

## Process Integration under Size Constraints: Logistical Fuels for Mobile Applications

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### Abstract

Current methods for resource management such as thermal and mass pinch analyses are aimed at processing facilities, i.e. stationary plants, where the overall goal is to balance reductions in operating cost against increased capital investments to maximize profitability. For a certain class of problems however, conventional pinch analyses fail to adequately address the resource management problems. For compact and/or mobile applications the deciding factor is not simply the resource utilization level or cost of equipment, but is often a trade-off between the achievable resource utilization and the weight and/or volume of the equipment. In this work, the integration potential of different reformation strategies has been evaluated for a variety of logistical fuel sources in size constrained systems.

**Keywords:** Process Integration, Fuels Processing, Size Constrained Systems

### 1. Introduction

The Center for Microfibrous Materials Manufacturing (CM<sup>3</sup>) at Auburn University has developed a bench scale testbed capable of running a portable

radar system of a Ballard Nexa™ PEM fuel cell stack by producing high purity hydrogen from steam reforming JP-8. Such systems inherently possess tremendous integration potential, not just limited to recycling unused material, but also in terms of energy recovery [1,2]. The objective of this work is to develop process simulation models for evaluating the integration potential of various reforming techniques when subject to restrictions on size or footprint. Experimental data from the testbed is used to specify the performance parameters of the different reactors, separation units and the PEM fuel cell [2].

## 2. Process Modeling

In previous work, a model describing steam reforming of JP-8 and the subsequent reformat clean-up system was developed based on data from the fuel processing test bed [2]. This validated model constituted the basis for developing models describing the three primary reforming strategies, i.e. steam reforming (SR), partial oxidation (POX) and auto-thermal reforming (ATR). Three hydrocarbon fuels of increasing complexity were evaluated for each reforming strategy, i.e. natural gas (approximated by methane), diesel (approximated by dodecane) and jet fuel (approximated by a mixture of C<sub>10</sub>, C<sub>12</sub>, C<sub>14</sub> and C<sub>16</sub> as these four components constitute about 80% of jet fuel [3]). The reforming and water gas shift reactors were specified using data from Seo *et al* (2002), while the remaining reformat cleanup steps and the fuel cell stack were specified using the testbed model [2]. A generalized schematic representing the models is given in Figure 1 below. For the ATR models the schematic is accurate, however for SR and POX there are slight changes, i.e. SR does not include the air feed, while POX does not include the steam feed, and consequently no water is recycled to the reactor either.

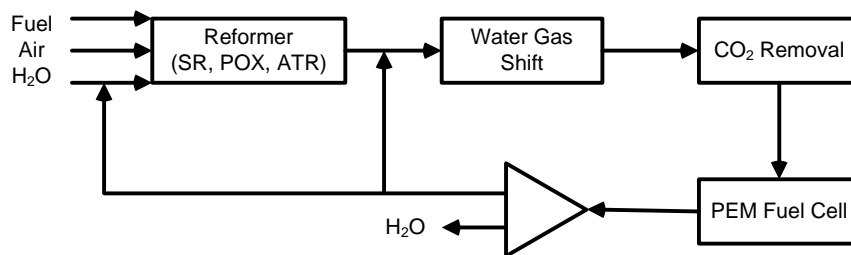


Figure 1. Generalized block diagram of fuel processing systems

## 3. Process Integration Analysis

The fuel cell produces electrical power and heat along with pure water, some of which is recycled back to the reformer and/or the water gas shift reactor. 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 steam reforming) in the system, the on board fuel processor is capable of providing drinking water for the personnel. After implementing the feasible water recycles, thermal pinch analyses were performed on each model to identify the minimum utility requirements of each system [5]. Note: Due to operational considerations the reactor duties are not included in the pinch analyses, thus the reactors are not allowed to be matched with the process streams directly.

Table 1. Integration potentials for isothermal reactor configurations (1 kg/s of fuel)

|             |  | SR           | POX         | ATR         |
|-------------|--|--------------|-------------|-------------|
| Natural Gas | Min. Heating (kW) [% red.]               | 20,240 [33%] | 1,996 [75%] | 1,820 [80%] |
|             | Min. Cooling (kW) [% red.]               | 1,987 [87%]  | 3,702 [72%] | 2,827 [79%] |
|             | Hydrogen production (mol)                | 247          | 172         | 174         |
|             | Electricity produced (10 <sup>4</sup> A) | 3.81         | 2.56        | 2.70        |
| Diesel      | Min. Heating (kW) [% red.]               | 19,560 [34%] | 6,767 [20%] | 6,618 [37%] |
|             | Min. Cooling (kW) [% red.]               | 2,170 [86%]  | 2,678 [85%] | 1,798 [90%] |
|             | Hydrogen production (mol)                | 215          | 130         | 134         |
|             | Electricity produced (10 <sup>4</sup> A) | 3.32         | 2.00        | 2.07        |
| JP-8        | Min. Heating (kW) [% red.]               | 18,210 [33%] | 6,717 [21%] | 6,463 [37%] |
|             | Min. Cooling (kW) [% red.]               | 1,638 [87%]  | 2,668 [85%] | 1,795 [91%] |
|             | Hydrogen production (mol)                | 215          | 130         | 134         |
|             | Electricity produced (10 <sup>4</sup> A) | 3.31         | 2.01        | 2.07        |

Table 1 summarizes the results of the thermal pinch analyses for each fuel and reforming strategy when all the reactors are operated isothermally. Switching the reactor operation to adiabatic conditions yielded very similar results and are thus not included in this paper. It is apparent that reforming natural gas yields the highest electricity production due to the higher hydrogen to carbon ratio (4:1) of the fuel compared to e.g. diesel (2.2:1). The additional water used in steam reforming adds to the overall hydrogen production, however, the increased thermal mass coupled with the endothermic reaction scheme results in SR having the highest heating utility requirement. The process integration analysis showed that regardless of the fuel type and complexity, auto-thermal reforming seems to be the best strategy as it has the lowest external heating utility requirements and only slightly higher cooling demands than steam reforming. The balanced nature of the ATR reaction scheme, where the exothermic partial oxidation is used to drive the endothermic steam reforming

reaction, has led to the general acceptance that ATR is the best strategy for hydrogen production in mobile applications [6,7]. Based on the results obtained in the thermal pinch analyses, this conclusion seems appropriate. However, when the size of the resulting equipment is taken into account, the results are no longer as straightforward.

#### 4. Size Constrained Systems

The thermal pinch analyses identified the minimum utility requirements, however in order to evaluate the total system size, the heat exchanger networks capable of realizing these minimum requirements must be designed [5]. A variety of software implementations are available for designing heat exchanger networks from pinch analysis data, e.g. AspenTech HX-Net™. All these tools attempt to trade-off the capital investment vs. the utility cost to obtain the overall minimum cost solution [8]. This means that the networks designed by the algorithms do not necessarily match the minimum utility requirements because doing so may result in exorbitant capital cost of the heat exchangers. For mobile systems and particularly for military applications, e.g. tanks and forward staging areas, cost is not the primary concern. System size, i.e. weight and volume, is! Therefore, it is necessary to evaluate the attainable power production as a function of the system size.

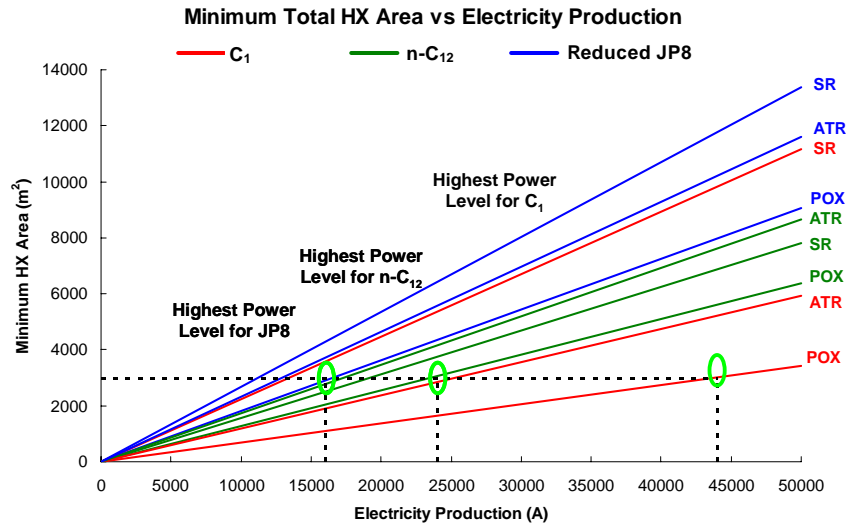


Figure 2. Attainable power production under size constraints.

The total required heat exchanger area can be translated to weight and volume by choosing a heat exchanger design, e.g. if using shell and tube exchangers, the

size and number of tubes in each will dictate the required head space, weight of the equipment etc. Circumventing the trade-off between capital investment and utility cost, enables identification of the size of the heat exchanger networks that are capable of actually meeting the minimum utility requirements identified in the pinch analysis. Due to the richness of the design problem, several heat exchanger networks are designed that all match the minimum utility requirements. In each case the network with the smallest total heat exchanger area was selected. In Figure 2, the results are presented for each reforming strategy and hydrocarbon fuel source.

Imposing an arbitrary constraint on the total available system size, i.e. heat exchanger area, leads to significantly different results than previously accepted [6,7]. As seen from Figure 2, the highest power production (regardless of fuel type) given a certain size limit ( $3,000 \text{ m}^2$ ) is obtained from partial oxidation (POX) of the fuel and not auto-thermal reforming. The storage volume of the fuel itself needs to be taken into consideration as well, otherwise the results depicted in Figure 2 may lead to the erroneous conclusion that when subject to size constraints the optimal solution is partial oxidation of natural gas. Although natural gas yields an increased power output (almost three times compared to JP-8 and twice compared to diesel), the difference in energy density between a gas and a liquid is considerable. For a given power output, the corresponding volumetric fuel flowrate is roughly 800 times higher of natural gas than the liquid hydrocarbon fuels. So unless the size constraints are imposed in terms of system weight only, the optimal strategy for mobile fuel processing appears to be partial oxidation of a liquid hydrocarbon fuel such as diesel or JP-8.

In Figure 3, the effect of switching the reactors from isothermal to adiabatic operation is illustrated. For POX and ATR, no significant difference was found, as the lower thermal mass of these systems diminish the impact of moving the duties from the reactors to the heat exchangers. Steam reforming becomes more attractive when operated adiabatically, thus challenging the notion that increased integration translates to increased equipment size. Because of the decision not to allow the reactors to be matched directly with the process streams, adiabatic operation allows for increased integration as the duties are included as part of the heat exchanger network and not just the utility network.

## **5. Conclusions**

In this work common reformation strategies have been compared based on utility requirements and energy integration potential for a range of logistical fuels. Although steam reformation produces the most hydrogen and thus more electricity, the energy costs to process the fuel outweigh the benefits of extra power production.

Analyses of the integration potential of the different reformation strategies showed that autothermal reformation produces about 60% of the hydrogen of steam reformation at less than half of the utility demands. Based solely on the

energy required to produce electricity, autothermal reformation appears to be the fuel processing strategy of choice. However, when accounting for limitations on equipment size, partial oxidation of liquid hydrocarbons shows the greatest potential.

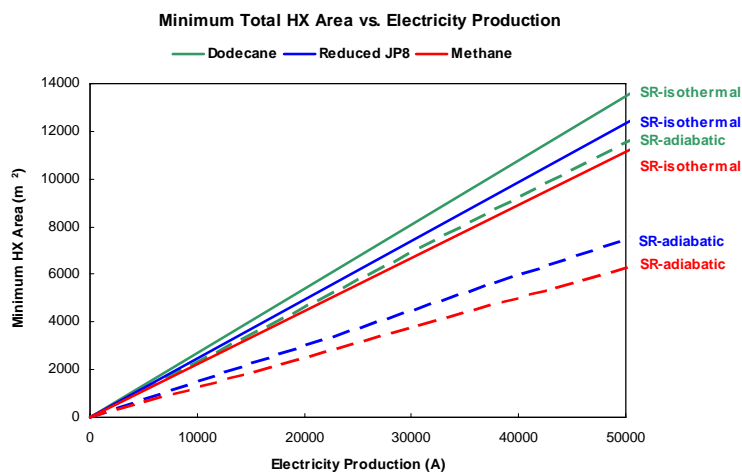


Figure 3. Effect of reactor operation on attainable electricity production under size constraints.

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