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Spiral Methanol to Hydrogen Micro-Reformer for Fuel Cell Applications

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A spiral microchannel methanol reformer has been developed to provide power in conjunction with a micro fuel cell for a portable, low-power device. The design is optimized for low pumping power and rapid operation as well as thermal efficiency, overall size, and complete generation of the available hydrogen. An iterative, implicit, finite-element solution code, which locates the boundaries between liquid, two-phase, and gaseous flow, provides a complete solution of the fluid and heat transfer properties throughout the device. The solution employs experimentally verified available microchannel fluid dynamics relations to develop accurate results. Based on this analysis, the proposed microreformer design will have an overall maximum energy efficiency of 70%.

INTRODUCTION

Many battery chemistries in use today are mature technologies nearing their theoretical limit in terms of power density and they usually require a period of 1 up to 4 h to fully recharge, which limits their utility and the distance that portable devices can be taken away from the power grid. The energy density of fuel cell systems is 3–10 times that of batteries [1]. Fuel cells can be “recharged” instantly simply by adding more fuel. Additionally, there is no need for the device to ever be plugged in to the power grid, which makes a fuel-cell-powered device that much more portable. Fuel-cell exhaust products include only water in some cases and perhaps also carbon dioxide depending on the fuel, and these pose no harm to people or the environment. Although hydrogen is the best choice of fuel, it is cumbersome to store, and presents unique hazards of its own. A more energy-dense and more inert fuel would be preferable, but many fuels used in fuel cells tend to be troubled by contaminants. A better option would be to produce the hydrogen on board the device from a safe, hydrogen-rich fuel like methanol. Applications for portable electronic devices abound all around us, including cell phones, satellite phones, global positioning system (GPS) receivers, personal digital assistants (PDAs), notebook computers, sensing devices, and many others. Customers continue to demand that even more applications be freed from wires and become portable. Those devices that are already portable show a continuing need for higher power levels to support additional functionality and longer life between charges to increase their portability. Methanol reforming is traditionally an energy-intensive, high-temperature operation conducted at chemical process plants. Methanol reforming or methanol–steam reforming converts a methanol–water mixture to vapor and then heats it to a high temperature and pressure. The mixture is passed through a catalytic reactor, where the outputs of the operation are carbon dioxide and hydrogen gas. Then the carbon dioxide is separated from the hydrogen to result in a pure product.

There is considerable challenge to conducting this operation on board a small portable system. The lowest temperature, currently available catalyst is copper–zinc oxide (Cu/ZnO), which operates at temperatures as low as 200°C. Since the size of this reformer must be minimized, the objective must be to provide just the minimum dwell time required of the mixture in the presence of the greatest possible amount of catalyst surface.

New manufacturing techniques have expanded the possibilities for microchannel devices beyond silicon into glass, polymers, and other materials [2]. Silicon was originally used, as the manufacturing expertise already existed for that material, it was acceptable for a wide range of applications, and the equipment required was already in place throughout industry and university laboratories. Silicon microchannel manufacturing has already

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demonstrated the thin-wall capability desired for this application [3]. The spiral microreformer studied in this article can provide an effective, miniaturized source for hydrogen gas to power a micro fuel cell, and a single microchannel is etched onto a small piece of silicon and the spiral geometry permits a very efficient use of space with which to provide the approximately 4 m of channel length required for this application.

A successful design for a methanol microreformer requires the application of several disciplines. Since traditional or classical fluid and heat transfer science may not be applicable for all micro-scale applications, new studies are required to accurately predict the behavior of various designs. The available research is outlined here that is utilized for development analysis of this microreformer design. A review of polymer electrolyte membrane (PEM) fuel cells by Prater [4] verifies the basic assumptions made about the operational requirements of proton exchange membrane (PEM) fuel cells for this article, to ensure that the proposed microreformer will successfully operate as part of a system. The fluid passing through this microreformer design will experience many flow conditions, and a much wider variety will be experienced when considering all of the geometric variations studied to arrive at an optimized design.

Morini [5] and others have studied the laminar flow of liquid through microchannels. Among the significant findings is that classical Navier–Stokes equations remain valid for microchannels with hydraulic diameters as low as 30 µm. For flows of thin gasses, the classical equations do not continue to have such a strong hold on the phenomena of fluid flow in microchannels. Many investigators have studied the flow of gasses in microchannels, and a review by Yener et al. [6] provides a good description of the current state of research in this area. Relations identified by this review as well as those developed by Turner et al. [7] will be used to analyze the flow conditions in the superheat and catalytic reactor regions of the microreformer. Most research on laminar gas flow in microchannels focuses on thin, single-constituent gasses, or refrigerants [8]. In some cases steam is investigated, but little in the way of anything approximating a water–methanol mixture, so the study produced here will be employing these experimentally derived relations on new ground, although not outside of their prescribed flow conditions.

There is a need for verification of the flow effects of curved channels at the micro scale. For macro scales, the effects on flow separation, pressure drop, and other effects are known for pipe or channel bends and corners, but most microchannel studies involve only straight channels. The analysis presented here utilizes the macro relations for this effect [9].

Flow boiling is a complex phenomenon under any circumstances, and is made even more so, considering flow boiling in microchannels. However, considering the intrinsic benefits of latent heat transfer, several researchers are studying the topic, although the published results are not always in the best agreement, and wide scatter between the variously proposed correlated relations is a sign of the current state of research in this area. Kuznetsov et al. [10] conducted a review of various experimental results in this field. Among the significant findings were that accepted macrochannel relations would either drastically overpredict or underpredict the flow conditions in microchannel boiling. The relations given by Kandlikar [11] have been used. Of interesting note are the flow regimes observed for microchannel boiling, such as described by Bontemps et al. [12], and their effects on the heat transfer coefficient. As with other boiling applications, however, the best data will come as a result of testing in the specific flow conditions expected for the microreformer. Pattekar and Kothare [13] developed one application similar to that presented in this article, creating a bead-packed millimeter-wide channel reactor for the production of hydrogen sufficient for 10 W of electrical power. Their experimental approach demonstrated the feasibility of the design of this component as they successfully converted over 88% of the available hydrogen with a copper–zinc oxide (Cu/ZnO) catalyst and an operating temperature of 200°C as proposed here. The width of their rectangular channels was 1 mm and the overall device was a square approximately 4 cm per side. Earlier research by this team demonstrated the problem of catalyst fouling and the criticality of sufficient surface area and fluid dwell time for complete chemical conversion [14].

The catalyst for use in the chemical conversion region of the microreformer is of critical importance in creating a feasible device. Harold et al. [15], as well as others given in this reference, have studied various catalysts available for methanol reforming applications. From these studies, the most efficient low-temperature catalyst for methanol reforming appears to be copper–zinc oxide. Some unpublished research may prove that some new noble metal catalysts (incorporating Pt or Pd) can reduce the required reaction temperatures by as much as 80°C. Until those catalysts are available, however, feasibility analysis of this microreformer must rest on what is currently available.

The design of the microreformer presented in this article can provide an effective, miniaturized source for hydrogen gas to power a micro fuel cell. As seen in the concept model in Figure 1, a single microchannel is etched onto a small piece of silicon. The spiral geometry permits a very efficient use of space with which to provide the approximately 4 m of channel length required for this application. The spiral geometry reduces the amount of pressure required to drive the fluid through the device. Insulation to protect the high-temperature component from touch temperature hazards and eliminate excessive heat loss forms the greater part of the component volume. The primary improvements of this design are reduced pressure drop as compared to alternative nonspiral configurations and reduced device size as compared to other channel configurations.

**DESIGN REQUIREMENTS**

Potential applications for this micro-reformer include cellular and satellite phones, navigation devices, and portable computers. A gross power level of 1.5 W will be utilized as a design requirement, with a net power supplied to the device of at least vol. 30 no. 14 2009
1 W. This should correspond to a wide variety of portable electronic devices, including multifunction cell phones and other personal electronic devices.

The chemical reaction of the methanol–water mixture into hydrogen follows an endothermic reaction, and requires the following heat of formation to sustain this reaction: $q_{\text{chem}} = 59.17 \text{ kJ/kmol}$. At these mass flow rates for this microreformer design, this results in a power rate required of 0.17 W. According to [14], a 20-W PEM fuel cell operating at 80% efficiency requires a hydrogen flow rate of 0.372 mol/h. The efficiency in this case means that the fuel cell realizes 80% of the potential electrical power from the supply of hydrogen provided. Therefore, a 1.5-W fuel cell operating at a similar efficiency will require 0.028 mol/h of H$_2$. To continuously supply hydrogen sufficient to provide 1.5 W of electricity, a water–methanol mixture feed rate of 0.6074 cc/h is required, assuming a conversion efficiency of 90%. This assumes that the fuel mixture is a liquid at room temperature ($\sim$20°C). In our case, the fuel supply is provided by a pressurized cylinder sufficient to maintain the proper flow rate. The pressure can be maintained at a nearly constant value by the use of a suitable two-phase propellant where any increase in volume of the propellant side of the cylinder will result in the vaporization of a portion of the remaining liquid-phase propellant until equilibrium is reached. A device using a total of 1.5 W would require a fuel cartridge approximately the size of a single AA battery ($\sim$6.2 cc) to power it for more than 10 h. This corresponds, for example, to the high-power mode or talk time of a cell phone. By comparison, most lithium ion batteries currently in use for cell phones can support only about 3 h of active operational time. This is an increase of 3 to 5 times the power capacity on approximately one-half of the volume, when considering the impact of carrying additional power for extended periods away from the grid or other centralized source. Active device time is equivalent to talk time for a cell phone.

The metal oxide catalysts for the reforming reaction of the water–methanol mixture generally operate at temperatures between 200°C and 250°C. Therefore, the temperatures of the fluid and catalyst must be maintained at a temperature of at least 200°C for a period of time. Previous research has demonstrated that a dwell time of at least 750 ms is required to fully develop all of the available hydrogen at 200°C [16]. In order to maintain the temperature of the microreformer at 200°C, heat is applied from the reverse side of the channels on the silicon chip. Silicon has a relatively good thermal conductivity, so with a small package such as this microreformer the entire assembly is easily maintained at the same temperature. This heater must be sized so that its output balances the heat loss to the outside environment, the heat required to conduct the chemical reaction, and the heat absorbed by the incoming water–methanol mixture.

The microreformer heater must have an on–off controller to prevent energy consumption when the powered device is turned off. In sizing the heater, a choice must be made between minimizing the transient response time and balancing the heater output with the total heat loss from the microreformer at the maximum temperature, which would mean that no active thermostat-type control would be necessary. With $q_{\text{chem}} = 0.17 \text{ W}$, $q_{\text{preheat}} = 0.026 \text{ W}$, $q_{\text{phase\-change}} = 0.22 \text{ W}$, and $q_{\text{superheat}} = 0.030 \text{ W}$ the total power utilized to heat the fluid and sustain the chemical reaction is 0.446 W. This is approximately one-third of the total energy available in the hydrogen fuel stream generated by this microreformer and reserves ample power for a device such as a cell phone (more than 1 W). The overall efficiency of the reformer should be maintained as high as possible, which includes minimizing the heat loss. Both the size of the microreformer and the thickness of the insulation material affect the heat loss. Increases in the flow rate will result in more power output in the form of hydrogen gas, but will also increase the power necessary for the heating and conversion of the fuel.
The microreformer heater should have an output of 0.446 W plus any heat lost to the environment to balance the inputs and outputs. A number of devices already in existence are capable of providing the necessary heat within a small volume. If commercial small-scale heating elements were not desired, a simple printed wiring trace applied to the reverse side of the microreformer could provide the necessary source through resistive heating. The concept modeled in this article includes a disk-type heating element. The overall design configuration is shown in Figure 1. Since the thermal mass of the microreformer including the insulation is fairly small, the transient response of the system to startup of the heater should be rapid. However, as the channel changes geometry the fluid velocity changes and the transit time for the fluid varies significantly. The transient heat-up time and the fluid transit time should each be no longer than 2 s.

ANALYSIS AND OPTIMIZATION

In order to design a microchannel device one must choose an orientation of the channel to be constructed. While many are possible, some are more beneficial to a microreforming application than others. Among the most important criteria for this design are ease of manufacture, available surface area created, ability to accept future surface enhancements, and ease of packing the channel cross section into a compact device. While various types of microchannels have been created in silicon, such as triangular, trapezoidal, and rectangular, most previous research and experience have focused on rectangular channels. The cross-sectional configuration of the channel affects the heat transfer and fluid flow parameters of the device, with each configuration being more useful depending on what phenomena the designer is seeking to maximize or minimize. In consideration of a range of variations, a rectangular channel with a width to height ratio of 2:1 was selected. As with the cross-sectional configuration of the channel, the overall configuration of the layout or packing of the microchannel into a device is important. The packing configuration affects the pressure required to drive fluid through the device, and it affects the overall size of the device. An efficient packing configuration is required to optimize the device. Once the channel dimensional ratio is chosen, the layout of the channel within the device must be decided. Two general options are considered, including Archimedes’ spiral, and a square layout where the channel follows a rectangular path. The layout of the channel affects how much of the overall device is functioning channel and how much is wall space or other additional structure; this also determines how large the overall device must be to contain the necessary channel length. The layout of the channel through the sharpness and number of corners also affects how much pressure drop will be required to force fluid through the device. These quantities are compared in Table 1.

While many spiral configurations exist, the concentric spiral or Archimedes’ spiral has been chosen to provide the layout for this microreformer design. An Archimedes spiral increases its radius by a constant amount with each full revolution. This allows the microreformer to contain a constant channel width and a constant wall thickness. If any variation were desired, such as a constantly expanding channel, another Archimedean spiral could be employed.

An additional factor to consider in the optimal layout of the channel in the microreformer is the wall thickness required. This wall thickness must resist the internal pressure applied to the fluid to force it through the reformer. A thickness greater than is necessary will increase the size of the device, making the system less efficient. In order to determine the optimal thickness, a stress analysis was conducted. The minimum feasible wall thickness for current micro-electromechanical systems (MEMS) manufacturing techniques in silicon is 35 µm [3]. A finite-element analysis conducted using a commercial finite-element method (FEM) software package for the distributed loads caused by fluid pressure against the silicon walls found that the internal walls should have a thickness of 40 µm, while the exterior walls require a thickness of 70 µm. These values maintain a factor of safety of at least 5.

The microreformer accepts a liquid mixture of methanol and water as an input, and through a catalyzed reaction outputs a gaseous mixture of hydrogen, carbon dioxide, and water vapor. To accomplish this fuel reforming operation, the fluids pass through a heated microchannel and experience four distinct regions: liquid preheating, phase change, vapor superheating, and the catalyzed reactor. Each of these regions must be analyzed by different relations. The solution parameters are depicted in Figure 2.

Table 1 Comparison of channel packing orientations

<table>
<thead>
<tr>
<th></th>
<th>Spiral</th>
<th>Square</th>
</tr>
</thead>
<tbody>
<tr>
<td>Outer dimension (mm)</td>
<td>31.6</td>
<td>28.5</td>
</tr>
<tr>
<td>Total area (mm²)</td>
<td>785.6</td>
<td>812.3</td>
</tr>
<tr>
<td>Area efficiency (ε)</td>
<td>44.6%</td>
<td>43.1%</td>
</tr>
<tr>
<td>Equivalent length due to bends (L_e/D)</td>
<td>1308</td>
<td>2280</td>
</tr>
<tr>
<td>Additional pressure drop (mm H₂O)</td>
<td>117.5</td>
<td>204.9</td>
</tr>
</tbody>
</table>

Preheat Region

This zone consists of heating the incoming liquid mixture from room temperature up to the boiling point of the mixture. The entrance of the fluid mixture is assumed to be at a static pressure of 1.06 MPa (10.46 atm) and a temperature of 20°C. The mixture is composed of water (H₂O) and methanol (CH₃OH) at a 1:1 molar ratio. The respective volumetric and mass fractions of methanol in the mixture are 69.2% and 64.0% and the molar...
flow rate of hydrogen required to supply 1.5 W of power is 0.028 mol/h. The fuel mixture supply rate necessary to provide this amount of hydrogen is 0.6074 cc/h. The microchannel wall is maintained at a constant temperature of 200 °C by resistive heaters.

The Nusselt number for fully developed liquid laminar flow in a microchannel is identical to the classically derived value for hydraulic diameters as small as 30 μm [5], which is equal to 3.391.

In addition to the pressure drop required to force the fluid through the rectangular channel, one must also consider the pressure required to drive the fluid past the curved channel. The effects of curved channels or pipes or corners are given in terms of the equivalent length, meaning that from a friction factor perspective the bent channel is equal to its real length plus an equivalent length to account for the bend. The equivalent length data is determined by the ratio of the radius of the bend over the channel diameter. A curve fit to the data provided in [9] provides the equivalent length for each cell in the solution routine. Table 2 includes each of the equations utilized for the solution of this region.

### Phase Change Region

This zone consists of converting the liquid mixture at the boiling point to a saturated vapor mixture at the boiling point. The 1:1 molar mixture of water and methanol is directly heated by the three sides of the silicon microchannel surface. The expected flow regime is that of a vapor core surrounded by a liquid film covering the channel surfaces until the film finally disappears as the vapor quality reaches 100%. The convection coefficient for this section is based on microchannel boiling correlation from Lazarek and Black [17] in terms of the given boiling number Bo, which is the ratio between the amount of heat that is available to be absorbed by the liquid and the energy required to transform the liquid into a vapor. The expression developed by Warrier et al. [18] and also that developed by Kandlikar [11] are compared against that of Lazarek and Black to evaluate the optimum microreformer design. The complex relations for pressure drop in two-phase flow in microchannels, developed by Lockhart and Martinelli [19] and by Qu and Mudawar [20], are both used and compared in the evaluation of the microreformer design. Table 2 includes each of the equations utilized for the solution of this region.

### Superheat Region

This zone consists of heating the saturated vapor mixture at the boiling point to a superheated vapor mixture at 200 °C. The value for the Reynolds number indicates that the flow is laminar in this region, even considering the lower laminar to turbulent transition value for microchannel flow. Microchannel

<table>
<thead>
<tr>
<th>Region</th>
<th>Relations utilized</th>
</tr>
</thead>
<tbody>
<tr>
<td>Preheat</td>
<td>( T_h = T_{wall} - \frac{T_{wall} - T_{in}}{\exp\left(\frac{\mu_{liq}}{\mu_{num}}\right)} ), ( Re_{n} = \frac{\rho_{liq} \cdot \mu_{num} \cdot D_{h}}{\mu_{n}} )</td>
</tr>
<tr>
<td>Phase change</td>
<td>( dP_{n} = f_{s} \left( L_{n} + E L_{D_{h}} \right) \frac{\rho_{liq}}{\beta_{liq}} \mu_{n} ), ( f_{s} = 62.2 \frac{Re_{n}}{K_{0}} )</td>
</tr>
<tr>
<td></td>
<td>( Nu_{3} = 8.235(1 - 1.883 \beta + 3.767 \beta^{2} - 5.814 \beta^{3} + 5.316 \beta^{4} - 2.000 \beta^{5}) )</td>
</tr>
<tr>
<td></td>
<td>( Nu_{4} = 8.235(1 - 2.042 \beta + 3.085 \beta^{2} - 2.477 \beta^{3} + 1.058 \beta^{4} - 0.186 \beta^{5}) )</td>
</tr>
<tr>
<td></td>
<td>( Bo_{n} = \frac{G_{h} \cdot C_{0} \cdot \mu_{n} \cdot (T_{in} - T_{out})}{\mu_{n} \cdot \rho_{liq} \cdot D_{h}} )</td>
</tr>
<tr>
<td></td>
<td>( h_{p} = N_{wall} \cdot h_{p, max}(E, S), \ h_{d} = 0.023(Re_{num})^{0.3} \left( \frac{Pr_{liq}}{Pr_{num}} \right)^{0.4} \frac{h_{in}}{Pr_{num}} )</td>
</tr>
<tr>
<td></td>
<td>( E = 0.6683Co^{-0.2} + 1058Bo^{0.7} ), ( Co = \frac{1 - V_{d}}{V_{d}} \left( \frac{Pr_{num}}{Pr_{liq}} \right) )</td>
</tr>
<tr>
<td></td>
<td>( S = 1.136Co^{-0.9} + 667.2Bo^{0.7} )</td>
</tr>
<tr>
<td></td>
<td>( \frac{h_{in}}{Pr_{num}} = 1 + \frac{c}{X_{S}} + \frac{c}{X_{C}} )</td>
</tr>
<tr>
<td></td>
<td>( C = 21 \left( 1 - e^{-0.339 \times 10^{3} D_{h}} \right) 0.006418G + 0.0613 )</td>
</tr>
<tr>
<td>Superheat</td>
<td>( Nu = Re_{num}^{0.62} ) [6], ( Nu = \frac{k_{x}}{D_{h}}, \ K_{n} = \frac{k_{x} T}{\sqrt{2 \pi}} )</td>
</tr>
<tr>
<td></td>
<td>( Re_{n} = \frac{\rho_{liq} \cdot \mu_{num} \cdot D_{h}}{\mu_{n}} ), ( T_{h} = T_{wall} - \frac{T_{wall} - T_{in}}{\exp\left(\frac{\mu_{liq}}{\mu_{num}}\right)} )</td>
</tr>
<tr>
<td></td>
<td>( \frac{dP_{n}}{X_{So}} = \frac{96}{\pi} \left( \frac{1}{T_{wall}} - \frac{T_{in}}{T_{in}} \right) \frac{1}{K_{n}} )</td>
</tr>
</tbody>
</table>

Table 2  Relations used for simulation model in each region.
The laminar–turbulent transition begins at Reynolds number equal to 1600 [11].

The Nusselt number variation with the Reynolds number for fully developed laminar flow in a microchannel given by [14] is used. Table 2 includes each of the equations utilized for the solution of this region.

**Catalytic Reactor Region**

This zone consists of chemically converting the superheated vapor mixture of methanol and water into a mixture of hydrogen and carbon dioxide. The key parameter in this zone is the dwell time of the vapor mixture in the presence of the Cu/ZnO catalyst. Previous research has demonstrated that a period of 750 ms is required to fully convert the mixture [16]. The length of the channel in this section is governed entirely by having the fluid experience the necessary dwell time of 750 ms. However, the fact that the mixture is changing chemical constituents results in other varying physical properties such as density, speed of sound, viscosity, and other properties, thus requiring an iterative solution in this section also. The model is based upon a linear curve that transforms an equal part of the whole mass for each fraction of time spent in contact with the catalyst.

The heat flux into the fluid throughout this section is governed by the amount of heat required to sustain the chemical reaction, since the fluid has already reached the wall temperature by the time this zone begins. It may be possible to utilize a catalyst operating at a lower temperature, which would permit us to design a smaller and more efficient reformer. The total time required to traverse the total channel length is important for minimizing the startup time of the reformer. A shorter startup time reduces the time required between turning a device on and the application of full power. This reactor utilizes a copper–zinc oxide (Cu/ZnO) catalyst, which has been shown to operate with greater than 88% conversion efficiency at 200°C [13]. This catalyst is deposited on the bottom surface of the microchannel.

In this region of the microreformer, the effects of pressure drop by slip flow could become significant. Additionally, an exponential model of the catalytic reaction will be utilized for the determination of effects on the overall fluid properties. The exponential reaction model assumes that the reaction proceeds exponentially, with the total reacted hydrogen gas reaching 99% at 750 ms. The maximum and minimum fluid properties are essentially unchanged by the use of either a linear or exponential model, but some cumulative properties such as pressure drop are affected by the use of one model over the other. From knowledge of previous experiments [14], the exponential model is likely to be more accurate. The general outline of the properties in reactor region is displayed in Figure 3. All of the relations in this region are equivalent to those of the superheat region (shown in Table 2); however, the fluid properties are changing due to the chemical conversion.

![Figure 3](http://example.com/fig3.png)

**Figure 3** Flow Properties for four stages of microreformer.
RESULTS AND CONCLUSIONS

All quantities considered in this section are evaluated from a minimum width of 20 µm to a maximum width of 400 µm. In the preheat, phase change, and superheat regions the channel length is determined by the heat transfer coefficient, while the length of the catalytic reactor is determined by the dwell time. The necessary channel length varies from a maximum of 2244 meters for a 20-µm channel to a minimum of 1.6 m for a 400-µm-wide channel. The overwhelming majority of the channel length is devoted to the catalytic reactor region. On average, less than 1% of the total channel length is devoted to the preheat, phase change, and superheat regions combined. The total channel length directly affects the total size of the device, but not in a simple linear fashion. An equal length of spiral channel can be cut into both sides of the device. One can observe that the packing efficiency of the spiral configuration is quite high, as over 2200 m of channel can be held on a circular surface only 10 cm in diameter.

Another reason that the device diameter is important is that it affects the amount of heat lost to the environment, and thus can decrease the efficiency of the reformer in providing more power than it uses. The heat loss is calculated by considering the device outer surface at an insulated temperature around 45°C, the maximum permitted for safe continuous skin contact [21]. Using a typical free convection model for air, the values for heat loss were derived. In reality, some of this heat could be used to maintain the temperature of the fuel cell, or some heat could be recaptured from waste heat given off by the supplied devices electronics. But the results, as shown in Figure 4, should be considered a good estimate of potential losses, although probably at the high end.

As the fluid is heated it expands and loses density, especially in its vapor form, and from that expansion the fluid must accelerate. As the channel size is decreased, the maximum velocity of the fluid increases. That continues without abatement until the fluid in very small channels approaches the speed of sound. However, since there is no nozzle to permit acceleration beyond that velocity, the flow is choked and the curve of resulting properties takes a different path.

The complication to the Mach number calculation in the catalytic reactor region is the changing chemical constituents of the fluid. As methanol vapor, steam, hydrogen, and carbon dioxide have different sonic values, the sonic value of the fluid account must take into account what stage of the conversion is in effect for the particular cell being analyzed. Figure 4 displays the maximum Mach number versus channel width for the microreformer. A good rule of thumb to avoid compressibility effects is to maintain the maximum Mach number below 0.15 [22]. In order to comply with this criterion, the microreformer channel width must be 85 µm or greater.

In addition to compressibility effects, the potential for turbulence must be considered. The small channel sizes and high fluid velocities have the potential to produce turbulence prior to the normal flow transition point. Typically, the laminar–turbulent transition point is said to begin around Re = 2300. However, in microchannels, the transition can begin as early as Re = 1600 [11]. All channel widths produce flow conditions that are expected to be entirely laminar. Due to this observation, no limitations on the optimum channel width will be made so as to avoid turbulent conditions.

In considering flows of thin gasses in very small channels, one must also be aware of the effects of rarefied flow conditions. While the gasses in this microreformer are not particularly thin, the molecule size of methanol is rather large, and so the same effects may be encountered in small channels as for thin gasses. These rarefied flow conditions challenge the continuum assumption made in most calculations. The Knudsen number provides a measure of how applicable the continuum assumption is for the flow being studied, with the assumption becoming less valid as the Knudsen number increases. The highest Knudsen number for each channel width was analyzed; for example, for a 20-µm channel, it was 0.0022. This means that the continuum assumption is valid for most channel widths, with only some small effects becoming evident for channels narrower than 50 µm.

The total time fluid takes to traverse the entire device is of importance to the operation of the microreformer. If an end user has to wait for 10 s after turning a system on before it reaches full power and becomes operational, that may be too long. The transit time increases as the channel width increases, but this quantity should be minimized for ideal operation. A maximum transit value of 2 s is established, which limits the channel width to less than 290 µm. Another quantity to consider is the available reactor surface area. By the present proposed method of depositing a layer of catalyst on the bottom, the surface area in the lower surface of the channel can be easily compared across the possible geometries. Since a greater amount of catalyst reduces the possibility of fouling and increases the efficiency of the conversion, this surface area quantity should be maximized. That leads one to favor the smallest possible channel width allowed by the other constraints.

Figure 4 Microreformer optimization displaying pressure drop, heat loss, Mach number, and transit time.
The total pressure drop of the device is equivalent to the static pressure at the inlet required to maintain the necessary mass flow rate through the device. Too much pressure drop, and the device could become infeasible due to the large pump or pressure vessel required to force the fluid through the microreformer. Figure 4 plots the total pressure drop of the device against the channel width. As would be expected, smaller channels require greater amounts of pressure than larger channels. The linear and exponential models for the chemical reaction do produce some difference on cumulative flow properties, such as total pressure drop, with the exponential model tending to require slightly lower pressures than the linear model. This is due to the fact that the end-product gases of hydrogen and carbon dioxide provide less flow resistance than input gases of methanol and water vapor. Collecting all of the criteria established in this section and plotting those relevant criteria and the applicable data on a single plot, as given by Figure 4, will give us a good understanding of the optimal channel width to select from these competing values. In addition, considerations of the reactor surface area lead one to minimize the channel width to the extent possible. Treating the various factors equally, the minimization of both transit time and heat loss occurs at their point of intersection, which is nearest the channel width of 255 \( \mu \text{m} \).

Based on the data realized on this design from the simulation model, we have calculated the maximum theoretical efficiency considering the energy required to perform the reforming reaction and the energy made available by that reaction as shown by the equation below. That efficiency was found to be 70%. Based on the amount of insulation provided to prevent heat loss to the environment, the actual efficiency would be lower. For example, only reducing the exterior temperature to 40°C, would result in an efficiency of 42%.

\[
\text{Efficiency} = \frac{\text{Total Potential Power from Reformed Hydrogen} - \text{Energy Required for Reforming} - \text{Heat Loss}}{\text{Total Potential Power from Reformed Hydrogen}}
\]

The microreformer design presented here has proven feasible based on the analyses performed to provide a safe, clean hydrogen source for a micro fuel cell. The scale and power requirements of this design are consistent with the needs of small-scale personal electronic devices. The cost of the materials involved is low, as well as the required assembly tasks. The flow conditions at each point of the microreformer have been determined by a finite-element code developed especially to optimize the geometry and flow conditions of this design. This analysis tool has demonstrated its value in that any changes to geometry, flow conditions, or thermal characteristics can be quickly evaluated for their effect on the fluid at each point along its travel and transformation process. While this design could likely be implemented into a portable power system, the current size and efficiency may only be sufficient for highly specialized portable electronic equipment for use by surveyors, military, adventurers, and pipeline or power line inspectors.
REFERENCES


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