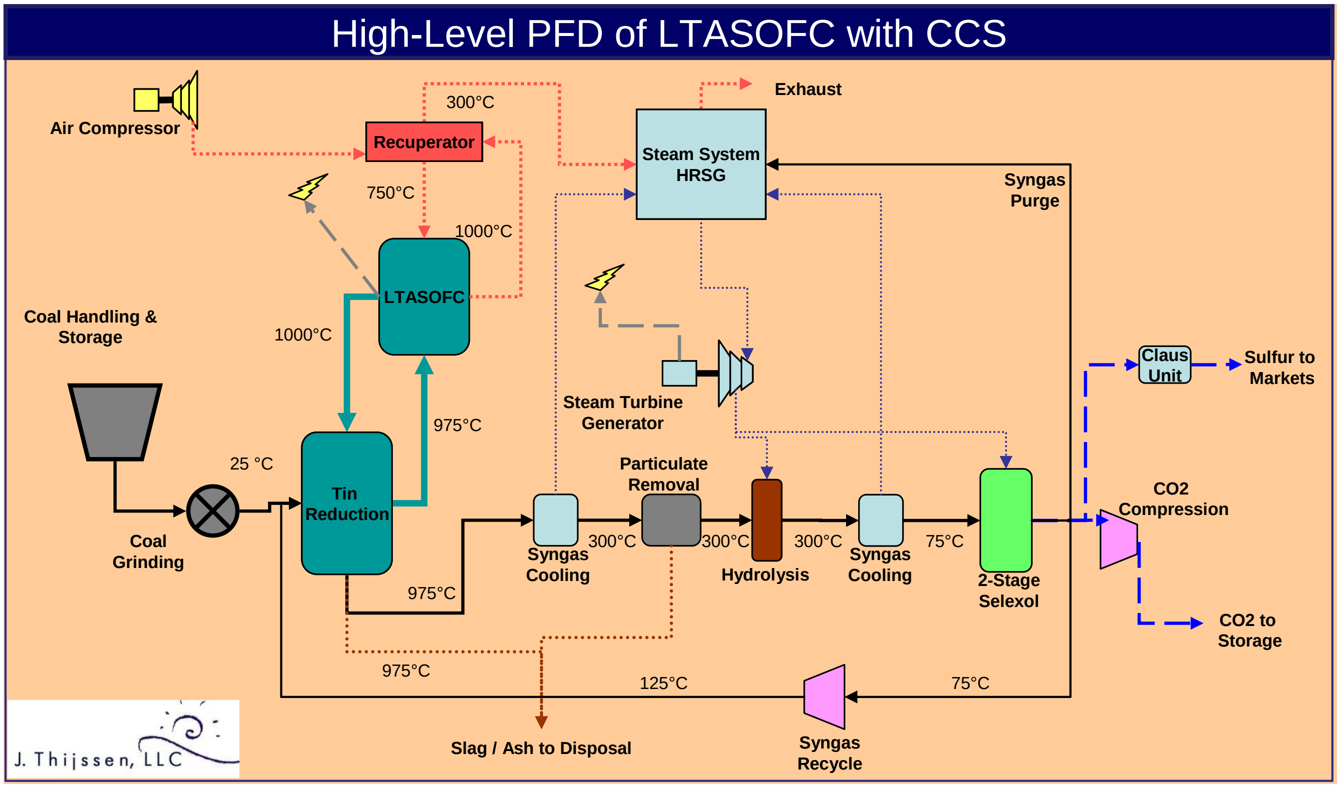


Figure 4: Phase I – Task 1 produced a comprehensive high level process flow diagram with provisions for separate coal feeding and syngas recycle.

Task 2a – Data synthesis and preliminary design of a 1 kW LTA Single Cell

CellTech Power has demonstrated the scientific feasibility of the Liquid Tin Anode – Solid Oxide Fuel Cell (LTA-SOFC) for smaller power applications, on a range of carbonaceous fuels. The current LTA design, Gen3.1, is capable of 170 mW/cm^{-2} (5 watts, active area 30 cm^{2}) on diesel or military diesel fuel (JP-8) without reforming or desulphurization. Utility scale applications will require a single cell with approximately 1kW output to minimize cell count, reduce cost and increase efficiency. Thus, one major task of this Phase I SBIR was to develop a preliminary LTA cell design suitable for megawatt power generation.

The first step in design of a larger cell was to collate and synthesize relevant information from previous testing and project design requirements for the 1kW cell. This allowed selection of a set of design parameters. Targets for power density, operating potential, electrical efficiency and the net power capacity of the cell were extrapolated from on-going CellTech Power cell development programs for small power. The performance of the Gen3.1 operating on JP-8 is shown in Figure 5.

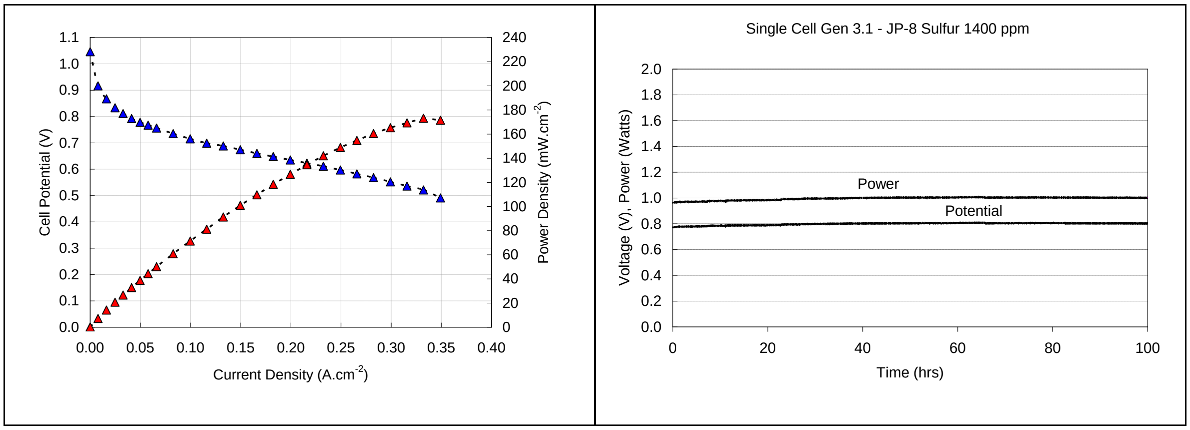


Figure 5: Gen3.1 cell can achieve 170 mW.cm-2 and has run for 100 hrs plus without noticeable decay on military diesel (JP-8).

The selected design parameters are summarized in Table 2. The power density target is conservative since it is only an 18% increase over our current cell test data. The Nernst potential under load is established to avoid formation of harmful tin oxide near the cell. The electrical efficiency target was established to yield high system level efficiency.

Table 2: Design parameters used to scale up cells for megawatt power production.

Design Parameters	Values
Power Density	0.2 W.cm^{-2}
Nernst Potential (under load)	0.8 V
Electrical Efficiency	91.25%
Net Power Capacity	1 kW
Operating Potential	0.73 V
Operating Current	1370 A
Resistance Target	**60 μΩ**
Cell Active Area	**5000 cm^2**

Several geometries were evaluated during the Phase I cell design effort to provide multiple options to mitigate the risk of cell scale-up. Three very different cell geometries were considered.

1. Tubular cell design
2. Flat tube (elliptical) design
3. Design similar to Siemens HPD cell

The tubular cell design scales from the current Gen 3.1 cells. It utilizes a single central cathode current collector with adjustments made to the number of and dimension of the current-carrying ribs. In contrast, the flat tube offers large flat surfaces to optimize cell packing in the stack. This concept also uses multiple current carrying ribs; however in this case, multiple cathode current collectors were used to increase the current carrying capability. The use of a configuration similar to the Siemens HPD cell design was suggested by CellTech Power as well as Jan Thijssen, a consultant for this program.

The next step in the cell design process was to demonstrate that the resistance target and cell active area are achievable in the selected geometries. The design process for each geometry started by using the cell active area to define the ratio of cell height to circumference. The generated sets of aspect ratios were studied using Fermi solutions to narrow the set of aspect ratios. The current paths from the electrolyte to the current collector were then described mathematically using cell geometric constraints. The resistance could then be calculated using the resistivity of the materials and the generic equations for resistance and summation of resistor circuits. The fundamental reference point was the Gen3.1 design that contains 4 current carrying ribs to a central current collector. The current path ways and resistor circuit used for the Gen3.1 is shown in Figure 6.

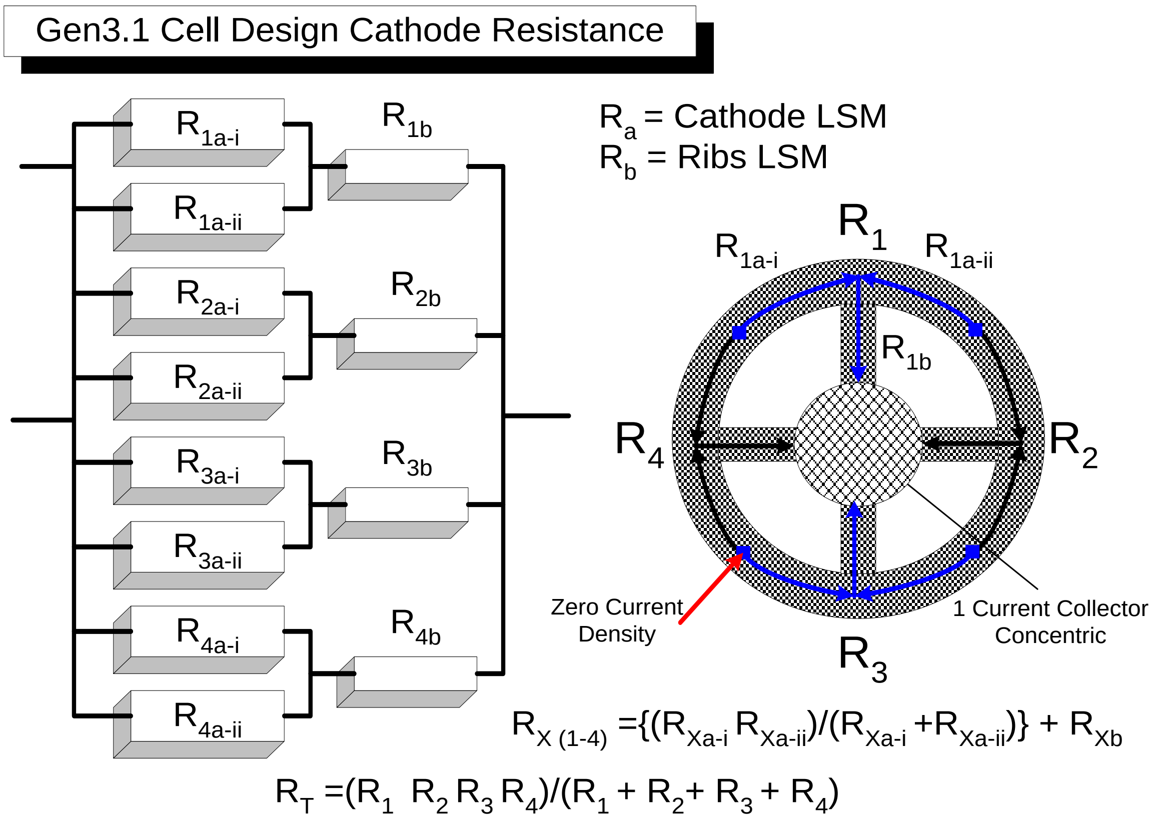


Figure 6: For the tubular design, the current paths were initially described for the 4 rib model to calculate resistances for the conceptual resistor circuit.

The resistance model for the Gen3.1 cell was applied to a 5000 cm^2 cell with varying aspect ratios of circumference to height. The resistance of the cell was then minimized by altering the number of current carrying ribs and shortening the current path along the ribs. One technique for decreasing the current path length along the ribs is to increase the diameter of the central current collector. However, in the case of the tubular cell, not all of the cross-sectional area of the current collect was needed to draw current longitudinally down the cell. This allows a tube shape for the current collect with a hollow current collector to minimize material utilization. For the flat cell, a number of smaller current collectors were used. The resistance was reduced as the spacing between the current collectors was reduced. In both the tubular and flat tube designs consideration was given to the manufacturability of the cell and the geometry of the cells changed accordingly. Initial CAD models are illustrated in Figure 7 and Figure 8 for the tubular and flat tube designs respectively.

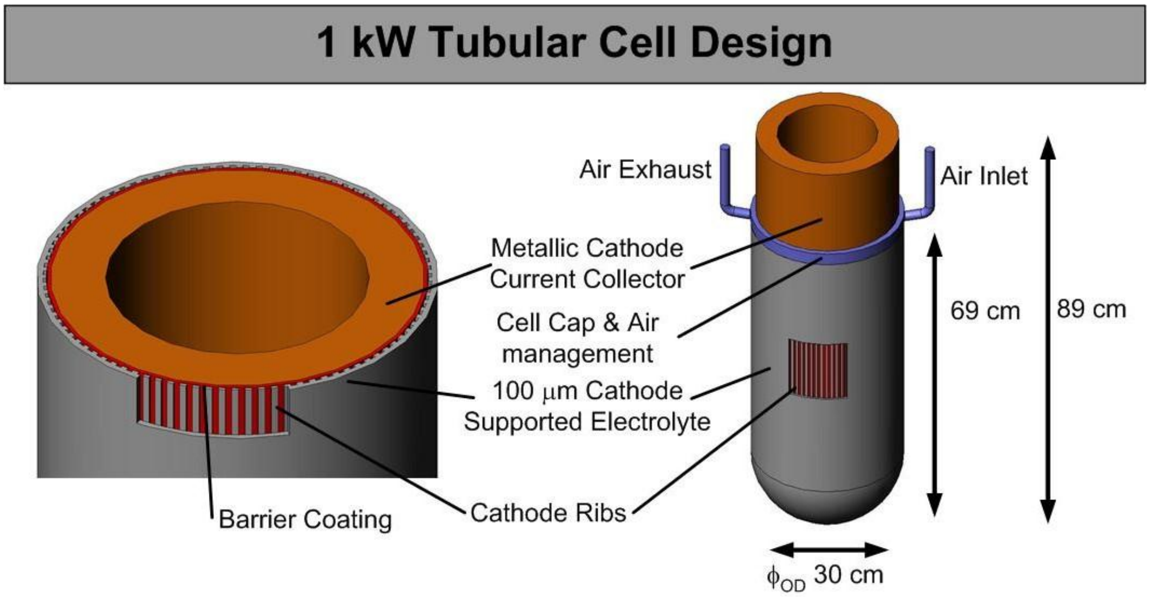


Figure 7: The tubular LTA-SOFC cell design for a 1 kW single cell is derived from CellTech's Gen 3.1 Direct JP- 8 cell design.

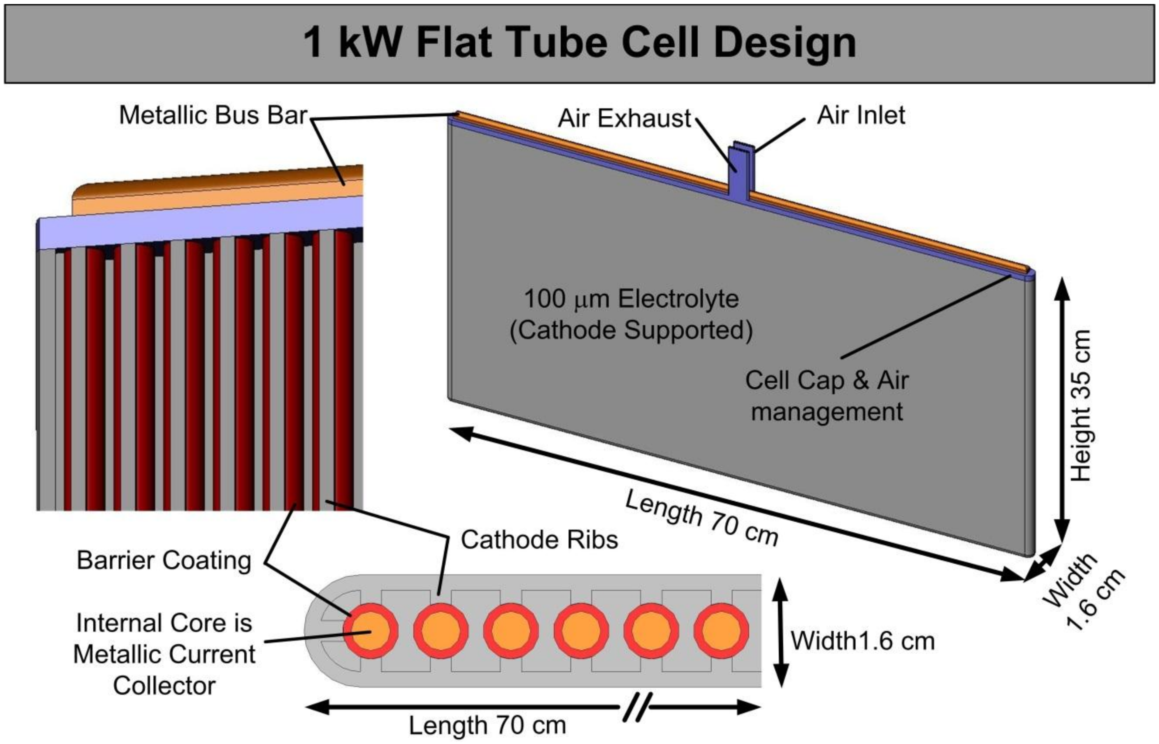


Figure 8: The flat tube design utilizes multiple small diameter current collectors to minimize resistance

Several key geometric factors could cause manufacturability issues for both the tubular and flat cell concepts. The cathode thickness for example needs to be reduced to lower resistance, but also needs to be mechanically strong enough to support the electrolyte of the cells. 5 mm was chosen and the resistance calculated. In future work a more detailed design review of the mechanical stress on the cell during operation will be required since the cells are subjected to a flowing stream of liquid tin. In addition to the cathode thickness, the current carrying ribs geometry optimization is also complicated. For resistance the ribs should be short and have a large cross sectional area perpendicular the direction of current flow. However, thicker ribs will create airflow dead spots within the cathode where oxygen diffusion is limited. Also, the extrusion of these ribs over a long length will be challenging. All of these considerations were taken in to account when generating the initial designs for 1 kW cells. An example of the end point is shown below for the tubular design, Figure 9. These charts will allow additional information from Phase II work to be quickly assessed to ensure the cell performance design goal is still achievable.

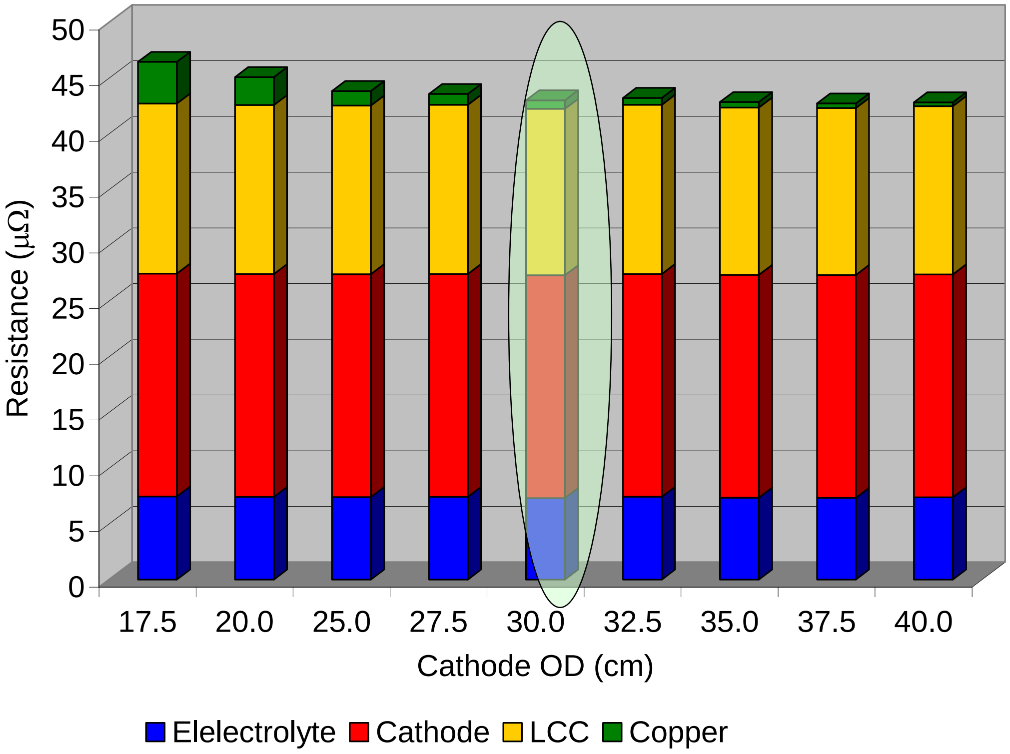


Figure 9: An example of an optimization chart for electrical resistance showing the optimal cathode diameter (highlighted bar) for the given geometrical constrains.

The resistance models have also allowed CellTech Power to focus on areas that offer the biggest gains from materials development and component redesign. For example CellTech Power used a resistance model to identify cathode resistance as a major barrier to the development of the Gen3.1 cell. This component was redesigned with a new ribbed approach which resulted in the power density increasing from 40 mW.cm-2 to 170 mW.cm-2 on military diesel fuel. For the proposed 1 kW cell design, the resistance break down of the tubular design, Figure 10, shows the cathode and proprietary material for current collection to be the largest contributors to resistance. The flat tube design shows a similar trend. Fabrication of these designs will be feasible with current manufacturing processes used at CellTech Power.

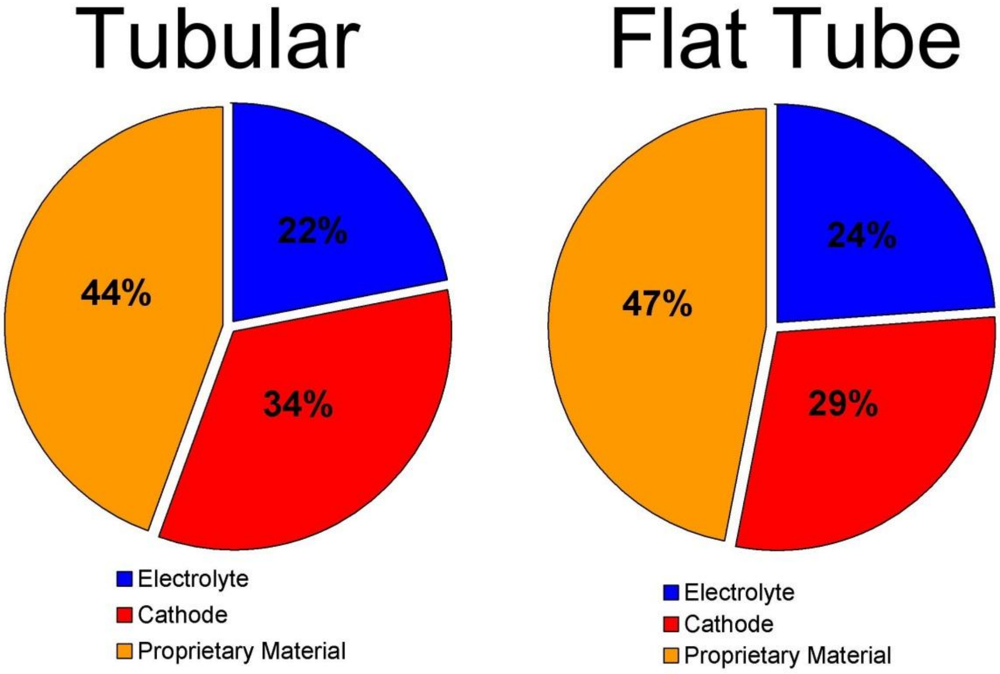


Figure 10: The resistance model showing the areas where the biggest gains can be made from materials development for the tubular design and the flat tube design respectively.

In summary, this Phase I task has identified the key characteristics for an LTA cell scaled for 100 MW scale applications. The performance characteristics for the cell have been defined. Three concepts have been developed and 2 of these, the Tubular and Flat concepts have been further analyzed. A resistance model, derived from CellTech's small scale cells, was modified to analyze the cell resistance. Both concepts appear to be able to meet the established cell resistance requirement, which is an important first step in concept evaluation.

Task 2b - Experimental Assessment of Tin Impurities and Cell Longevity.

A key step in reducing development risk for the Direct Coal concept is to understand the effect of coal impurities on the LTA-SOFC electrolyte and their impact on performance. Experimental work for this task was performed jointly under a co-operative award with DOE and Phase I of this SBIR. CellTech has identified 10 elements that are detrimental to the LTA-SOFC electrolyte YSZ, they are As, Se, V, Cr, Mo, Nb, Ta, W, Mn and U. To investigate the fate of coal impurities in molten tin, a laboratory scale Tin-Coal Reactor was built and a number of samples were produced by reacting tin dioxide with Wyoming coal. Glow Discharge Mass Spectroscopy (GDMS) analysis was selected to allow identification of ppb levels of contaminants. Coal and tin were fully reacted and cooled. In the narrow diameter laboratory reactor stratification of ash and tin was incomplete. The GDMS data from these unconsolidated samples are shown in Table 2. It is thought that most of the measured impurities are contained as compounds within the coal ash. Some of the cooled samples were subjected to a consolidation process of reheating the tin to 450°C which allowed the coal ash trapped in the tin to float to the surface. This consolidation step results in removal or dramatic reduction in the amount of coal ash/solid particulates. This observation demonstrates a simplistic method to clean unwanted coal ash/solid particulates from the tin that can easily be achieved on a large industrial scale.

The contamination study resulted in two major observations:

1. Small trace amounts of coal ash/solid particulates were present in tin samples that were tested.
2. The consolidation of the tin by reheating to 450°C removes and/or dramatically reduces the trace levels of coal ash/solid particulates in the tin.

It is probable that the rejection of coal impurities from the tin in a large scale reactor will occur at 1000°C without the consolidation step because gravimetric stratification will be aided by the bubbling dynamics associated with coal feeding/devolitalization and the radically different form factor (larger diameter) of the full scale TCR. The rejection of impurities via gravimetric separation has been observed experimentally for coal and coal ash which had larger particles sizes and was not intimately mixed with the tin.

Summary of Phase I Task 2b: results, conclusions and discussion

Coal-tin reactor chemical analysis – impurities in tin

The GDMS results and prior and subsequent thermodynamic analysis indicated fundamental trends about the fate of coal impurities in molten tin under conditions where the tin-coal reactor is projected to operate. It has been observed that molten tin may indeed be able to provide a media for separation, purification or even elimination of harmful elements and impurities found in coal under certain conditions similar to those expected in the tin-coal reactor. These preliminary results/data/analysis suggest 2 major conclusions discussed below:

(1) Successful demonstration of direct reduction of tin oxide by coal and feasibility of coal ash separation from molten tin.

Tin oxides were found to be reduced by raw coal to tin at 1,000C, leaving ash behind. The main components of coal ash may be oxides/sulfates of Si, Fe, Ti, Al, Na, Mg and Ca, etc, in form of particulates or slag. Separation of these lighter reaction products from molten tin is feasible through filtration or gravitational separation (skimming off, for example), although embedment of particulates in molten tin remained an issue at very small scale (less than 10 cc of tin) where these Phase I tests were conducted. A scale up of reactor size to one kg or larger is needed to evaluate coal ash separation from molten tin in the future;

(2) High attenuation of impurities by molten tin.

(2.1) type of impurities dissolved in molten tin – Gibbs Free Energy of oxidation

Consolidated tin samples (free from visible embedded coal ash particulates) were found to contain far fewer elements than coal itself. Tin standard samples (reduced from SnO_2 by H_2 with 3% H_2O) also contained certain elements. Only those elements with Nernst Potentials (an electrochemical expression of Gibbs Free Energy) lower than 0.9V at 1,000C were found in molten tin. This is a most important and intriguing finding that many elements which have been predicted to be harmful such as V, Mo, W, Cr, Nb having Nernst Potential higher than 0.9 V were found to be absent in molten tin at projected operating conditions.

The absence of V, Mo, Cr, Nb and W in consolidated tin samples (even though some of these elements were present in the coal and the SnO_2 starting material itself) suggests that these species were not in the form of elements (virtually all elemental metals were found to be able dissolved in molten tin), but in the form of compounds or oxides. In the coal tin reaction, the ratio of coal to SnO_2 was kept near stoichoimetric but with a slight excess on the reducing side, that means, the equivalent Nernst potentials to be around 0.9V to 1.0V (giving $CO:CO_2$ ratios at equilibrium from 50:50 to 95:5). This suggests only noble metals and those with Nernst Potentials less than a threshold (somewhere from 0.8V to 1.05V) would accumulate in molten tin and those elements which remain dissolved in tin such as Ag, Au, Pt, Ni, Cu, Pb, Sb, Bi, etc were generally expected to cause no harmful impact on the electrolyte YSZ.

Under certain conditions molten tin was projected to be capable to reduce or eliminate many harmful elements found in coal. Such purification properties makes Liquid Tin Anode solid oxide fuel cell unique and very appealing for direct coal conversion.

The Phase I study is rather preliminary with limited data. In the future a systematic study must be conducted to verify and to establish the correlation of partial oxygen pressure inside the tin-coal reactor (TCR) with solubility of coal impurities in molten tin.

(2.2) levels of coal impurities found in molten tin.

A more fundamental long term research project would allow definitive links between impurity levels and the thermodynamic/kinetic reactions of the TCR. It is clear that as the impurity level builds over time, the solubility limits of the impurities will influence the tin melt chemistry. Although estimating the total accumulated impurities seen by the TCR based on the coal feed rate is a trivial calculation, it is not possible to accurately estimate the amount of coal impurities absorbed into the tin melt from the current set of GDMS analysis. It is also not possible to accurately predict the effect of tin dilution in a full scale TCR due to the 0.2 wt% oxygen solubility limit. It is suggested that a full scale TCR may treat impurity rejection and segregation to the tin melt significantly differently since the tin melt will be dynamic, in contrast to the static tin melt in the laboratory TCR. Some of these questions will need to be explored in detailed in the future.

The consolidation process of reheating the tin to 450°C which results in removal or dramatic reduction in the amount of impurities present is a very significant observation. It is currently thought that this process demonstrates a simplistic method to clean unwanted impurities from the tin. However, the key questions that remain are:

> A) what is the critical concentration of impurities in the tin melt that would cause significant damage to the fuel cell stack, and thus warrant cleaning of the tin melt; and,
>
> B) How many mega-watt hours of operation result in a critical concentration of impurities?

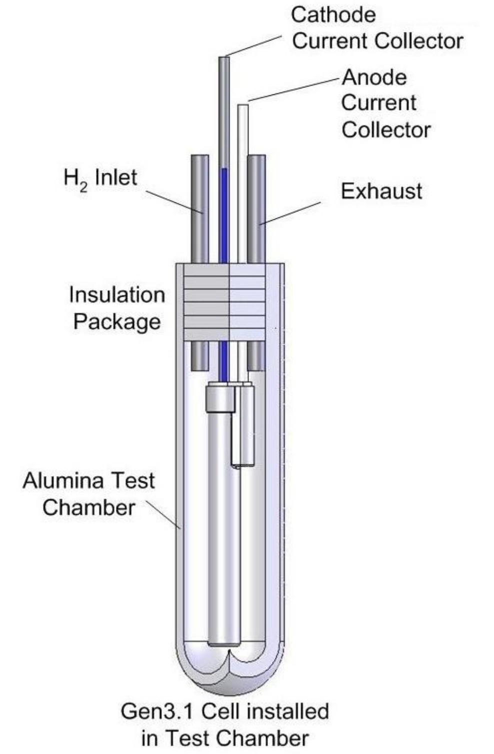
To start to understand the scope of study for cell degradation due to coal impurity segregation to the tin melt, it was agreed that CellTech Power would conduct limited electrochemical testing using tin spiked with coal impurities.

Coal tin reactor – electrochemical testing

The electrochemical testing was conducted on the current generation, Gen3.1, of CellTech Power's Liquid Tin Anode – Solid Oxide Fuel Cell. The Gen3.1 cell produces 3-5 W of power using 30 g of tin. Normalizing for peak power with respect to weight gives 167 $mW.g^{-1}$. The key difference between the Gen3.1 cell and the proposed mega-watt coal power plant is the separation of the electrochemical reaction from the chemical reaction – tin being confined and stationary in Gen 3.1 cell vs. being mobile and circulated in a MW scale coal plant. In the proposed power plant, the electrochemical reaction of oxygen ions with tin will occur at the fuel cell stack. The tin containing tin oxide species would then be transported from the fuel cell stack to the Tin-Coal Reactor. The coal would be fed into the TCR to reduce the tin oxide species back to tin. The loop would be completed by transporting refreshed tin back to the fuel cell stack. In contrast, the current Gen3.1 cell relies on the tin oxide concentration gradient across the 500 µm tin layer to drive diffusion of the tin oxide species from the electrolyte interface to the fuel interface. Given the tin thickness in the Gen3.1 cell is 500 micron compared to an undefined but substantially longer path from fuel to electrolyte in the power plant it is suggested that the power output *per gram of tin* for the power plant will be at least an order of magnitude less than the 167 $mW.g^{-1}$ for the Gen3.1 cell.

The estimated difference between the Gen3.1 cell and the mega-watt power plant in terms of watts per gram tin was the basis for deciding the initial impurity concentrations for electrochemical testing, though such estimation was somewhat arbitrary. Assuming an operational power density of 0.2 $W.cm^{-2}$ and using the active area of a Gen3.1 cell 30 cm^2 the amount of coal consumed can be calculated and therefore the amount of coal impurities exposed to the tin. The detailed calculation is presented in Appendix H of Reference 2. One extreme of such estimate was that all of the impurities present in the coal were segregated to the tin, thus simulating a worst case scenario. After discussing these levels with NETL it was decided that a factor of 10 dilution should be applied for the initial testing. For practical/operational reason the impurities were added to a 1/3 of the tin charge as metal powder and the rest 2/3 of the tin charge was pure tin. It was assumed that a homogenous mixture formed over time, although this has not yet been confirmed. The loading of tin into the cell and heating of the cell to operational temperature mimicked the standard testing methodology of Gen3.1 cells at CellTech.

The Gen3.1 cells and their setup is shown in Figure 11. The tin used in the Gen3.1 cells was spiked with 5 elements that are present in coal as impurities, V, Cr, As, Nb, and Mo. CellTech Power's previous experience with tin alloying and proprietary modeling was used to select the 5 most detrimental impurities present in the coal. The spiking levels were 400ppm for V, Cr and As, while 200ppm was used for Nb and Mo based on the calculation of between 1 and 10 years of operation as described above. As such, this test was a worst case scenario. The cell was run on hydrogen and air.



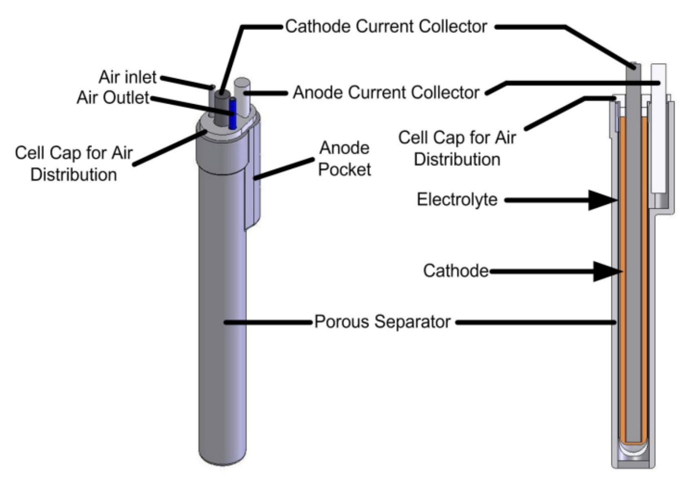


Figure 11: Typical setup of a Gen3.1 for operation on hydrogen and air. For DOE electrochemical experimentation, the coal impurities were mixed with the tin powder before testing. In this experiment the tin is static opposed to a circulating loop between the TCR and fuel cell stack in the megawatt power plant.

The purpose of the electrochemical testing was to observe decay in the cell performance when subjected to a large amount of impurities in an accelerated longevity test. Testing of standard Gen3.1 cells has allowed a baseline for cell degradation over time to be collected. To normalize out cell degradation due to contamination from other sources the DOE cells were tested in a similar manner to standard Gen3.1 cells. For longevity testing, the experimental methodology is to characterize the performance of the cell with an initial IV curve. Then the cell is loaded at a constant current while monitoring its cell voltage. The value of current is set at 60% of the maximum stable current determined from the IV curve, giving 4.2A as shown in Figure 12.

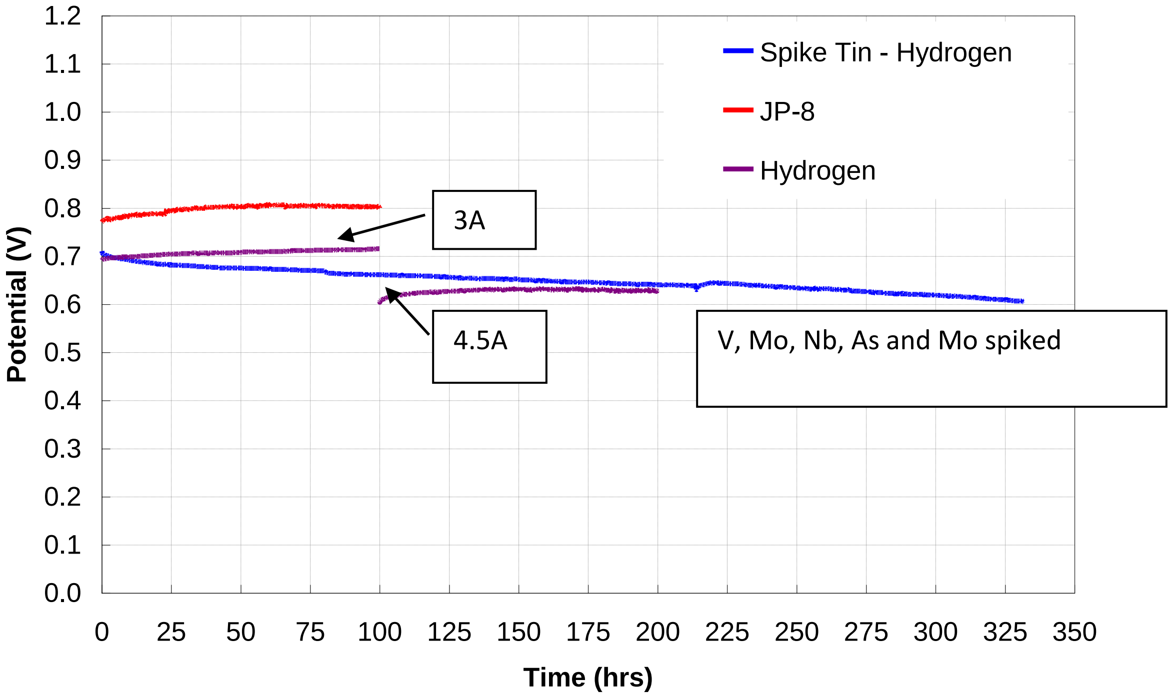


Figure 12: The potential decay profile as a function of time for a load of 4.2 Amps which was 60% of the peak load for the initial IV curve on this cell.

As the time this report is being written, the spiked tin cell has continuously run for more than 400 hours. After the first 24 hrs, degradation of its cell voltage (Delta V/V) became stable, at decay rate of about 30% / 1000hrs. As a comparison, Gen 3.1 cells had their voltage decay rates below detection limits or less than 0.1%/1000 hrs with JP-8 and hydrogen as fuels and regular tin without spiking.

The spiked five elements (As, V, Mo, Cr and Nb) had a total concentration of 1,600ppm. Indeed these five elements as a whole were found to cause degradation of the cell performance. Post mortem analysis has yet to be performed to determine the cause. The impact of individual elements on the decay rate should be studied in future programs such as Phase II. Nevertheless this study has established a baseline for impact of coal contaminants on cell performance (likely due to electrolyte degradation but yet to be confirmed).

The voltage decay rate is estimated as:

0.02% per 1,000hours per 1 ppm (harmful elements)

For example, it suggests that in order to maintain 5-year (43,800 hrs) continuous plant operation with less than 10% fuel cell degradation, the maximum concentration of harmful elements (the ten elements) in molten tin would have to be less than 11 ppm.

Task 3- System Analysis

The baseline flowsheet developed in Task 1 was used as the basis for plant-level performance and cost estimates. In order to make the results of the system performance analysis consistent with DOE's analyses of other coal based systems, the detailed system analysis for LTA Direct Coal was conducted by Jan Thijssen, a consultant who has conducted similar assessments on behalf of NETL. The scope of the analysis is a 250W-500 MW Greenfield plant. Multiple analyses have been conducted on different plant sizes and fuel cell conditions (250MW, 500MW, different cell operational voltages, etc.). The basis of assumptions for the system efficiency and cost analyses lies in NETL's 2007 "Cost and Performance Baseline for Fossil Energy Plants" (August 2007) including coal composition and the approach to Cost of Electricity calculations. Performance assumptions for LTASOFC cells and stacks were based on CellTech's baseline assumptions:

- Oxygen content of melt: 0 – 0.1% (wt% oxygen, fuel cell inlet – outlet)
- Cell voltage: 0.78 V @ 200 mW/cm^2
- Conditions: 1000 °C, atmospheric pressure
- Carbon: CO/CO_2 = 1/5 (equilibrium)
- Hydrogen: H_2/H_2O = ¼
- Sulfur: 80% to H_2S (gas phase), remainder dissolves in melt
- Nitrogen: 100% to N_2 (gas phase)
- Oxides: 100% partition to floating slag (removed periodically)
- Metals: based on equilibrium partition between gas and melt

System performance predicted by thermodynamic analysis is summarized in Table 3. Thermodynamic analysis of the system predicts a 61% to 63% system efficiency including energy requirements for carbon capture. The carbon emissions are also very low, 30g/kWh$_{net}$, due to the ability of the LTA-SOFC to produce an undiluted carbon dioxide exhaust stream (nitrogen free) which can be easily handled for carbon capture operations. The Sankey diagram shown in Figure 13 illustrates the importance of capturing waste heat to maintain high efficiency while capturing carbon. The independent analysis conducted in Task 3 has shown that the high system level efficiency is achievable by LTA technology in the context of high carbon capture.

The Phase II project will look at the technical risk by developing a number of alternative flow sheets. The oxygen solubility, tin circulation, coal impurities solubility in molten tin, cell polarization losses, system heat losses and taking advantage of existing cell technology are the important parameters in the Phase II. For example: the injection of the TCR exhaust gas directly into the fuel cell tin containment area may offer several advantages. This approach would reduce the effect of tin solubility and heat losses on the system by allowing localized reduction of the tin which will reduce the flow rate of tin between the TCR and stack. A lower tin velocity would result in a less turbulent flow and thus lower heat losses through the pipes. The other Phase II alternative would be a direct coal conversion LTA-SOFC using current cell configuration (Gen 3.1) of which tin was a thin layer sandwiched between a ceramic porous separator and the electrolyte, instead of circulation of tin.

Table 3: The projected system performance of a 250 MW LTA-SOFC predicts 63% efficiency.

Projected System Performance		
Fuel Cell Stack	Maximum O Content (mass/mass)	0.1%
	Cathode Stoichiometry	1.22
	Stack Temperature	1000°C
	Air Inlet Temperature	500°C
	Cell Voltage	0.69 V
	Fuel Cell Gross Power	250 MW
TCR	Coal/O (mass/mass)	0.51 kg/kg
	Anode Recycle	75%
	Temperature Drop	26.5°C
BoP	Steam Cycle Efficiency	40%
	Steam Cycle Power	45 MW
System	Parasitic Load	13 MW
	Exhaust Temperature	180°C
	System Efficiency (HHV Basis)	63.0%
	Carbon Emissions	29 g/kWh

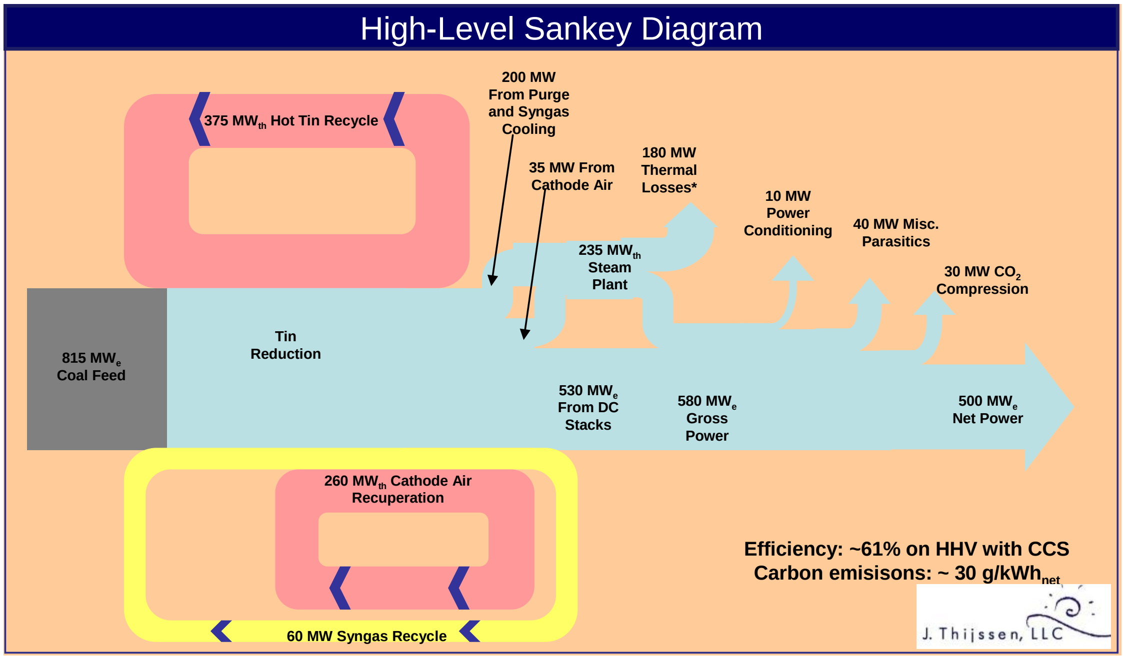


Figure 13: A high level Sankey diagram of a 500 MW fuel cell power plant illustrates that high (61%) efficiency is possible even with a high degree of CCS, but a considerable amount of thermal circulation and tin circulation is required.

Task 4 – Identification of Risk Areas

The purpose of this task was to identify some of the most significant technical risks to developing and commercializing a full scale Direct Coal fuel cell. CellTech Power is conducting two Direct Coal LTA-SOFC programs for DOE. The risk identification process described here focuses on the two technical areas which are the subject of these combined programs:

1) Scalability to MW power plant – 1000W single cell design and
2) Coal impurities and their impacts on electrolyte YSZ.

This was the first step in a continuous process of identifying and addressing the multiple levels of challenges which any advanced technology like the Direct Coal LTA-SOFC faces. In addition to the cell-level technical risk which is discussed here, there are other risks which will be addressed during later stages of development including:

- Coal impurities and their impacts on fuel cell components other than electrolyte (anode current collectors, sealing, cap, anode chamber, pipes, etc.);
- Other technical risks including stack and system level materials, design and performance uncertainties (for instance risks associated with development of a tin/coal reactor, tin circulation, electric current interruption, etc.);
- Cost risks associated with achieving the necessary cost structure to be competitive. These risks may exist at the cell, stack and system level.

- Market development risks such as:
  - The competitive performance of Direct Coal Liquid Tin Anode systems compared with other Direct Coal technologies and other power generation technologies.
  - The achievement of the necessary financial resources required to develop test and commercialize this technology.
  - The regulatory and government incentive environment for coal power, carbon emissions and competitive technologies.

The cell-level risk factors for large scale coal plants can be placed in two major categories:

(1) The technical risk associated with scaling known LTA-SOFC cell designs up to one kilowatt per cell.

(2) Risk factors relating to fuel, especially impurities in coal, and how they will affect fuel cell performance. These are expected to be substantial. The proposed coal plant process flowsheet and the results of impurity testing in Task 2 offers the very important prospect that tin itself may act as an impurity barrier. Coal impurities are expected to have little impact on tin itself and tin oxide reduction. However it is still uncertain whether any impurities in coal will be wholly or partially dissolved in tin and be subsequently transferred to the fuel cell stack. If indeed harmful impurities are dissolved in tin, mitigating techniques could involve a purification process (pressure swing, temperature swing, purging, or chemical precipitation, ect.) that would remove them from tin before being transferred to the stack. To our knowledge no scientific studies other than the work now ongoing at CellTech have been conducted to address these concerns. We shall identify these risk factors in the proposed work.

Table 4 Risk items associated with LTA cell scale-up

Risk Items Cell Performance	Description and Consequence of Risk	Recommended Actions to Further Define Risk	Potential Actions to Mitigate Risk
1. Cell lifetime	Cell cannot provide threshold performance for the specified lifetime. **DOE Goal: 40,000 hrs**	Long term single cell testing Build and test small scale cells	Materials improvement. CellTech design uses cathode, electrolyte, sealing materials which are common to other SOFC and will benefit from ongoing R&D by SECA etc.
2. Cell power density	Failure to achieve target power density will result in larger, more costly stacks and systems. **Goal: 200mW/cm^2 @0.7 V**	Build and test a full scale cell Continue the development of small scale technology which has already achieved 170 mW/cm^2 on hydrocarbon fuel.	Improved cell design Improved electrolyte and cathode materials
3. Cell Internal resistance	Failure to achieve required cell resistance will result in more costly stacks and systems, and lower plant efficiency **Goal: 51 micro-ohms**	Detailed cell analytical model Materials property testing Build and test a full scale cell	Improved current collector materials and design. Cell design to reduce current path
4. Cell Interconnect	Common, conductive tin anode may make it difficult to place cells in series. Without build up of stack voltage, amperage may be technically unfeasible **Goal: Stack voltage of 50 V min**	Technical problem is clearly identified. The risk is that design measures may not be workable.	Potential cell design changes to allow isolation of tin in-between cells. Bipolar flat cell design using tin as interconnect

Table 5 Risk items associated with Coal Contamination

Risk Items Contamination	Description and Consequence of Risk	Potential Actions to Further Define Risk	Potential Actions to Mitigate Risk
1. Coal impurities attack cell electrolyte	Coal impurities dissolved in tin attack YSZ electrolyte causing degraded cell performance and/or mechanical failure. **Goal: Determined by cell lifetime goal.**	Electrochemical testing at longer time scales to evaluate YSZ interaction with contaminated tin. Coal-tin chemical testing to further define contamination levels in tin.	Impurity removal such as vacuum stripping or sparge stripping, or Precipitation. Improved electrolyte materials or processing to improve resistance to degradation. Thicker electrolyte.
2. Coal impurities attack other components exposed to anode environment	Coal impurities dissolved in tin attack anode current collector or seals exposed to tin or anode gas environment causing degraded cell performance and/or mechanical failure. **Goal: Determined by cell lifetime goal.**	Long term electrochemical testing to evaluate anode current collector interaction with contaminated tin. Coal-tin chemical testing to further define contamination levels in tin (some testing has already been conducted). Chemical testing to evaluate component interaction with contaminated tin or anode headgas.	Impurity removal such as vacuum stripping or sparge stripping, or precipitation Improved component materials which are resistant to degradation. Cell design to isolate vulnerable components from contact with tin or anode environment.
3. Coal impurities degrade tin	Tin conductivity or oxygen solubility may be affected by accumulation of impurities. **Goal: tin lifetime of 40,000 hours**	Analysis of equilibrium levels of contaminants in tin at operating conditions. Long-term coal/tin testing with periodic analysis of tin.	Impurity removal such as physical filtering, vacuum stripping or sparge stripping. Replacement of tin. Potential for re-refining spent tin.

The listed risk items and mitigation techniques point to the importance of further, longer duration testing in establishing the durability of cell components. Thus, the focus of the proposed Phase II efforts (under this SBIR and other DOE funded programs) is on obtaining longer duration test data on critical components (electrolyte, anode current collector, cap etc.) that are a) unique to the LTA design and b) key to long cell life.

Task 5 Development Plan

Commercialization of Direct Coal power plant technology using LTA will require very large resources and a significant amount of time. CellTech has developed a stage-gate plan for Direct Coal development which is shown in Figure 14. Several validation and risk reduction programs have already been completed with most of the results discussed in Tasks 1-4. The proposed Phase II work will continue risk reduction activities by addressing key durability issues. Upon completion of Phase I and II, CellTech Power will take advantage of the technical progress made on Gen 3.1 design, to implement commercialization of small power (1 kwatt) generators. We envision the first commercial LTA-SOFC will be for generators in the range of 500W. Next, a bench scale model of the complete Direct Coal flowsheet will be constructed, using Gen 3.1 LTA cell hardware and an experimental Tin-Coal Reactor. Following bench scale validation of performance and the Tin-Coal Reactor, a subscale 50 kW design will be built to validate process parameters at a realistic scale. A first commercialization step will follow at the 100 kW to 5 MW power range, probably using biomass as a distributed fuel resource. This step and the final step of demonstrating a 100+ MW Direct Coal powerplant will be taken with industrial partners.

Bench scale Direct Coal activities over the next several years will be significantly aided by CellTech's small generator development activities. The impurities and performance testing during Phase I of this SBIR have demonstrated the value of having actual LTA cell hardware from CellTech's small generator programs available for testing. The development plan places an emphasis on near-term actions, including implementation of activities for demonstrating feasibility at pilot scale and addressing risk areas indentified in this SBIR. More details on CellTech's plan for commercialization of LTA-SOFC technology is provided in the separate section of this proposal dedicated to Commercialization.

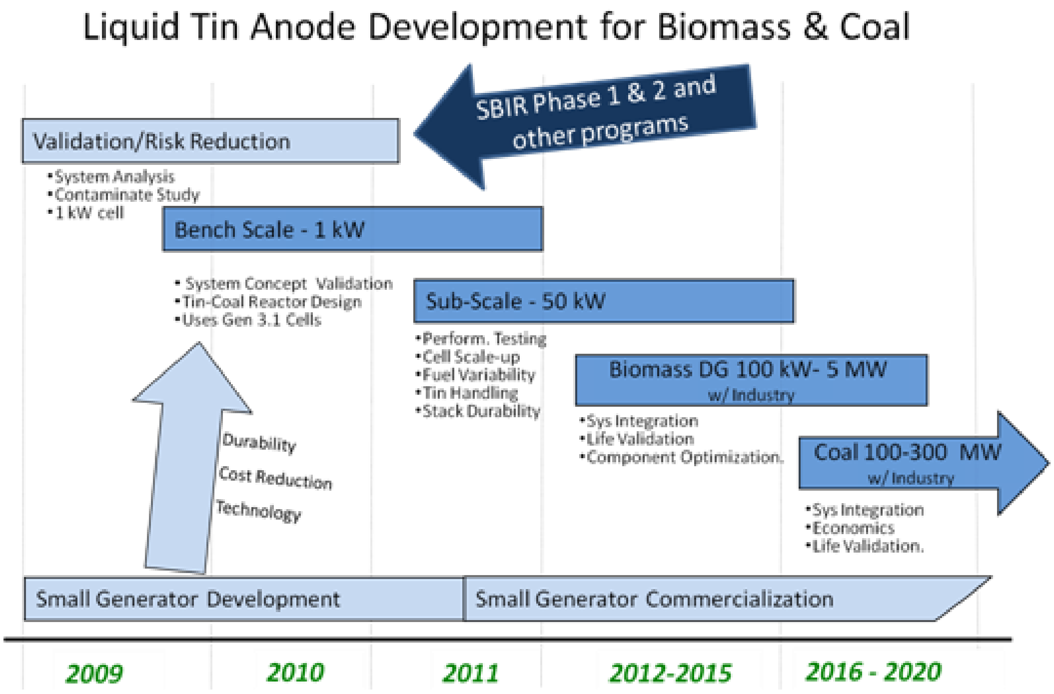


Figure 14 CellTech has developed a phased approach to commercializing Direct Coal technology. A significant element of this plan is the ability of the LTA fuel cell to address earlier commercial markets such as portable power, creating technical and commercial experience which will benefit the Direct Coal commercialization effort.

Phase II Results

Based on the Phase I development, the objective established for Phase II was to develop LTA cell technology which addresses the key issue of LTA cell durability in a coal environment. The method of identifying durability issues is through long-term testing of single cells. In order to accomplish this testing, test stands are required which can reliably maintain test conditions over the duration of testing. Also, more information, is required regarding the behavior of impurities likely to be present in tin, in order to establish the level of contaminant spiking of elements of interest. This impurity data will be obtained by analysis and test. Cell testing with single component spiking will allow the identification of specific contaminants which cause degradation and allow evaluation of degradation mechanisms. Finally, the durability data and failure mechanism knowledge will be used to propose materials and flowsheet changes to minimize durability impacts. These changes can also be evaluated on the test stands constructed during Phase II.

Task 2 - Study coal contaminants and their solubility in tin

CellTech's proprietary analytical techniques for predicting which elements will cause electrolyte damage have been presented during thePhase I program. The Ionic Oxide Model which predicts Lattice Coulombic Energy (CE) has successfully predicted doped zirconia electrolyte phase stability in the presence of other elements. Based on this analysis, the metallic elements of posing the greatest concern to the electrolyte were identified as: As, Se, V, Cr, Mo, Nb, Ta, W, Mn and U. In the LTA-SOFC, the electrolyte is protected by a liquid tin layer which will block gas phase transport. The question is whether these elements are soluble or remain in molten tin at the conditions of the tin-coal reactor will drive the scale of mitigation strategies. The testing in the second phase was expanded to include non-metallic elements of halogens (F, Cl, Br, I) as well as S,Si and P.

Coal contamination solubility in tin may pose a threat to the ceramic components, namely the stabilized zirconium oxide electrolyte and current collection, over time. For the solubility analysis, each concerned element was spiked into tin and was exposed to conditions similar to tin-coal reactor. One difference from the full scale concept is that the metallic elements were spiked in the metallic form. It is more likely that the elements in question will be in a compound form and retain an oxidized state. Contaminant spiking levels were set at 4,000ppm for metallic elements and compounds of the other elements. The initial contaminant amounts are shown in Table 1. Powders of the contaminant and tin were pre-blended and put into a YSZ crucible for the test. Figure 15 shows the experimental

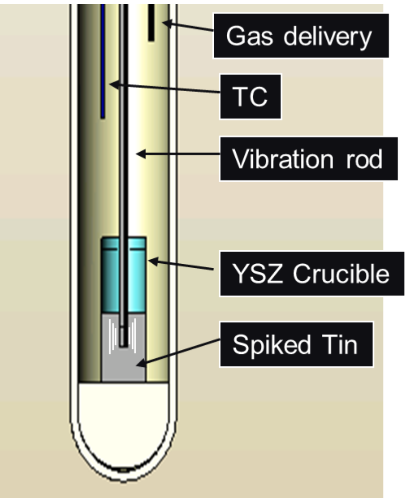


Figure 15 - Experimental configuration for contaminant solubility testing.

configuration. Humidified H_2 (with 1% H_2O) was introduced into the chamber to maintain a 1.1V environment. The 1.1V environment was selected since it represents the least oxidized condition for the tin returning from the tin coal reactor to the electrochemical pod. As such, this represents the last chance to oxidize any contaminants.

Samples were cut from the center of the tin slugs and analyzed by ICP-OES. Table 6 shows the residual contaminant solubility results from the ICP testing. In the same table, the analysis from the tin is presented for comparison.

Spiked Element	Spiked as	Initial amount (ppm wt)	ICP-OES Results (ppm wt)	Spiked Element	Pure Sn GDMS results (ppm wt)
Cr	metal	4060	1098	Cr	0.02
V	metal	4039	10	V	< 0.001
Mo	metal	4000	9	Mo	< 0.01
Nb	metal	4038	115	Nb	< 0.005
As	metal	4019	2535	As	1
Mn	metal	4020	2405	Mn	0.01
W	metal	4020	60	W	< 0.01
Ta	metal	4000	8	Ta	< 5
Se	metal	4020	44.7	Se	< 0.01
Si	element	4000	5	Si	< 0.01
Cl	NaCl	1732	n/a	Cl	< 0.01
S	SnS	862	8	S	2.8
P	Sn_3P_4	652	203	P	0.08
F	$SnPO_3F$	347	n/a	F	< 0.5
Br	$SnBr_2$	2323	n/a	Br	< 0.05
I	SnI_2	2760	n/a	I	< 0.05

Table 6 - Element solubility in tin at 1.1V conditions

The visual results can be categorized into 1) visible oxide particulates, 2)surface oxide with no soluble contaminant and 3) no visible contaminant. Examples of the discrete oxide particulates include: Cr and Ta. Condition 2 was shown by Mn, As, V, Nb and Se. The remainders of the elements were very clean in appearance. Figure 16, Figure 17 and Figure 18 show examples of the tin solubility samples.

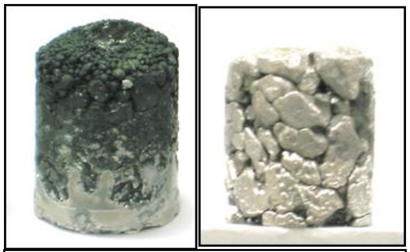


Figure 17 - Chrome (left) and tantalum (right) slugs showing separated tin.

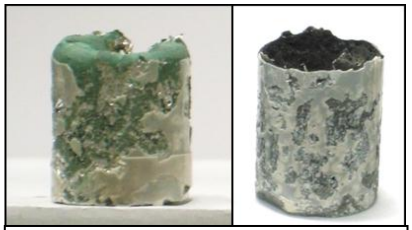


Figure 16 - Manganese (left) and vanadium(right) results having surface coating.

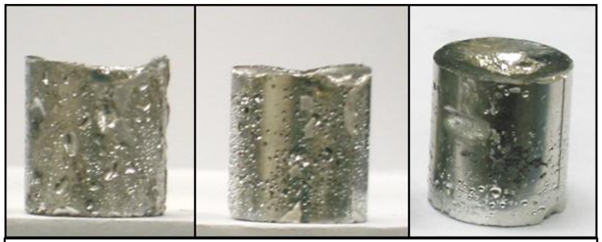


Figure 18 - Tungsten(left), selenium(middle) and Molybdenum(right) showing very little evidence of the contaminants.

Table 7 presents the data sorted by descending contaminant level in comparison with the amounts of the contaminants found in two coal sources, Wyodak (DECS-26) and Illinois #6 (DECS-24) obtained from the Penn State Coal Bank and Database. The highest residual element concentrations in tin belong to As, Mn and Cr. These elements are present in both coal samples, but in lower concentrations than the initial spiking levels. Phosphorous shows similar levels within the coal, indicating that the retention of phosphorous could be a concern.

Contaminant	1.1 V starting contaminant (ppm)	1.1 V final contaminant (ppm)	1.1 V remaining contaminant (%)	Wyodak DECS-26 contaminant levels (ppm)	Illinois #6 DECS-24 contaminant levels (ppm)
As	4019	2535	63.07	1	2
Mn	4020	2405	59.83	10	53
Cr	4060	1098	27.05	3	23
P	652	203	31.15	260	170
Nb	4038	115	2.85		
W	4020	60	1.49		
Se	4020	44.7	1.11	2	4
V	4039	10	0.25	11	27
Mo	4000	9	0.23		
S	862	8	0.93	4300	55300
Ta	4000	8	0.20		
Si	4000	5	0.13	10000	26000
Cl	1732	n/a			1400
F	347	n/a			
Br	2323	n/a			
I	2760	n/a			

Table 7 - Residual contaminant levels compared to Wyodak and Illinois coal contaminants.

The contaminant exclusion from the liquid tin was tested at a single condition and demonstrated that the elements are reduced. The effectiveness of contaminant exclusion will be increased with larger scale tin circulation and cell operating conditions. The form of contaminant tested represents the most drastic case. Appendix A lists coal elemental contaminants in their mineral form. The predominant forms are oxides, carbonates and sulfur compounds.

Task 3 - Conduct long-term testing of key contaminants in LTA-SOFC cells.

The effect of contaminant accumulation in the TCR concept on the longevity of cell components under operating conditions is critical to understand in order to develop mitigation strategies for stable long term operation. Individual LTA-SOFC cells spiked with contaminant levels determined by Task 2 were tested under a constant current condition of 4.8 amps, or > 60% maximum current, for a target of 100 hours or until instability. Table 8 summarizes the test results for each contaminant, in descending order, for run time, percent degradation and percentage of maximum current. Graphical presentation of the test data is shown in Figure 19 and Figure 20 for the metallic and non-metallic elements respectively.

Contaminant	Spiked contaminant (ppm)	Short duration electrochemical test (hrs / degradation)		Cell load (% max current)
Pure Tin		**100**	**2 %**	**Load = 4.8A (64% max)**
As	2,535	47.6	29 %	Load = 4.8A (60% max)
Mn	2,405	10	2.5 %	Load – 1.25A (36% max)
Cr	1,098	23.5	13%	Load = 4.8A (80% max)
P	203	0.2		Load = 0.5A
Nb	115	100	34 %	Load = 4.8A (69% max)
W	60	100	8 %	Load = 4.8A (69% max)
Se	45	100	3 %	Load = 4.8A (56% max)
V	10	65	10 %	Load = 4.8 A (64% max)
Mo	9	65	30 %	Load = 4.8A (69% max)
Ta	8	100	5 %	Load = 4.8A (60% max)
S	8	70.7	4 %	Load = 4.8A (80% max)
Si	5	22.8	12 %	Load = 4.8A (56% max)
Cl	500	100	6.5 %	Load = 4.8A (56% max)
Br	500	100	10 %	Load = 4.8A (64% max)
I	500	1.3	0.7 %	Load = 2 A (40% max)
F	500	100	5.5 %	Load = 4.8A (56% max)

Table 8 - Cell test results for 100 hour contaminant performance tests.

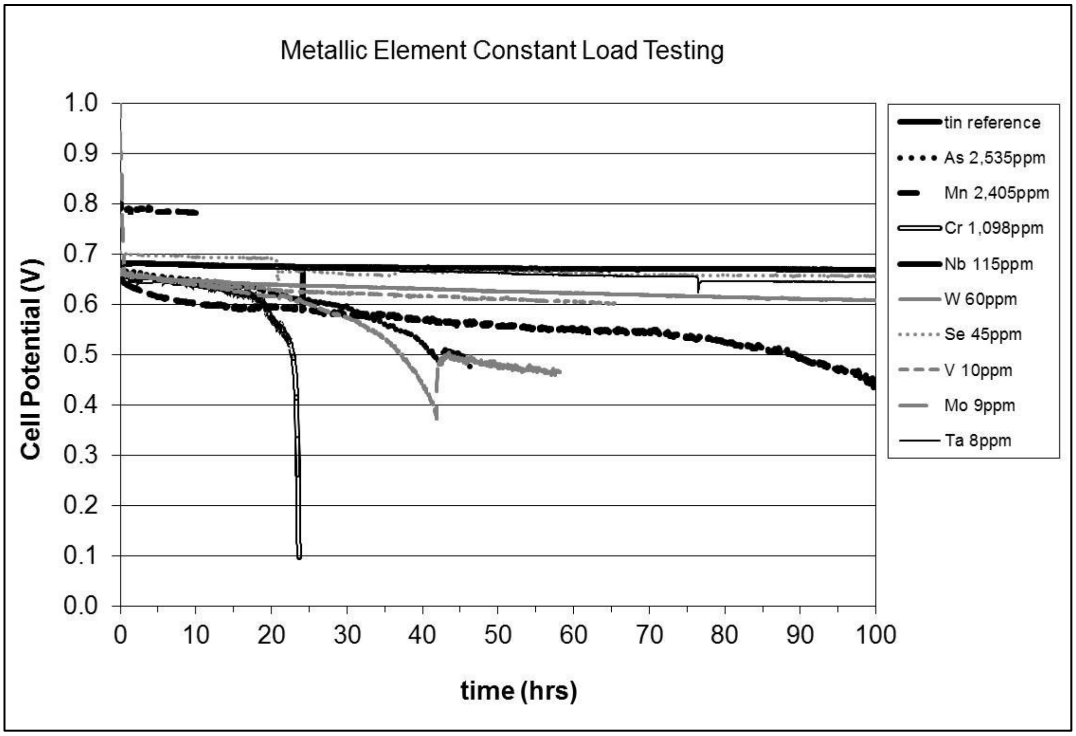


Figure 19 - Constant current testing voltage curves for metallic contaminants.

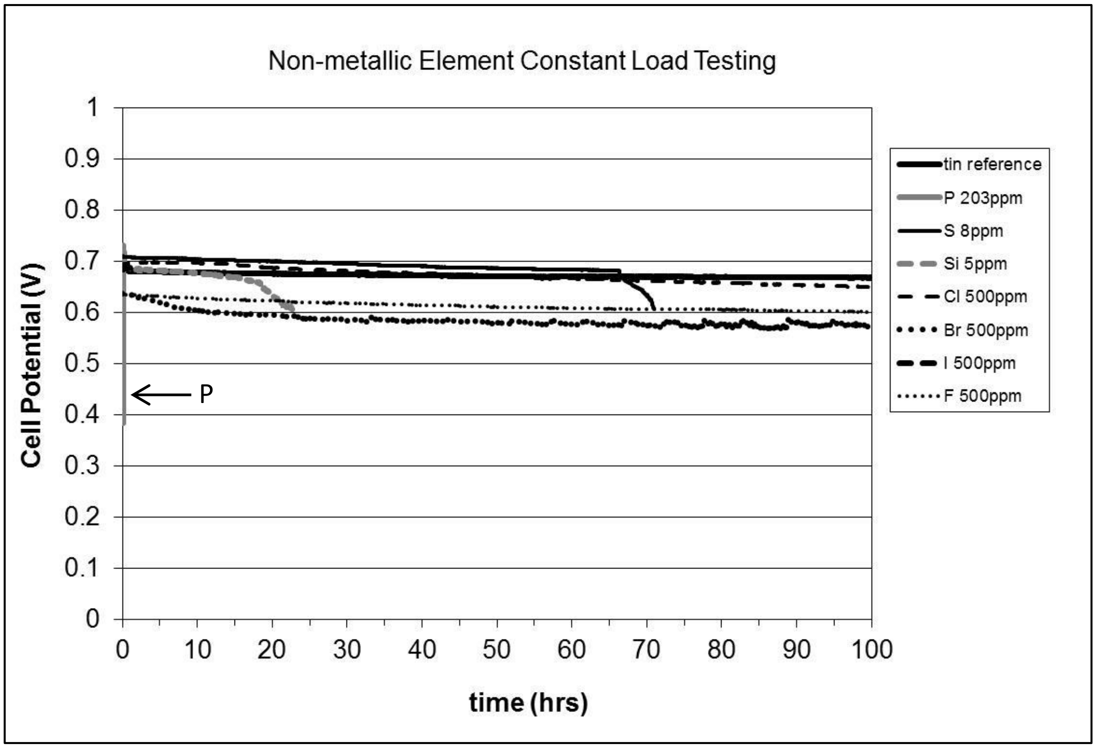


Figure 20 - Constant current testing voltage curves for non-metallic elements.

The testing of the ‘harmful’ elements to the LTA-SOFC electrolyte did show an impact on the long term performance. Figure 21 shows second phase crystalline deposits on the electrolyte surface for manganese and phosphorous. The identification of the degradation mechanisms enables strategies for successful contamination mitigation in future programs.

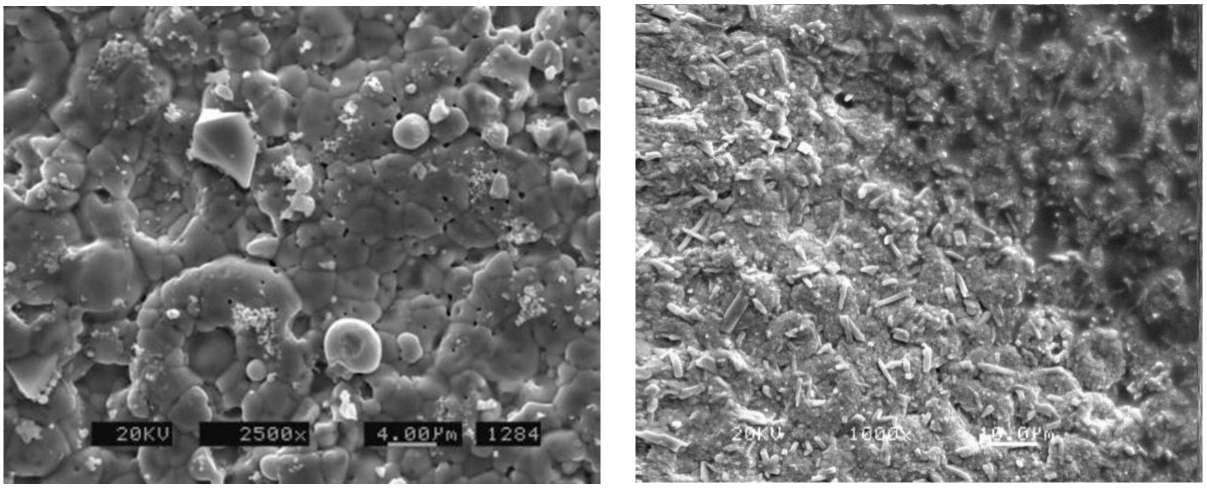
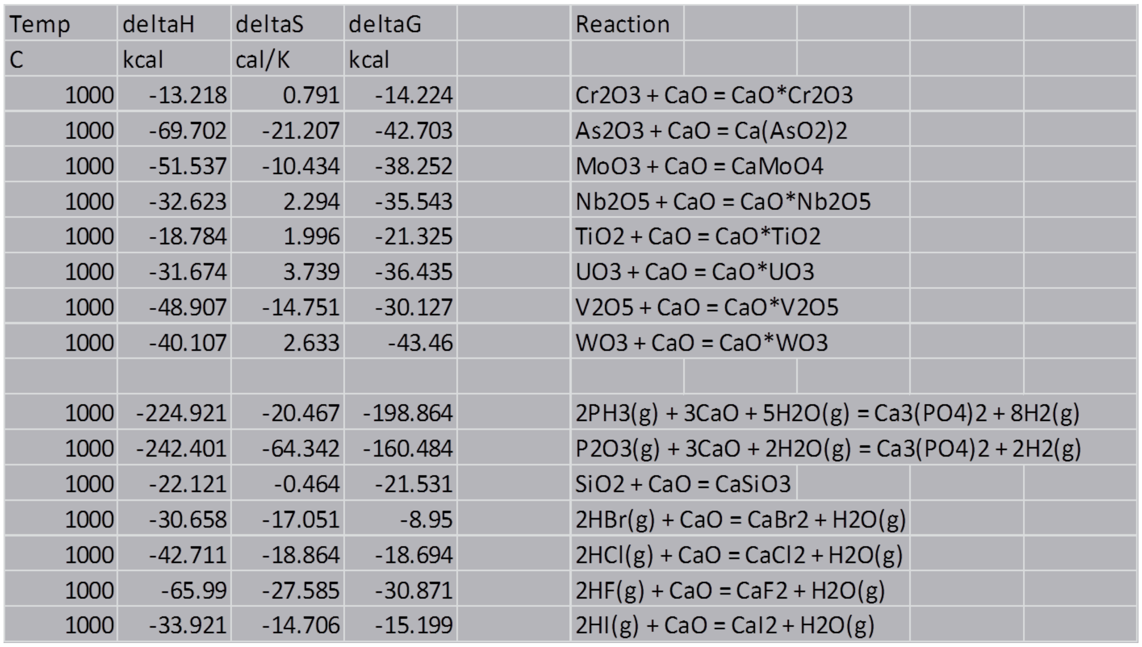


Figure 21 - Second phase on electrolyte surface for manganese(a) and phosphorous(b).

Contaminant Mitigation Strategies:

The mechanism of electrolyte degradation is the removal of the stabilizing ions, such as yttrium. One reasonable approach to neutralize the harmful elements is to react them out with calcium before they can interact with the electrolyte. Table 9 shows that at 1000°C, it is thermodynamically favorable for all the elements tested to form compounds with calcium.

Experimental results showed that calcium carbonate, or calcium oxide at high temperatures, is successful in reducing the residual phosphorous amount in tin from 216ppm to 60 ppm. In another experiment, CaO was mixed with several contaminant oxide powders. Analysis by xray diffraction showed that the samples run in an oxidizing environment completely reacted with the CaO, but samples run in a reducing environment only partially reacted. The concept of the calcium capture has been demonstrated on a small scale to be simple, inexpensive and easily integrated into the architecture of the LTA-SOFC. Future investigation and verification will need to address the effective window in terms of oxygen partial pressure and practical mechanisms to scale the approach.



Temp	deltaH	deltaS	deltaG		Reaction
C	kcal	cal/K	kcal		
1000	-13.218	0.791	-14.224		Cr2O3 + CaO = CaO*Cr2O3
1000	-69.702	-21.207	-42.703		As2O3 + CaO = Ca(AsO2)2
1000	-51.537	-10.434	-38.252		MoO3 + CaO = CaMoO4
1000	-32.623	2.294	-35.543		Nb2O5 + CaO = CaO*Nb2O5
1000	-18.784	1.996	-21.325		TiO2 + CaO = CaO*TiO2
1000	-31.674	3.739	-36.435		UO3 + CaO = CaO*UO3
1000	-48.907	-14.751	-30.127		V2O5 + CaO = CaO*V2O5
1000	-40.107	2.633	-43.46		WO3 + CaO = CaO*WO3
1000	-224.921	-20.467	-198.864		2PH3(g) + 3CaO + 5H2O(g) = Ca3(PO4)2 + 8H2(g)
1000	-242.401	-64.342	-160.484		P2O3(g) + 3CaO + 2H2O(g) = Ca3(PO4)2 + 2H2(g)
1000	-22.121	-0.464	-21.531		SiO2 + CaO = CaSiO3
1000	-30.658	-17.051	-8.95		2HBr(g) + CaO = CaBr2 + H2O(g)
1000	-42.711	-18.864	-18.694		2HCl(g) + CaO = CaCl2 + H2O(g)
1000	-65.99	-27.585	-30.871		2HF(g) + CaO = CaF2 + H2O(g)
1000	-33.921	-14.706	-15.199		2HI(g) + CaO = CaI2 + H2O(g)

Table 9 - Thermodynamic analysis results for contaminant-calcium reactions.

Conclusions

Coal may contain each element existed on the earth. In this study only these metallic elements of As, Se, V, Cr, Mo, Nb, Ta, W, Mn and U, and non metallic elements P have been predicted based on CellTech Power's modeling as potential harmful components toward electrolyte YSZ;

Molten tin has been demonstrated to have the ability to exclude or to reduce these potential harmful elements at liquid tin anode SOFC operational conditions, i.e. OCV from 0.8 to 1.06 volt. That means any harmful metallic element in coal would be eliminated or its amount would be reduced in molten tin anode;

These harmful elements when intentionally added to the tin anode with the highest possible concentration indeed demonstrated various degrees of degradation of fuel cell performance;

A mitigation strategy of using CaO as a getter or eliminator of these harmful elements has been evaluated and initial modeling results and experimental data supported such approach;

Therefore Liquid Tin Anode (LTA) SOFC has been demonstrated as a potential viable direct coal conversion fuel cell with a projected fuel efficiency of 61%.

APPENDIX A

Table 1. Common minerals found in coal and their elemental compositions.

[Although more than 120 different minerals have been identified in coal samples, only about 33 of these occur in most coal samples; of these, only about 8 generally are abundant enough to be considered as major constituents. Data from R.B. Finkelman (U.S. Geological Survey, written commun., 2000).]

Mineral name	**Chemical composition**	**Remarks**

Major Mineral Constituents
(In general order of abundance)

Quartz	SiO_2	
Clay Minerals:		
Kaolinite	$Al_2Si_2O_5(OH)_4$	
Illite	$KAl_4(AlSi_7O_{20})\,(OH)_4$	
Montmorillonite	$(1/2\ Ca,Na)_{0.7}\,(Al,Mg,Fe)_4\,[(Si,Al)_4\,O_{10}\,]_2\,(OH)_4 \cdot nH_2O$	
Chlorite	$(Mg,Al,Fe)_{12}[(Si,Al)_8\,O_{20}]\,(OH)_{16}$	May have Mn. (Clays may also contain Be, Cr, Ni, and other trace elements.)
Pyrite	FeS_2	May contain As, Cd, Co, Hg, Ni, Sb, and Se.
Calcite	$CaCO_3$	
Siderite	$FeCO_3$	May contain Mn.

Minor Mineral Constituents

Analcime	$NaAlSi_2O_6 \cdot H_2O$	
Apatite	$Ca_5(PO_4)_3\,(OH,F,Cl)$	
Barite	$BaSO_4$	
Chalcopyrite	$CuFeS_2$	
Clausthalite	PbS	
Crandallite Group		
Crandallite	$CaAl_3(PO_4)_2\,(OH)_5 \cdot H_2O$	
Florencite	$CeAl_3(PO_4)_2(OH)_6$	
Gorceixite	$BaAl_3(PO_4)_2\,(OH)_5 \cdot H_2O$	
Goyazite	$SrAl_3(PO_4)_2\,(OH)_5 \cdot H_2O$	
Dolomite	$CaMg(CO_3)_2$	

Feldspars	(Ca,K,Na)$AlSi_3O_8$	
Galena	PbS	
Marcasite	FeS_2	May contain same elements as pyrite.
Monazite	(Ce,La,Y,Th,Nd)PO_4	
Rutile/Anatase	TiO_2	
Sphalerite	ZnS	May contain Cd.
Xenotime	YPO_4	
Zircon	Zr[SiO_4]	

Trace Mineral Constituents

Chromite	$FeCr_2O_4$	
Gibbsite	$Al(OH)_3$	
Gold	Au	
Gypsum	$CaSO_4 \cdot 2H_2O$	
Halite	NaCl	
Magnetite	Fe_3O_4	
Muscovite	$KAl_2(AlSi_3O_{10})(OH)_2$	

http://pubs.usgs.gov/circ/c1143/html/text.html