Computer Modeling of a Fuel Processor

By: Zain Horning, M.S. Candidate
Advised by: Xingwu Wang, Ph.D.

College of Engineering and Professional Studies
Alfred University
Alfred, NY 14802-1205

April 7, 2003

Table of Contents

Abstract

Computer simulation of reactors is needed for the design of a fuel processor to be utilized in PEM fuel cells. An Aspen software package, Aspen Plus, has been utilized in this project to simulate a steam reformer, an auto thermal reformer, a selective oxidizer and a shift converter.

I. Introduction

In recent years, there has been a growing interest in the area of fuel cell study. Fuel cells are a clean and efficient source of electricity and potentially, have a wide range of applications. Due to the desirable characteristics of fuel cells, it is projected that in the future, fuel cells may replace some functions of the internal combustion engine. To date, there is no commercial fuel processor available at hydrogen production rates of 100 SLPM for PEM fuel cell applications.

A fuel processor (reformer) is a device that converts hydrocarbon fuel to hydrogen. In this paper, Aspen Plus was used to perform simulations of a steam reformer and auto thermal reformer (ATR).[1] In each reformer, methane is used as fuel. The simulation output is the amount of hydrogen produced, and the variables are the temperature and the concentration of reactants.[2-4]

In addition, simulations of a selective oxidizer and a shift converter were performed. The purpose of these experiments is to reduce the amount of carbon monoxide in the reformate gas.

II. Procedure

Simulations were carried out by constructing models of fuel processors with Aspen Plus. The modeling process began by developing a "process flowsheet" which is a visual representation of the reaction sequence. Each flowsheet utilizes an arrangement of heaters, reactors and streams to define a process. Heaters are used to vaporize the water entering a reactor and begin the initial reaction. The reactor is the chamber where chemical reactions occur. Streams (represented by arrows) direct the gas mixture throughout the process.

Next, the input components (air, steam, methane, etc.) of the reaction must be defined. After the models are complete, the fuel processors were simulated under varying conditions such as different temperatures and different ratios of reactants.

III. Steam Reformer

Figure 1 illustrates the flowsheet for a steam reformer.

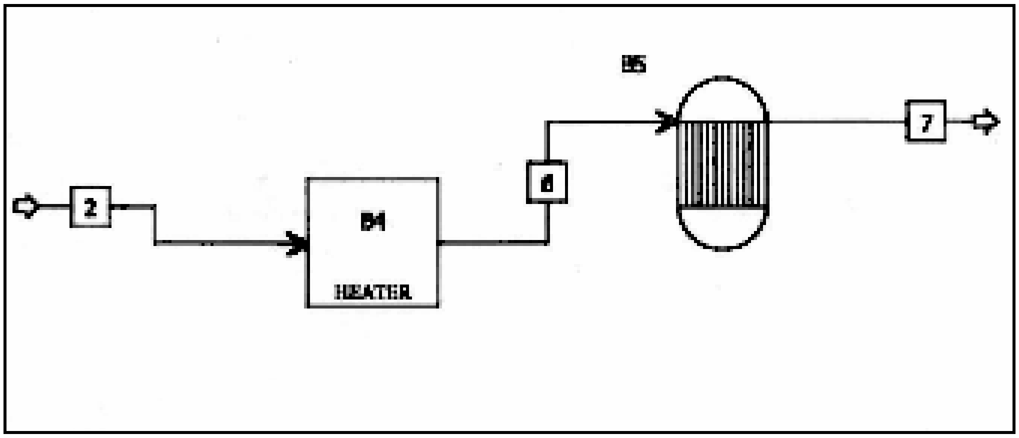

Figure 1 Steam Reformer Flowsheet

In this model, methane and water are fed into the system through stream 2. Stream 2 directs the mixture into a heater which is represented by block B4. Next, the steam and methane mixture enter a reactor through stream 6, where the chemical reactions occur. The results of this reaction can be observed in stream 7. It was observed that a water to methane ratio of 4:1 yielded the greatest amount of hydrogen.

IV. ATR

Figure 2 illustrates the process flowsheet for the ATR.

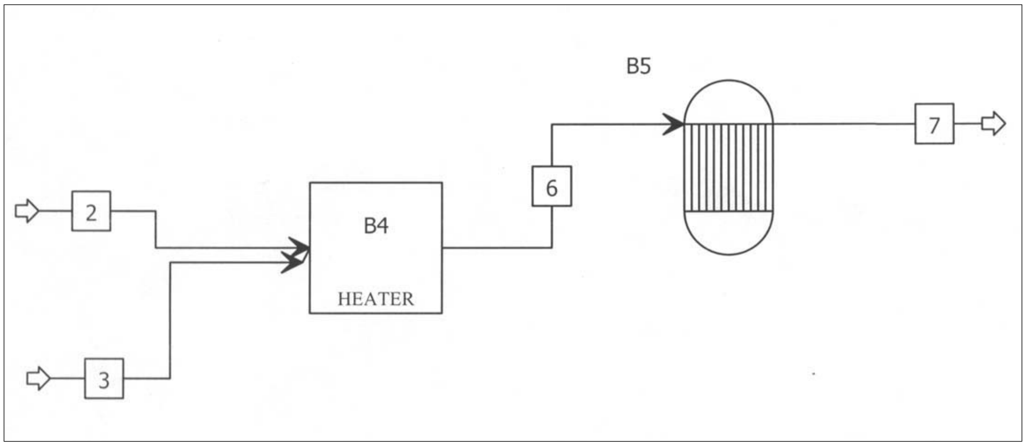

Figure 2 ATR Flowsheet

In this model, methane, water and air enter the process through streams 2 and/or 3. Stream 2 feeds methane and water into the processor. Air is added to the reaction through stream 3 and is expressed as 80% N_2 and 20% O_2. Streams 2 and 3 pass through a heater, which preheats the mixture to 700°C. After the mixture has passed through the heater, it is channeled into reactor B5. The products of the reactor can then be observed in stream 7.

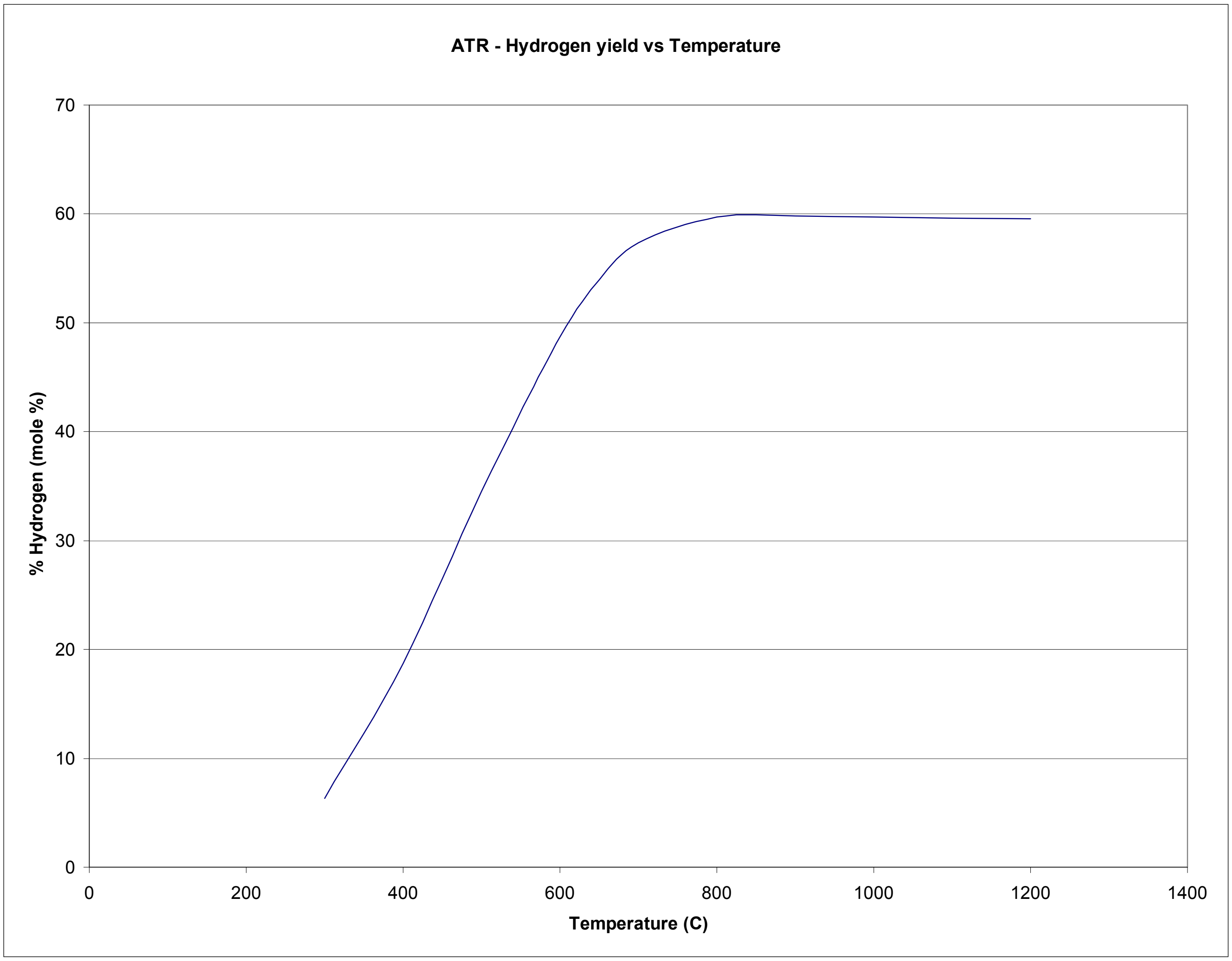

Figure 3. Hydrogen yield vs ATR temperature

Figure 3 illustrates the relationship between the temperature and the amount (mole %) of hydrogen produced by the reactor. During this simulation, the number of moles of air, methane and water remained at a 1:1:1 ratio while the ATR temperature was varied. As the temperature is initially incremented, there is a steady increase in the concentration of hydrogen until a temperature of 700°C is reached. After 700°C, the change in the concentration is small.

Next, the second simulation illustrates the hydrogen yield of the ATR for various amounts of methane. The amount of air and methane were kept at a constant 1 mole each.

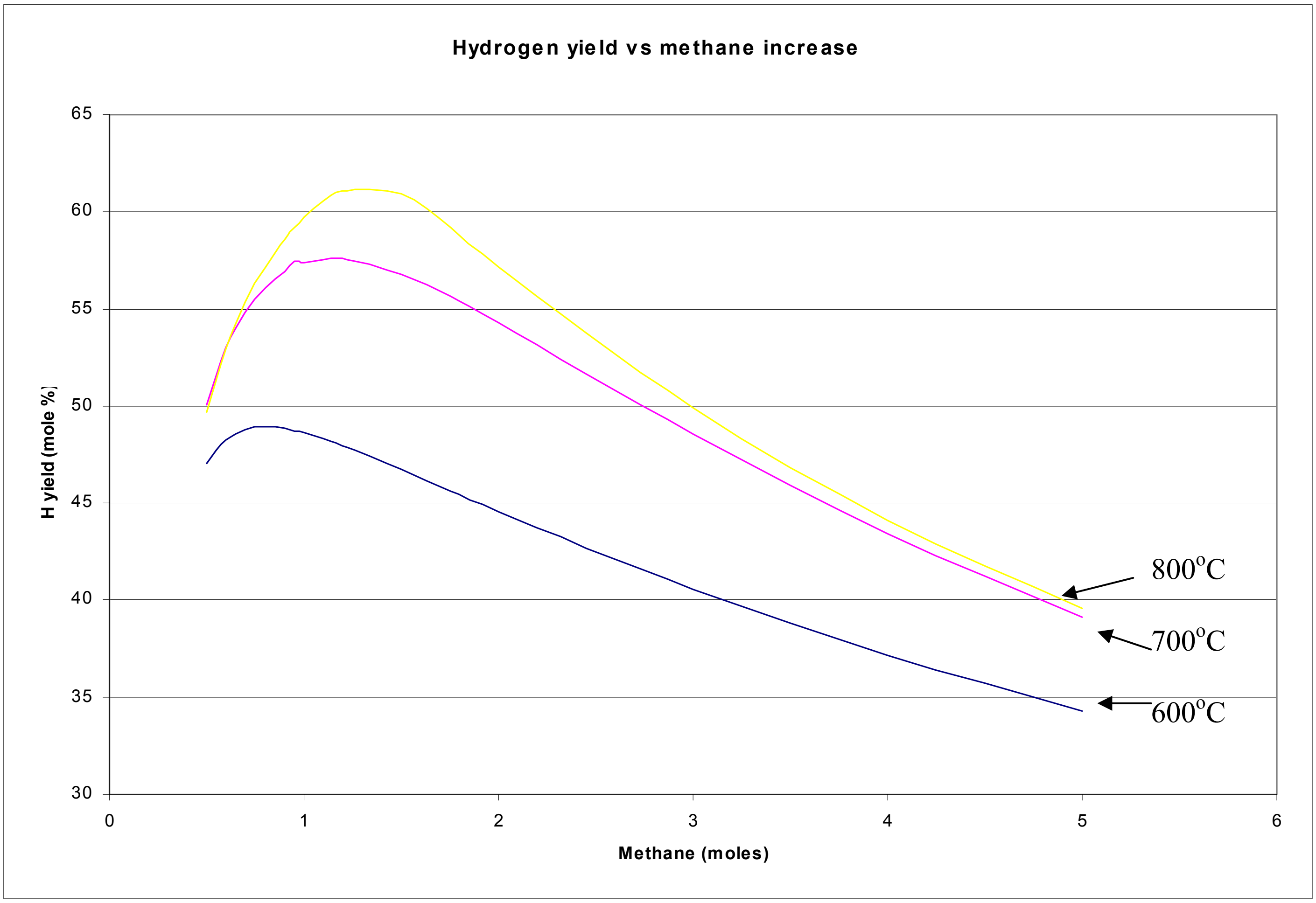

Figure 4 – ATR methane vs Hydrogen yield

The chart shows that as the number of moles of methane are increased, the concentration of hydrogen also increases. However, hydrogen production will peak around 0.95 moles of methane and then begins a steady decrease. It is also observed, that as the temperature of the reactor is increased; the concentration of hydrogen will also increase.

The third simulation illustrates the amount of hydrogen produced for various amounts of water. The amount of air and methane was delivered at a constant 1 mole per unit time.

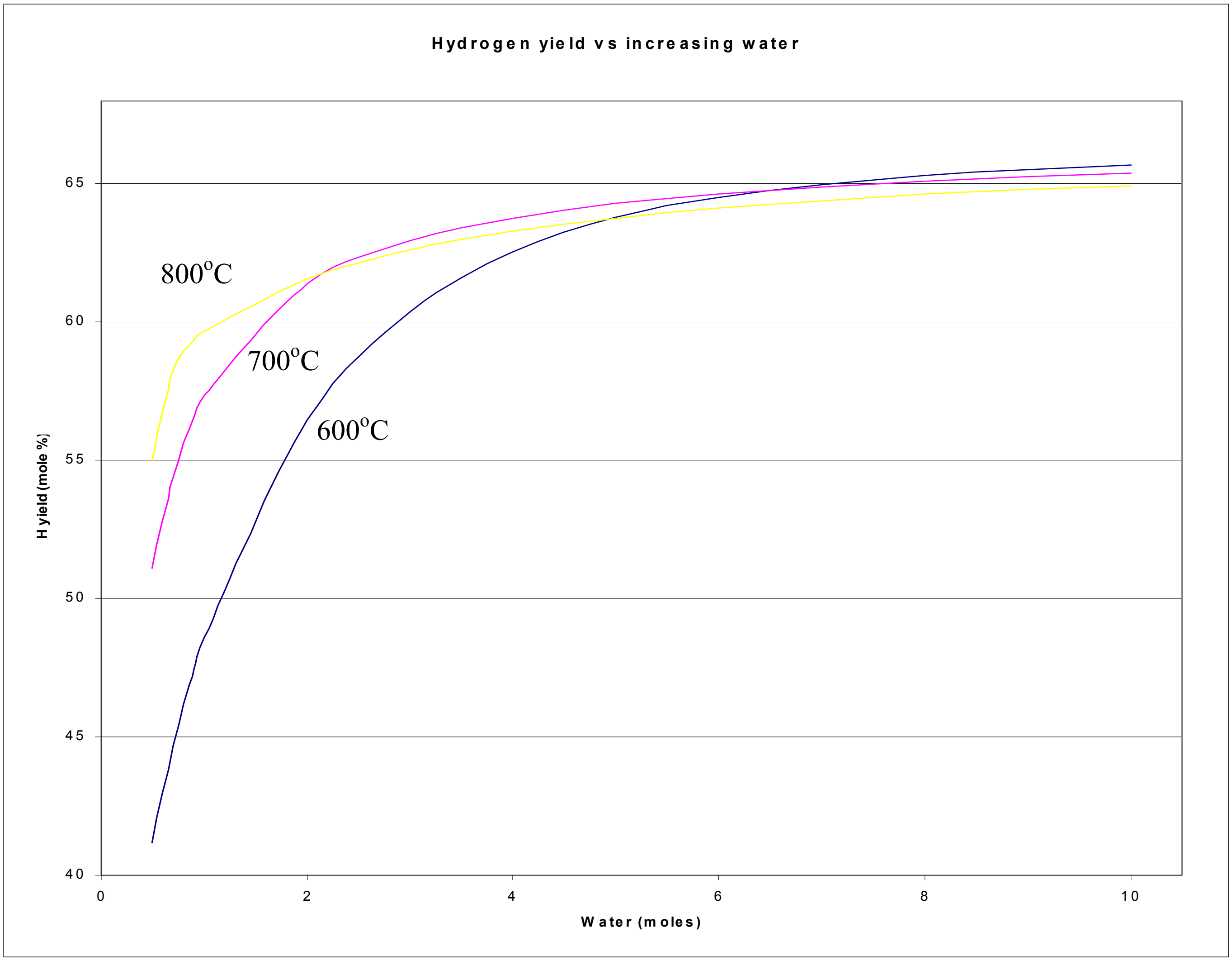

Figure 5 ATR Water vs Hydrogen yield

Figure 5 illustrates the relationship between the amount of water used in the reaction and the concentration of hydrogen. As the number of moles of water used in the reaction is increased, the concentration of hydrogen increases. In addition, it was observed that as the temperature of the reactor increases, the maximum attainable concentration of hydrogen decreases. However, after the water supply exceeds 7 moles per unit time, fewer moles of water are necessary to attain a maximum hydrogen concentration.

The fourth simulation illustrates the hydrogen yield for various amounts of air. In this case, the other reactants (steam and methane) were kept at a constant 1 mole per unit time.

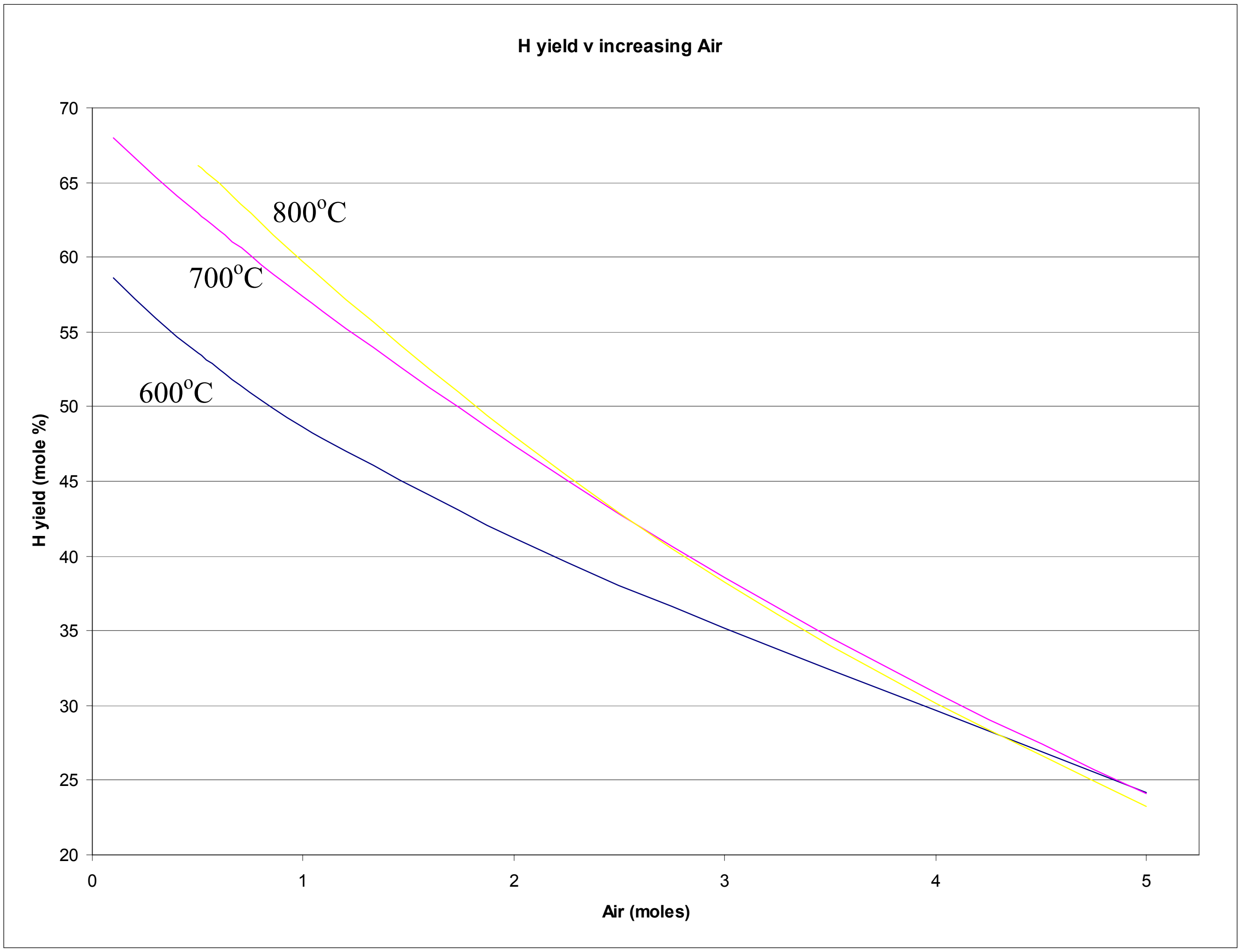

Figure 6 ATR Air vs Hydrogen yield

Figure 6 depicts the relationship between the moles of air used in the reaction and the concentration of hydrogen. As the moles of air delivered per unit time are increased, the concentration of hydrogen decreases. The graph also suggests that as the temperature increases, the hydrogen concentration will decrease more rapidly.

V. Shift Converter

A shift converter and a selective oxidizer are normally used for the removal of CO in a fuel processor. Essentially, a shift converter is constructed like a steam reformer; gas and steam mixtures are introduced into a shift converter where they react. The resultant mixture should yield a lower concentration of CO.

The results of a shift converter simulation are shown in figure 7. During this simulation, a mixture of CO and steam were reacted at different temperatures. It is illustrated that a minimal amount of CO is produced at lower temperatures.

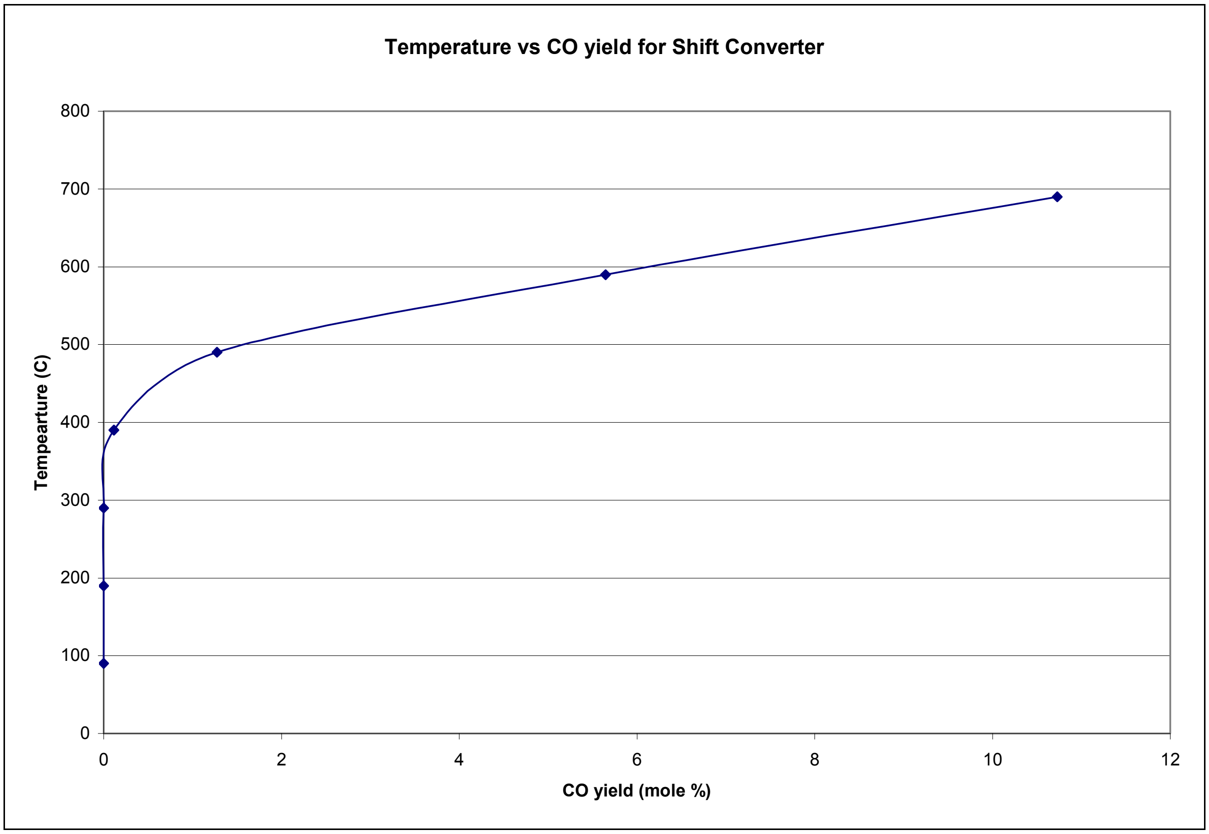

Figure 7 Shift Converter

VI. Selective Oxidizer

The selective oxidizer is similar in construction to the ATR; a mixture of gas, steam and air are combined in a reactor. The selective oxidizer is generally used to (ideally) eliminate any CO that was not removed by the shift converter.

The results of a selective oxidizer simulation are shown in figure 8. During this simulation, a mixture of CO, steam and air were reacted at different temperatures. The simulation demonstrates that the greatest amount of CO is removed at lower temperatures.

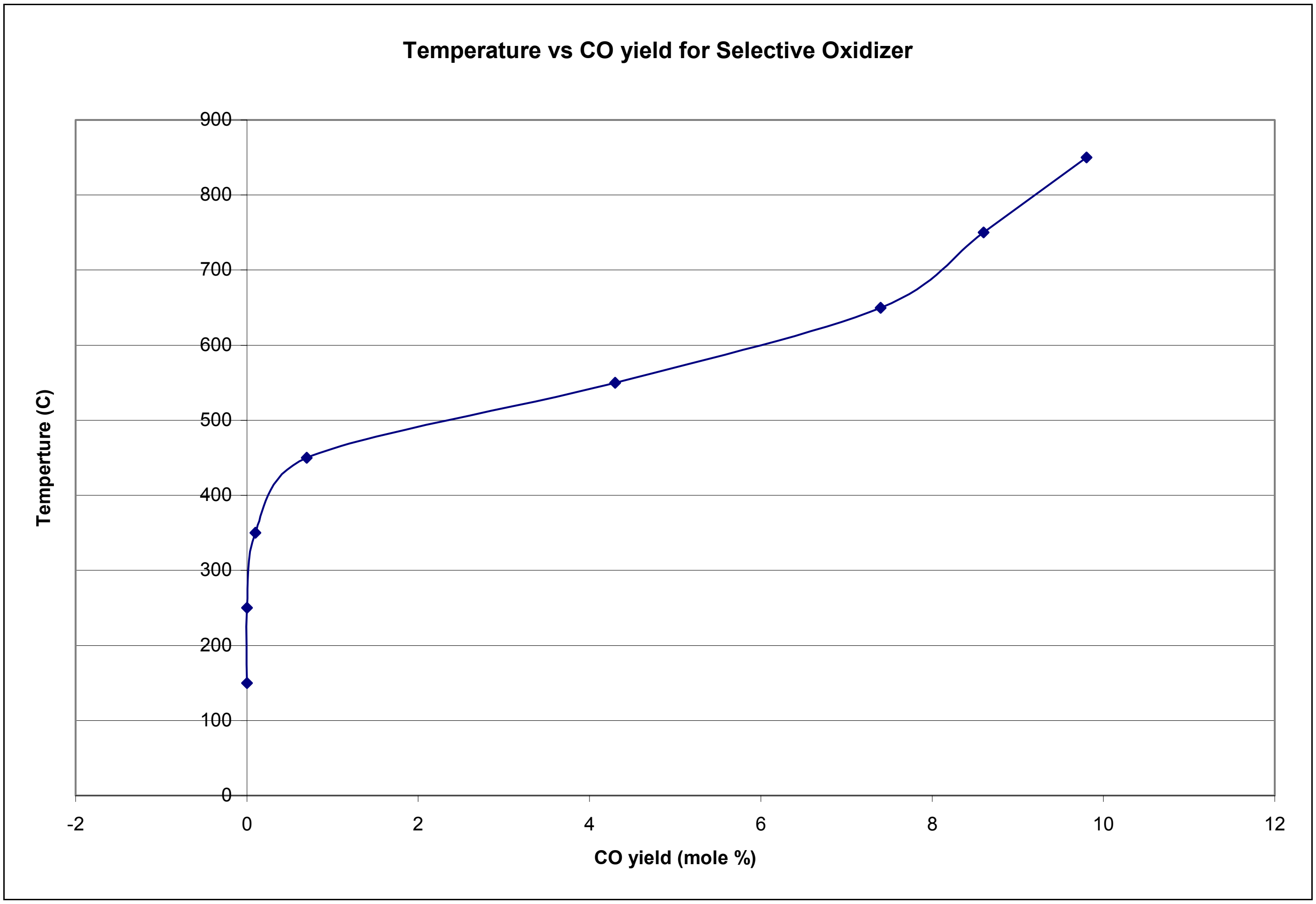

Figure 8 Selective Oxidizer

VII. Conclusion

The simulations presented in this report are useful for establishing some basic relationships but further experimentation may provide additional insight.

VIII. References

1. Aspen Plus is owned by and is a registered trademark of Aspen Technology Inc, Cambridge, MA 02141, USA (www.aspentech.com)
2. Xingwu Wang, Bigang Min, Huihui Duan, Art J. Peterson, "Modifications of Fuel Processing Techniques for Fuel Cell Applications", in Proceedings of Fifth European Solid Oxide Fuel Cell Forum, 1-5 July 2002, Lucerne, Switzerland.
3. Bigang Min, "Fuel Processor Studies", M.S. Thesis, Alfred University, May 2002.
4. Huihui Duan, "Fuel Processor for PEM Fuel Cells", M.S. Thesis, Alfred University, May 2002.