

Process Integration and Optimization of Logistical Fuels Processing for Hydrogen Production

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Abstract

In this work, the preliminary results of a process integration analysis of a logistical fuels processing plant is presented. A simulation model of a bench scale test bed was developed using a commercial simulator (Pro/II) and used to generate the necessary data for performing a thermal pinch analysis. The analysis shows that considerable savings can be obtained through increased thermal integration of the system. The specific application of the fuel processing system is to power a portable radar system, thus reductions in energy requirements translates into equally important reductions in equipment size. To further increase the integration potential the use of heat pipe technology has been investigated. Heat pipes allow for near isothermal heat transfer and thus significantly reduce the required temperature driving force. A simple, systematic method for identification of optimum heat pipe usage in heat exchange networks is presented in this work.

Keywords: Fuels processing, process integration

1. Introduction

Fuel cells are emerging as an important component of a renewable energy future for many utility and mobile applications. Proton exchange membrane (PEM) fuel cells are capable of achieving much higher energy efficiency levels since a fuel cell is not limited by the traditional Carnot cycle found in combustion engines. A very promising technique is to obtain the required hydrogen by reforming a liquid hydrocarbon fuel, which has a significantly higher energy density than gaseous hydrogen. Recent efforts are focused on reforming existing logistical fuels, e.g. diesel or JP-8 for use in fuel cell systems (Amphlett et al., 1998). This is particularly important for military applications, as it would allow for the US armed forces to move towards using one single logistical fuel. Since the overall energy efficiency of a fuel cell system is approximately three times higher than a combustion engine based generator, it would provide substantial savings for the US Army if alternative means of power production could be developed.

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To meet these ends the Center for Microfibrous Materials Manufacturing (CM³) at Auburn University has developed a bench scale test bed for investigating running a portable radar system of a Ballard NexaTM PEM fuel cell stack by producing high purity hydrogen from reforming JP-8. The PEM fuel cell system consists of the fuel processing section and the fuel cell itself, with the former being the reformer and post-combustion cleanup steps. Such systems inherently possess tremendous integration potential, not just limited to recycling unused material, but also in terms of energy recovery (Godat and Marechal, 2003). The objective of this work is to develop a process simulation model of the fuel processing test bed and use it to generate the data required for subsequently performing a thermal pinch analysis in order to identify the potential energy savings attainable. As this system is targeted for mobile applications reductions in utility requirements will automatically result in reductions in the system size.

2. Process Description and Model Development

A schematic of the fuel processing test bed is given in figure 1. A central theme for the test bed is the use of microfibrous entrapped catalysts and sorbents. These microfibrous materials provide high contacting efficiency through a high surface area to volume ratio. This enhanced heat and mass transfer capability presents an opportunity for miniaturization of the processing units compared to conventional catalyst supports, such as packed beds. In figure 2, 500 μm water gas shift catalysts particles are entrapped in 10-50 μm Nickel fibres. Similarly 150 μm particles of a precious metal catalyst on alumina support are depicted in figure 3 (Karanjekar et al., 2004). The simulation model was developed using a commercially available process simulator Pro/II (Simulation Sciences, 2004) augmented with a customized model for the fuel cell. It should be noted, that the simulation model is specified to match the experimental data.

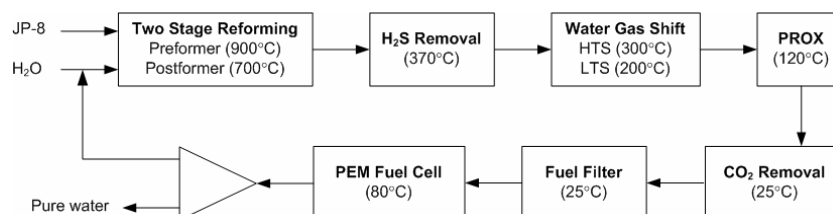


Figure 1. Fuel processing test bed schematic

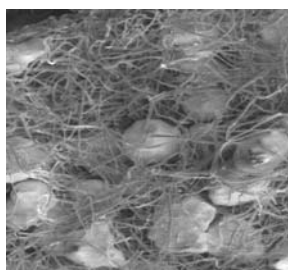


Figure 2. WGS catalyst in Nickel fibres



Figure 3. PROX catalyst on Al_2O_3 support

2.1 Reforming section

There is no standard formula for jet fuels such as JP-8. The exact composition depends on the crude oil from which they were refined. Variability in fuel composition occurs because of differences in the original crude oil and in the individual additives. As a result of this variability, little information exists on the exact chemical and physical properties of jet fuels (Custance et al., 1992). JP-8 consist of a variety of hydrocarbons ranging from C_7 to C_{16} , however the bulk of the fuel (over 80%) is made up by decane, dodecane, tetradecane and hexadecane (US Air Force, 1991). The steam-to-carbon ratio in the feed is 2.4, which has been reported as being the optimal choice (Zalc and Löffler, 2002). The mixture of steam and fuel is heated to 900°C and fed to the first reactor, which performs the majority of the reforming according to equations (1)-(3), while the second reactor reduces the methane content from approximately 15% to 1%. Chromatographic analysis of the effluents for the preformer and postformer is presented in figures 4 and 5, respectively and the reactor models are specified to match the performance of the experimental test bed.

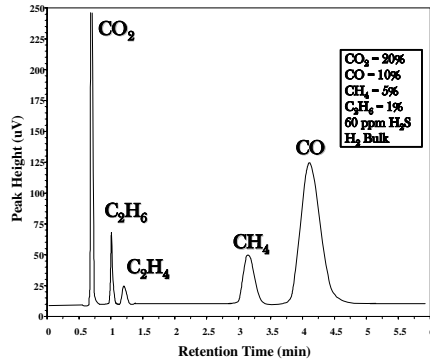


Figure 4. Analysis of preformer effluent

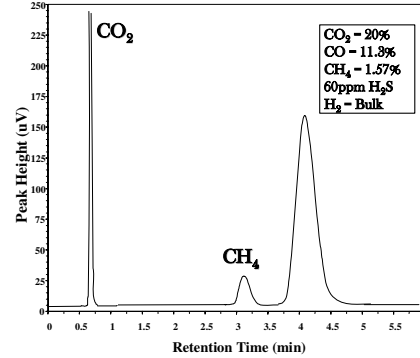


Figure 5. Analysis of postformer effluent

2.2 Reformate cleanup

The purpose of the next sequence of units is solely to purify the hydrogen by removing or converting the reforming by-products. Analogous to the reformer models, the model specifications are based on experimental data. First step is removal of hydrogen sulphide as it serves as a catalyst poison. The removal is performed by a microfibrinous entrapped ZnO/SiO_2 catalyst. The removal rate is greater than 99%, thus reducing the H_2S content to less than 1 ppm. Next are two water gas shift reactors, which convert carbon monoxide (which poisons the PEM fuel cell) into carbon dioxide as described by equation (3). The CO content after the shift reactors is reduced from 15% to less than 0.75%. The remaining CO is converted to CO_2 through preferential oxidation (PROX), which reduces the CO content to less than 10 ppm. The selectivity of the PROX catalyst

(Pt-M/Al₂O₃) is 60% towards the oxidation of CO, while the remaining 40% reacts with hydrogen to form water. The CO₂ is then removed by adsorption on a microfibrinous entrapped alkaline sorbent. The last unit before the hydrogen rich gas enters the fuel cell is an inline fuel filter, which is a series of microfibrinous entrapped sorbents that can remove traces of H₂S, NH₃, CO and CO₂ (Karanjekar et al., 2004).

2.3 PEM fuel cell

The high purity hydrogen stream is sent to the PEM fuel cell along with a feed of atmospheric air. The fuel cell produces electrical power and heat along with pure water, some of which is then recycled back to the steam production section. For the specific application envisioned by the military, i.e. power supply for a portable radar system, this presents an additional benefit. Since there is a net production of water (on a molar basis roughly 6 times the water supplied for the steam reforming) in the system, the on board fuel processor is capable of providing drinking water for the personnel.

3. Process Integration Analysis

Once the simulation model had been developed based on the experimental data obtained from the fuel processing test bed, a process integration study was performed to identify the potential energy recovery. By employing pinch analysis methods the global flow of energy in the system was mapped and analyzed. Assuming a 20°C minimum allowable temperature driving force, the pinch analysis showed that by extensive integration the external heating duty could be reduced by 58%, while the external cooling duty could be reduced 54%. These are quite significant savings when keeping in mind that these reductions in energy can be translated to reductions in equipment size as well. Furthermore, the fresh water requirement for steam production has been completely eliminated due to the fact that there is a net production of water in the system. Further investigations include dynamic simulation of the system, which may reveal that the hold-ups in the system require the water the recycle to be increased in order to run the system continuously. However it is still anticipated that a considerable amount of the fresh water produced can be used as drinking water.

4. Enhancing HEN Performance using Heat Pipes

Implementation of heat pipe technology has the potential of significantly increasing the attainable integration potential for process systems as the required driving force is decreased (Gaugler, 1944; Chi, 1976). A heat pipe is a heat transport device that utilizes evaporation and condensation to transport high rates of heat almost isothermally. Figure 6 outlines the structure of a generic heat pipe, where the heat transport is realized by evaporating a liquid contained in the wick in the heat inlet region and then subsequently condensing the vapour in the heat rejection region. Closed circulation of the heat transfer fluid is maintained by capillary and/or bulk forces. Heat is transferred radially through the casing and into the wick causing the liquid to evaporate and thus transferring mass from the wick to the vapour core. This increases the pressure in the vapour core at the evaporator end of the pipe, thus allowing vapour to flow to the condenser end of the pipe. Heat is removed through a suitable heat sink attached to the pipe casing at the condenser end. The condensing vapour replaces previously

evaporated liquid mass to the wick and capillary forces feeds the liquid back to the evaporation section (Harris et al., 2001). Besides the inherent benefits associated with nearly isothermal heat transport, an additional advantage of using heat pipes rather than conventional heat exchangers is that the pipe and the heat transfer liquid provides additional separation between the two streams exchanging heat. This ability reduces the dangers associated with transferring energy between incompatible materials, thus relaxing some of the conventional constraints encountered when designing heat exchanger networks (Harell, 2004).

4.1 Identification of optimal heat pipe placement

Since heat pipes are an emerging technology available to the processing industry and thus still quite costly, it is imperative to use them efficiently. For a conventional heat exchanger network the minimum allowable temperature difference ($\Delta T_{\min}$) is usually between 10 and 20°C. Hence, for a given heat exchanger network the pinch analysis is first performed with $\Delta T_{\min}$ equal to e.g. 20°C. Next, the utility targets for a heat pipe only network are identified by performing a pinch analysis with a significantly lower value of $\Delta T_{\min}$, e.g. 2°C. Now, an iterative procedure as outlined in figure 7 is employed to identify the placement and minimum number of heat pipes required to achieve these targets. The rationale behind the developed iterative approach is that in a standard heat exchanger network the thermal pinch point is the bottleneck, which must be overcome in order to transfer additional energy. Therefore the pinch location is the ideal point to implement a heat pipe. Once the first heat pipe has been implemented, the pinch analysis is redone and the utility targets evaluated. If another pinch point is identified, then a second heat pipe is added to remove this bottleneck. This procedure is continued until the utility targets identified from the 2°C pinch analysis have been matched, and thus no benefits will be obtained by adding additional heat pipes.

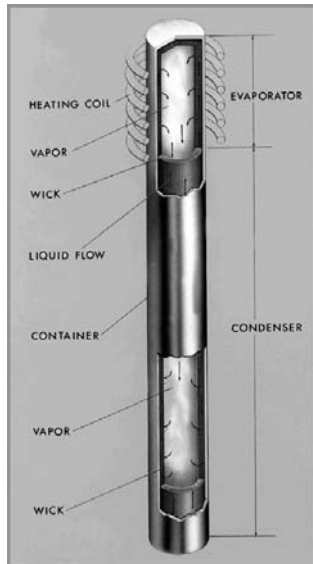


Figure 6. Capillary force heat pipe

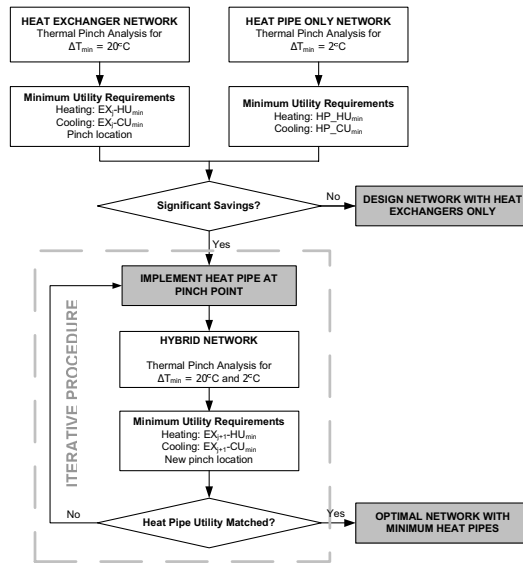


Figure 7. Iterative procedure for heat pipe placement

The iterative procedure outlined in figure 7 ensures that wherever possible the bulk heat transfer requirements are carried out using conventional heat exchangers and the more expensive heat pipes are only implemented, where a lower temperature difference is required in order to achieve the desired utility targets.

5. Conclusions and Future Work

Using commercial process simulation software a model of a logistical fuel processing system for mobile applications has been developed based on data from an experimental test bed. A process integration analysis showed that energy savings in excess of 50% are achievable through thermal integration of the system. A systematic method for evaluating the effect of using heat pipes in heat exchange networks has also been presented. The method is a simple extension to conventional pinch analysis methods. The presented method utilizes an iterative procedure where heat pipes are implemented at the pinch locations to overcome the thermodynamic bottlenecks. The implementation of heat pipes in the fuel processing system was found to potentially reduce the external heating and cooling demands by an additional 5% as well as providing a technology for reducing the physical size of the system. Future efforts will be focused on further developments of the simulation model including the use of alternative fuels, e.g. diesel, and different reforming schemes, i.e. partial oxidation and auto-thermal reforming. Furthermore, the design changes suggested by the thermal pinch analysis will be implemented on the test bed and the performance validated. Finally, the presented methodology for augmenting heat exchange networks with heat pipes will be extended from the current targeting approach to include actual network design.

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