A Numerical Study of the Performance of an Autothermal Reformer for Use in a Fuel Cell Powered Auxiliary Power Unit for Trucks

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An autothermal reformer of a type that is suitable for use with an on-board fuel cell powered auxiliary power unit (APU) in large long-haul trucks has been numerically studied. Such APU's have the potential to significantly reduce engine fuel use associated with long periods of idling and consequently to significantly reduce the amount of greenhouse gas emissions produced. The APU considered would utilize the engine fuel and convert it into a hydrogen rich gas stream for use in a fuel cell stack. Because experimental results for a reformer of the type being numerically studied here were available for the case where isooctane was used as the representative input "fuel" attention has here been restricted to this case. In the numerical work it was found that small modifications to the available catalyst model were required to improve the agreement between the numerical and experimental results. With this change in the model it was found that relatively good agreement between the numerical and experiment results was obtained. The effects of changes in the reformer design were then studied. It was found that by using a solid rod made of high thermal conductive material down the centre of the reformer and by reducing the length of inert porous region at outlet of the catalyst bed the hydrogen output can be increased by about 25%.

1. Introduction

Large transport vehicles require large engines when operating on the highway. However, these engines are also frequently used to supply electricity when the vehicle is parked which often means that the engine is run (or idled) for long periods with the vehicle at rest. Under these conditions, i.e., with the engine idling, the fuel efficiency tends to be very low and significant amounts of greenhouse gas emissions are produced. On-board fuel cell powered auxiliary power units (APU's) that would supply the energy requirements of the truck when it is parked have the potential to significantly reduce engine fuel use associated with long periods of idling and consequently to significantly reduce the amount of greenhouse gas emissions produced. These APU's would utilize the engine fuel and use a reformer to convert it into a hydrogen rich gas stream to be used in a fuel cell stack. Idling emissions could be reduced by 90% by using such an on-board fuel cell based APU. A vital component of such an on-board APU system is the reformer and the purpose of the present study is to numerically investigate in a basic

way the performance of a type of reformer that could be used in such a system. An autothermal reformer which can be considered to use a combination of steam reforming and partial oxidation has here been considered.

Experimental results for such a reformer are available and the purpose of the present numerical study was to determine whether the numerical model used could adequately predict these experimental results and then to use the model to investigate possible design changes to the reformer that would improve its performance. The reformer design tries to use heat transfer from the exothermic oxidation reaction region of the reformer to the endothermic steam reaction region of the reformer so that no heat need be supplied or removed from the system. In the present study iso-octane was used as the representative input "fuel" since this was the surrogate fuel used in an associated experimental study. The catalyst used in the reformer was a proprietary platinum on ceria (2% Pt) manufactured by NexTech Materials Inc.

The autothermal reforming of iso-octane has been studied experimentally by Caners (2005), Shaw (2008), Villegas (2006), and Moon et al. (2001). Pacheco et al. (2003) developed a model describing the reaction kinetics and performance for an iso-octane autothermal reformer. The model was validated using experimental results. This model has been used by Sylvestre (2007), McIntyre (2005) and others to numerically study the performance of an iso-octane autothermal reformer. The reaction model developed by Pacheco et al. (2003) is based on the assumption that the following reactions occur:

(i)   Oxidation: $C_8H_{18} + 12.5O_2 \rightarrow 8CO_2 + 9H_2O$
(ii) Steam Reforming A: $C_8H18 + 8H_2O \rightarrow 8CO + 17H_2$
(iii) CO2 Reforming: $C_8H_{18} + 8CO_2 \rightarrow 16CO + 9H_2$
(iv) Steam Reforming B: $C_8H_{18} + 16H_2O \rightarrow 8CO_2 + 25H_2$
(v)   Water-Gas-Shift: $CO + H_2O \rightarrow CO_2 + H_2$

One of the major disadvantages of using this simple reaction mechanism is that it does not account for the formation of lighter hydrocarbons that have been shown to exist in the reformate of autothermal reformers, e.g., see Roychoudhury (2005).

2. Solution Procedure

The reformer considered in the experimental study by Shaw (2008), on which the present numerical study is based, is shown in Fig. 1. The reformer was sized to ensure plug flow through the catalyst bed. In order to achieve a uniform velocity profile in the reformer before the catalyst bed an inert porous region 3cm in length was added before the catalyst bed. A 3cm long inert porous region was also added after the catalyst bed.

 The numerical study was based on the use of reaction model developed by Pacheco et al. (2003). The flow through the reformer was assumed to steady and axis-symmetric. The solution was obtained using the commercial cfd code FLUENT. Extensive grid independency testing was undertaken.

3. Results

In the experimental study to which the present numerical study is related the main parameters controlled were the O/C and H_2O/C ratios at the inlet to the reformer and the gas hourly space velocity (GHSV). It should be noted that the O/C ratio used refers to molecular oxygen-carbon ratio and not to the O_2/C ratio that is sometimes reported in
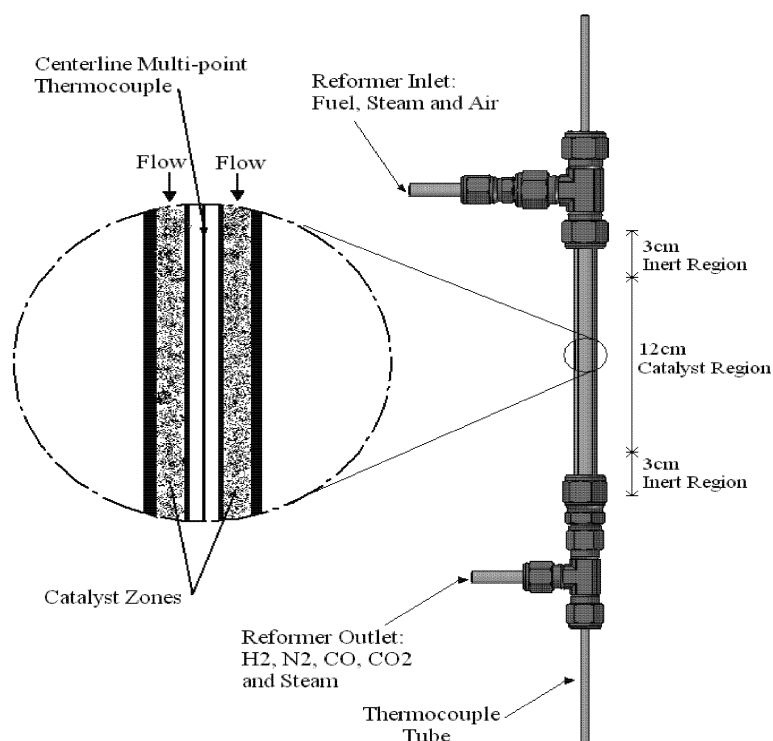
Figure 1 Reformer design considered.

literature. The gas hourly space velocity (GHSV) has been defined in various ways in the literature. Here it is defined the ratio of the volume flow rate of all inlet species in cc/h divided by the catalyst volume in cc and was always calculated at STP. Tests were undertaken using the conditions shown in Table 1. A GHSV value of 20 000h^{-1} was used in all tests. In all cases the gases entered the reformer at a temperature of 500°C.

Table 1 Conditions used in the testing of the autothermal reformer.

Experiment Number	GHSV h^{-1}	O/C Ratio	H$_2$O/C Ratio	Isooctane Flow Rate ml/m	Air Flow Rate ml/m	Water Flow Rate ml/m
1	20,000	0.7	1.0	0.52	1.02	0.45
2	20,000	0.7	2.0	0.38	0.75	0.67
3	20,000	0.7	3.0	0.30	0.60	0.79
4	20,000	1.0	1.0	0.42	1.16	0.36
5	20,000	1.0	2.0	0.32	0.90	0.53
6	20.000	1.0	3.0	0.27	0.74	0.69
7	20,000	1.3	1.0	0.35	1.26	0.30
8	20,000	1.3	2.0	0.28	1.02	0.49
9	20,000	1.3	3.0	0.23	0.85	0.61

Table 2 Measured molar percentages at the reformer outlet for the various tests undertaken.

Experiment Number	O/C Ratio	H_2O/C Ratio	H_2 Molar %	CO Molar %	CO_2 Molar %
1	0.7	1.0	25.2	12.1	6.7
2	0.7	2.0	27.7	14.4	4.6
3	0.7	3.0	28.6	14.9	2.4
4	1.0	1.0	28.6	10.0	7.4
5	1.0	2.0	32.1	12.0	4.8
6	1.0	3.0	32.4	12.9	2.8
7	1.3	1.0	20.4	9.10	7.9
8	1.3	2.0	22.2	11.5	5.1
9	1.3	3.0	22.0	12.7	3.0

The measured results for these test conditions are shown in Table 2.

The value of the effectiveness factor for the reactor catalyst bed was first determined by matching the outputs predicted by the numerical model with different effectiveness factor values with the measured results. A typical such a comparison is shown in Fig. 2. It will be seen from these results that an effectiveness value of 0.0032 appears to give a numerical result that is in the best agreement with the experimental result and this value was used in all calculations.
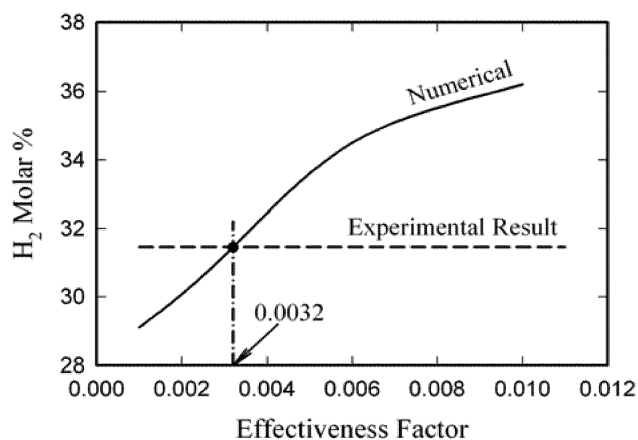

Figure 2 Comparison of numerically predicted molar percentage variation with effectiveness factor with the experimentally measured value for a GHSV of 20000h-1 and the conditions used in experiment number 5.

Using the value of the effectiveness factor so determined, numerical results were obtained for the same nine sets of conditions as those used in the experimental study. The results obtained are shown in Table 3. A comparison of these numerical results with

Table 3 Numerically predicted results for the conditions used in the experimental study.

Experiment Number	O/C Ratio	H$_2$O/C Ratio	H$_2$ Molar %	CO Molar %	CO$_2$ Molar %
1	0.7	1.0	27.8	12.0	4.28
2	0.7	2.0	27.8	12.6	3.58
3	0.7	3.0	28.4	12.0	3.48
4	1.0	1.0	30.2	14.5	4.88
5	1.0	2.0	32.6	14.8	4.22
6	1.0	3.0	31.3	13.6	3.79
7	1.3	1.0	29.0	14.2	5.31
8	1.3	2.0	32.0	14.8	4.74
9	1.3	3.0	29.5	13.0	4.20

Table 4 Numerically predicted results for the modified reformer with a solid rod on the centre-line and with an inert porous material at outlet with a reduced length and a lower thermal conductivity than used in the original reformer.

Experiment Number	O/C Ratio	H$_2$O/C Ratio	H$_2$ Molar %	CO Molar %	CO$_2$ Molar %
1	0.7	1.0	37.7	18.7	4.19
2	0.7	2.0	43.6	20.4	3.52
3	0.7	3.0	45.1	20.4	3.05
4	1.0	1.0	34.7	17.7	4.83
5	1.0	2.0	40.8	19.4	4.20
6	1.0	3.0	42.5	19.5	4.12
7	1.3	1.0	32.4	17.0	5.27
8	1.3	2.0	38.2	18.5	4.66
9	1.3	3.0	40.2	18.7	4.20

the experimental results given in Table 2 shows that relatively good agreement between the numerical and measured values is obtained at the lower O/C values. However at the higher O/C values considered the numerically predicted H$_2$ molar percentages are significantly higher than the measured values. This is the result of inadequacies in the reaction model used.

One of the aims of the design of the reformer was to have heat conducted along the outer tube from the region near the inlet where the high temperature exothermic partial oxidation reaction was occurring to the lower temperature region near the exit where the endothermic steam reforming reaction was occurring. An examination of the numerical results indicated that a relatively small amount of heat was in fact being conducted down the tube and that the relatively high thermal conductivity inert porous media at the reformer exit was transferring heat away from the steam reforming reaction section to the exit section. For this reason a modified reformer design was considered. This involved the insertion of a 3.2mm diameter solid rod made from a material with a thermal conductivity of 100W/mK down the centre-line of the reformer and a reduction in the length of the exit inert porous material layer from 30mm to 10mm and the use of

a different material for this porous layer that had a lower thermal conductivity. The numerical results obtained with this modified design for the same conditions as used in the experimental study are shown in Table 4. A comparison of the results given in Table 4 with those given in Table 3 shows the modified reformer does in most cases give significantly higher molar percentages of H_2, the increase being on average about 25%.

4. Conclusions

The results obtained in the present numerical study indicate that:
1. The effectiveness factor for the reactor catalyst bed is 0.0032.
2. Relatively good agreement between the numerical and measured reformate composition is obtained at the lower inlet O/C values considered. However at the higher O/C values considered the numerically predicted H_2 molar percentages are significantly higher than the measured values.
3. The modified reformer design considered does give a significantly improved performance.

Acknowledgements

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