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A "Swiss-Roll" Fuel Reformer: Experiments and Modeling

Chien-Hua Chen[1], Bradley Richard[1], Ying Zheng[1], Howard Pearlman[1],
Shrey Trivedi[2], Srusti Koli[2], Andrew Lawson[2], and Paul Ronney[2]

[1]*Advanced Cooling Technologies, Inc., 1046 New Holland Ave., Lancaster, PA 17601*
[2]*Department of Aerospace and Mechanical Engineering, University of Southern California,*
Los Angeles, CA 90089
[*]*Corresponding Author: chien-hua.chen@1-act.com*

Abstract: A Thermal Partial Oxidation (TPOX) based "Swiss-Roll" Reformer is being developed to efficiently convert hydrocarbon fuels (e.g., propane, n-heptane, JP-8) into hydrogen rich syngas for subsequent use in a solid oxide fuel cell (SOFC) for power generation. Similar in concept to the "Swiss-roll" combustor, the reformer is a countercurrent heat exchanger that efficiently recuperates heat from a hot reformate stream generated internal to the reformer and preheats the cold reactants entering the device. Effective heat recuperation enables superadiabatic temperatures to be achieved within the reformer and drive the reformate composition towards chemical equilibrium without the need for catalysts (avoiding their associated problems, i.e., coking, sulfur tolerance, deactivation, etc.) and external energy sources. In the paper, two modeling methods have been developed. The first one is a reactor based model that separates the Swiss-roll reformer into three reactors in series: plug flow reactors for the inlet and outlet channels and a perfect stirred reactor to model the center reaction zone. The second approach is a 2D CFD model with detail chemistry (GRI Mech 3.0) using commercially available software, i.e., FLUENT and CHEMKIN CFD. Comparison of the computational and bench-scale experimental test data will also be reported.

Keywords: Swiss-roll, Thermal partial oxidation, Fuel reformer, Syngas

1. Introduction
Partial oxidation may be the simplest way to convert hydrocarbon fuels to hydrogen-rich syngas. Hydrogen (H_2) and carbon monoxide (CO) are the major equilibrium state products that can be direct use with SOFC's. The exothermicity associated with partial oxidation is however typically too low to raise the reaction temperature to a sufficient extent needed to achieve high conversion efficiencies within the available residence time. Therefore, catalyst is typically needed to lower the activation energy. However, many practical fuels contain sulphur compounds and aromatics that may cause catalyst degradation due to poisoning and coking.

To address the issue, using external energy such as with plasma to accelerate the reaction rate has been proposed [1]. But such system requires electricity, which ultimately comes from additional fuel consumption. Efficiently recuperate heat from the hot reformate to the cold reactants to increase the reaction temperature and therefore reaction rate is probably the most thermally efficient non-catalytic reforming method. With the excess enthalpy in the reactants, the reaction temperature is able to achieve higher than the adiabatic temperature. The 'superadiabatic' temperature makes it possible to reform rich fuel-air mixtures and achieve high syngas yields. Several types of non-catalytic thermal reforming reactors based on the use of porous media [2] have been developed. The basic principle is to use the heat released during the partial oxidation process to preheat the rich fuel-air premixture through solid conduction and

solid-to-solid radiation from the post-flame zone to the pre-flame zone, thus raising the reactant temperature and promoting thermal partial oxidation. Stationary (flame stabilized) and transient systems (filtration combustion) have been developed with key challenges including managing the propagation of the reaction front in the porous media, conductive heat loss and soot formation/ clogging.

Swiss-Roll Reformer

An alternative non-catalytic thermal partial oxidation (TPOX) based reformer is developed via effective heat recirculation through a counter current spiral heat exchanger (Figure 1). In this configuration, the chemical reaction occurs within a spiral heat exchanger that has a large heat transfer to heat loss area ratio and therefore provides efficient heat exchange in a compact volume [3, 4]. In this reactor, the reaction zone, which has the largest propensity for heat loss, can conveniently be stabilized in the center of the spiral heat exchanger, where the most heat recirculation happens. The existing of a flow recirculation zone in the center also helps to stabilize the reaction. The curvature of the channels leads to the development of a centrifugal instability and causes Dean vortices. This is beneficial as it further enhances the gas phase heat transfer between adjacent spiral windings at lower Reynolds number that typically cannot be benefited from the turbulence heat transfer enhancement. Additionally, the long channels at elevated temperature provides a long residence time that helps to promote the reformates to the chemical equilibrium state.

While the Swiss-roll combustor/ reformer has several advantages, the manufacturing challenges and the complex thermal chemical interaction prevents it from practical applications. In this work, metallic Swiss-roll reformers made by two fabrication methods: brazed and 3D printing (Figure 2) were tested. Two modeling approaches: reactor based model and CFD model were developed to help understand the physics and design optimization.
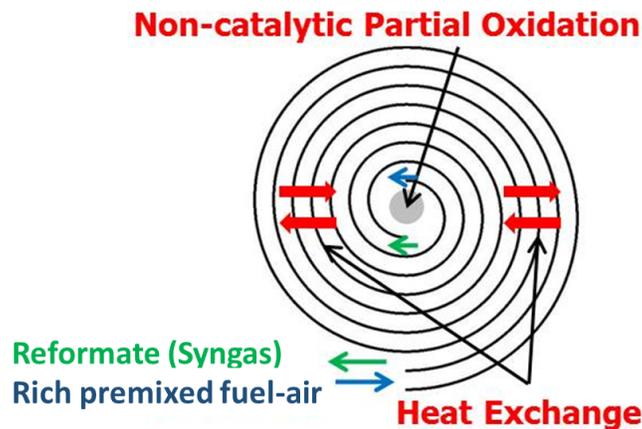
Figure 1: Swiss-roll reformer concept.

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(a)   (b)
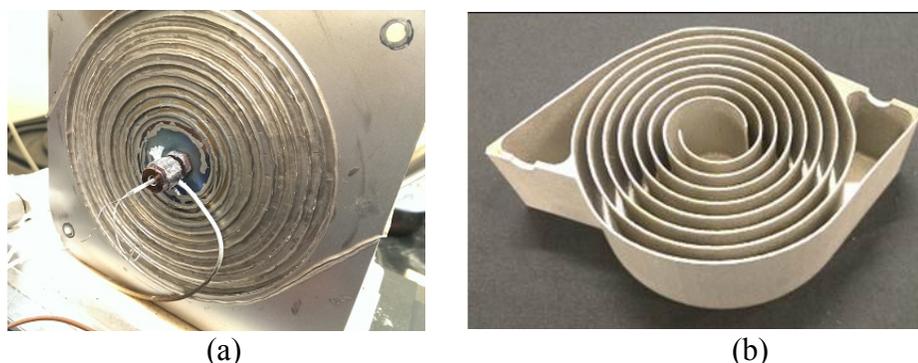
Figure 2: "Swiss-roll" reformer prototypes: (a) brazed inconel, (b) 3D printed stainless-steel cross-sectioned to show internal features.

2. Experiment

Experimental Setup

A schematic of the experimental test facility for the reformer experiments is shown in Figure 3. Air and gaseous fuel are metered using mass flow controllers and a liquid fuel injection and vaporization system was also developed for testing liquid fuels. This subsystem includes a pump with Meinhard nebulizer and temperature-controlled vaporization chamber used to control equivalence ratio upstream of reformer inlet. Ignition was initiated by a hot wire igniter (Kanthal A1) inserted through a Swagelok port located at the center of one of the reformer endplates. The power for the hotwire ignition was ~30 W supplied by a DC power supplier. After the reaction zone was established, the igniter was turned off, and the reaction was self-sustained by exothermic partial oxidation and heat recirculation.   Several K-type thermocouples were used to monitor the reaction and exhaust temperature. The downstream reformate was analyzed with an SRI Gas Chromatograph (GC) outfitted with a thermal conductivity detector (TCD) and a flame ionization detector (FID) equipped with a methanizer. An Omega DAQ with DASYLab was used to acquire all data and control the mass flow controllers and liquid fuel pump.
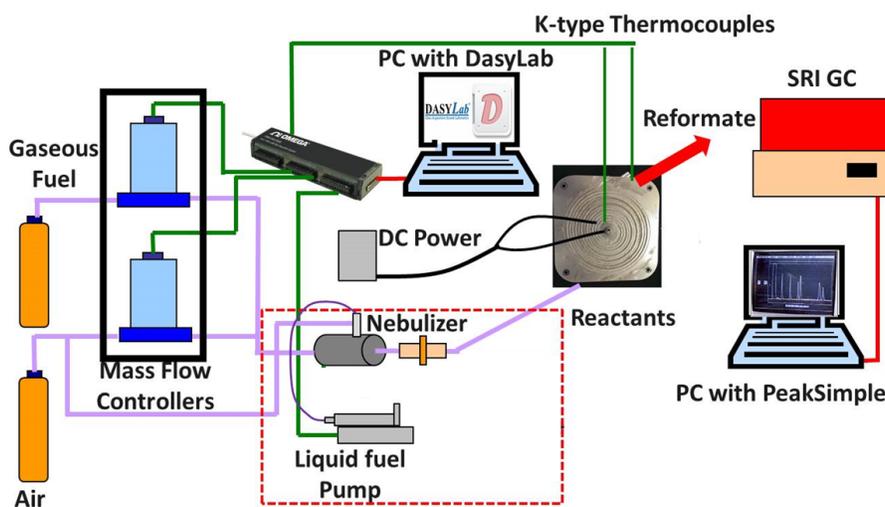
Figure 3. Schematic of the experimental apparatus for testing the 'Swiss-roll' reformer

Composition in the Reformate

Reforming tests have been conducted using different fuels including methane, propane, and n-heptane with current work is now focused on JP-8. Here, representative results for propane-air at an equivalence ratio of $\Phi = 3.0$ and Re = 157 are reported. Representative GC chromatograms are also shown in Figure 4. As shown, hydrogen accounts for 13.6% and CO for 16.8% of the reformate composition. The theoretical equilibrium composition for H_2 and CO is 28.8% and 21.5%, respectively. The H_2 yield is therefore about half of the equilibrium value while CO yield is about 20% below its equilibrium value.   Future testing will focus on optimizing the reformer design to further increase these yields.

Table 1: Reformate composition using propane-air in a six-turn reformer ($\Phi = 3$, Re = 157).

Measure Composition (vol %) of the Reformate						
H_2	CO	O_2	CH_4	CO_2	C_2H_6	C_3H_8
13.6	16.8	1.6	3.1	2.1	2.1	0.74
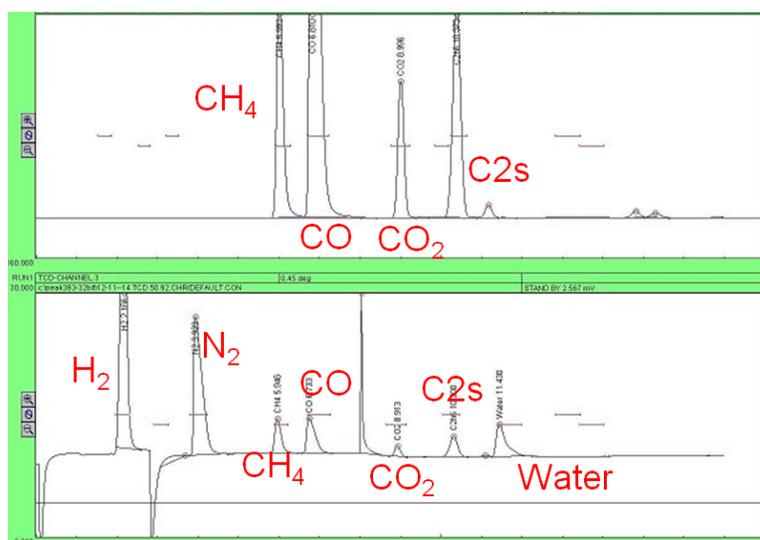
Figure 4: Representative GC chromatograms of the reformate composition.
Top: FID signal. Bottom: TCD signal.

3. Modeling

Reactor Based Model

Previous work [6, 8] has shown that under highly heat recirculation, the reaction zone of the Swiss-roll is more like a broad reaction zone instead of a thin flame. This result suggests that at highly heat recirculation condition, the center reaction zone can be treated as a Perfect Stirred Reactor (PSR) that internal diffusion effect is insignificant.   A reactor based model was developed using CHEMKIN. Here, the inlet channel was modeled as a 1D Plug Flow Reactor (PFR), the center reaction zone was modeled as a PSR, and the outlet channel was modeled a second PFR. The use of such a three reactor model system to model the Swiss-roll reformer is justified knowing that the reforming reactions largely take place in the center of the reformer, here modeled as a PSR. From the model, the transient and/or steady state temperature and species concentrations can be obtained as a function of initial composition, temperature, pressure, and flow residence time. Figure 5 shows an unrolled Swiss-roll reformer divide into inlet

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channel, center zone, and outlet channel sections. These three sections are model as PFR, PRS, and PFR in CHEMKIN as shown in Figure 6.

Figure 5. Unrolled Swiss-roll and divided it into three section: inlet channel, center zone, and outlet channel.
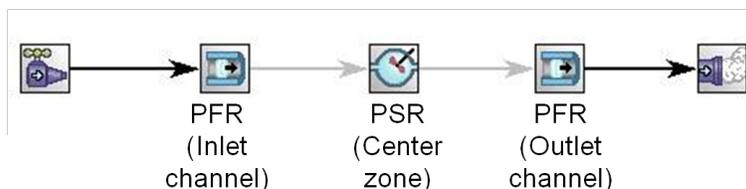
Figure 6. CHEMKIN graphic interface of unrolled Swiss-roll reformer.

The PFR + PSR + PFR reactor model verification was first performed by comparing the model predicted results with previous propane reforming experimental data. The propane reaction mechanism was downloaded from Lawrence Livermore National Laboratory (LLNL) contributed by Dr. Pitz and Dr. Westbrook's group [10].

A reactor model was built with the reactor dimension and operation condition similar to the experiment. The inlet and outlet channel were simulated as two PFRs with the channel length ~ 5 ft. The PFR reactor channel width is 4 mm and the center PSR reactor size is 70 cm^3. Both geometrical parameters are similar to the 6-turn prototype reactor. The operation condition is 50 cm/s (Re = 126) with Φ = 2.4. The thermal profile in the model is prescribed to match the experimental measurement. Figure 7 shows the model predicted result of the mole fraction of CO and H$_2$ in the outlet PFR. The comparison between model predicted result and experimental data is shown in Table 2.
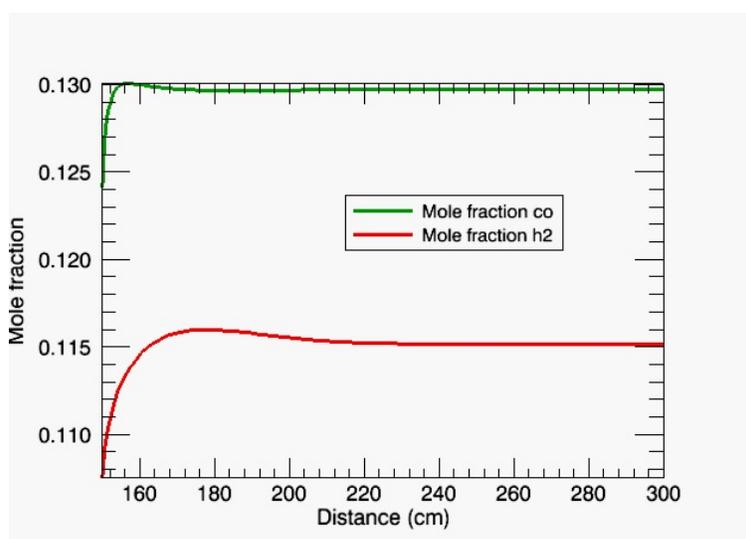
Figure 7: The mole fraction of H$_2$ and CO along the channel length in the outlet PFR model at the operation condition Re = 126 and Φ = 2.4.

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Table 2: Comparison of the mole fraction of H_2 and CO in the exhaust between experimental data and CHEMKIN model predicted result.

Species	Experiment	CHEMKIN Model
H_2	10%	11.5%
CO	16%	13%

CFD Model

A 2-D computational CFD model was developed using Fluent coupled with CHEMKIN CFD to compute the flow, species concentration, and temperature profiles in a Swiss-roll reformer. To illustrate the concept, computational results are reported here for rich methane-air at $\Phi = 2.6$ and Re = 220 (corresponding to a 1 m/s inlet velocity). The chemistry model used was GRI Mech 3.0. The computed temperature and velocity profiles are shown in Figure 8 showing the reactants are heated by the countercurrent hot reformate stream and reach a peak temperature near the center of the Swiss-roll reformer of 1776K. This is 559 K higher than the computed adiabatic flame temperature for this methane-air premixture (which is 1217K).

Velocity (m/s)   **Temperature (K)**
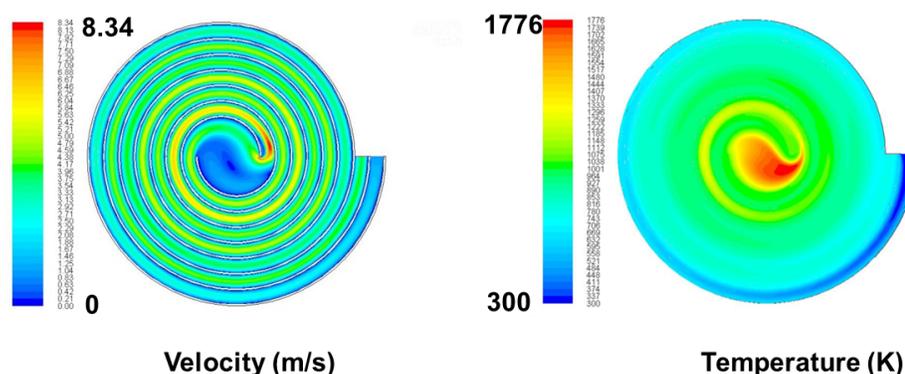
Figure 8: Computed velocity and temperature contours for rich CH_4-air reformation within a 3.5-turn Swiss-roll reformer.

The corresponding species profiles for this computational result for CH_4, H_2, CO, CO_2 and H_2O are shown in Figure 9. The H_2 and CO are first formed in the high temperature central reaction zone with some continued reaction in the entrance region of the exhaust stream eminating from the central core.

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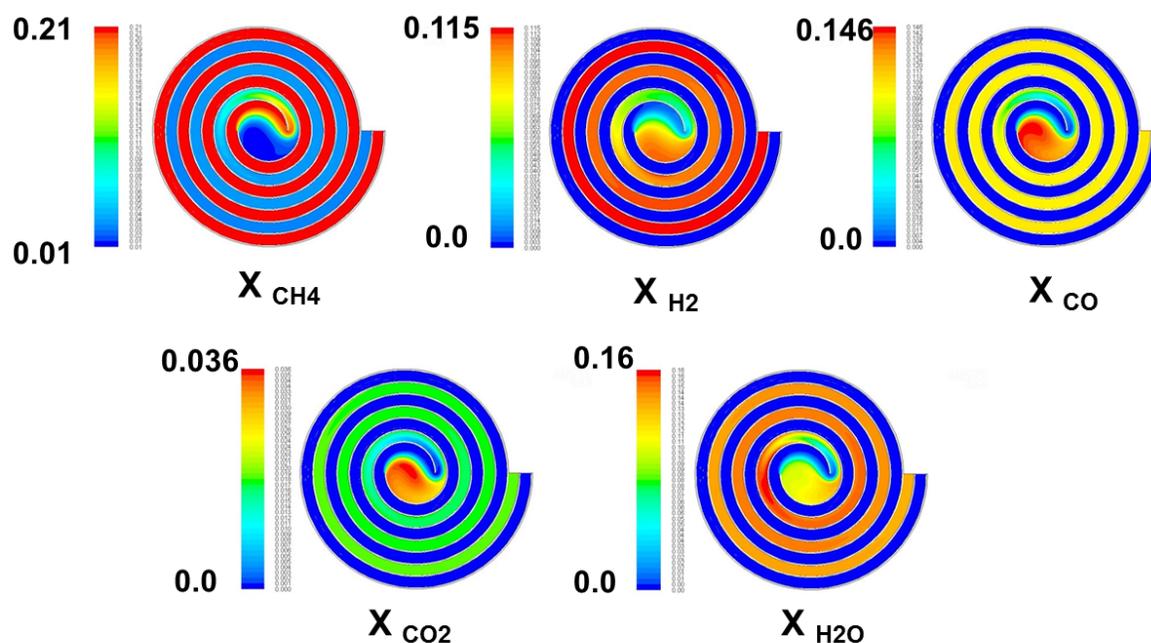
Figure 9: Computed species concentration contours for rich CH4-air reformation corresponding to the same conditions as in Figure 8.

For this case shown in Figure 9, the exhaust temperature and reformate species concentrations are summarized in Table 3 showing 11.5% H_2 and 11.0% CO. For comparison, the equilibrium yields for H_2 and CO are 27.3% and 14.5%, respectively.

Table 3: Comparison of the exhaust reformate species and temperature between FLUENT + CHEMKIN CFD and CHEMKIN at the same condition (1 m/s inlet velocity, $\Phi = 2.6$).

Species	FLUENT	CHEMKIN
CH_4	2.8%	2.95%
CO	11%	9.4%
H_2	11.5%	13.4%
CO_2	1.85%	1.87%
H_2O	13%	15.74%
C_2H_2	1.85%	2.11%
C_2H_4	0.4%	0.16%
C_2H_6	0.09%	0.04%
N_2	58%	54.3%
Total	99.99%	99.97%
T	757K	732K

4. Conclusions

Experiments and modeling works were performed to explore the use of a non-catalytic Swiss-roll TPOX-based reformer for converting hydrocarbon feedstocks to syngas mixture for use in solid oxide fuel cells or other combustion devices. Metallic Swiss-roll reformers made via both braze and 3D printing methods were successfully tested. Two model approaches (1D and 0D reactor based model and 2D CFD model) were developed and results shows good agreement with each other. The experiment results also show reasonable agreement with model predicted data. Further work is now being done to better understand the reforming process within the spiral heat exchanger through CFD simulations and additional experiments.

5. Acknowledgements

6. References

1) L. Bromberg, D. Cohn, A. Rabinovich, and J. Heywood, Int. Journal of Hydrogen Energy 26 (2001) 1115-1121.
2) M. Dixon, I. Schoegl, C. Hull, J. Ellzey, Combustion and Flame, 154 (2008) 217-231.
3) S. Lloyd and F. Weinberg, Nature, 251 (1974) 47-49.
4) A. Jones, S. Lloyd, F. Weinberg, P. R. Soc. London Section A.360 (1978) 97-115.
5) P. Ronney, Combustion and Flame, 135 (2003) 421-439.
6) C.-H. Chen and P. Ronney, Proc. Combust. Inst. 33 (2011) 3285-3291.
7) C.-H. Chen and P. Ronney, Combustion Theory and Modelling, 17 (2013) 888-905.
8) C.-H. Chen, PhD Thesis (2011).
9) C.-H. Chen, S. Sur, J. Thayer, H. Pearlman, P. Ronney, 8th U. S. National Combustion Meeting, May 19-22, 2013, Paper # 070MI-0132.
10) Marinov, N. M., W. J. Pitz, C. K. Westbrook, A. M. Vincitore, M. J. Castaldi, and S. M. Senkan, Combustion and Flame, 114, (1998) 192-213