Mathematical modeling of transport phenomena in chemical reactors

Junjie Chen (cjmmmm@163.com)
Department of Energy and Power Engineering, School of Mechanical and Power Engineering, Henan Polytechnic University, Jiaozuo, Henan, P.R. China

Research Article

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Junjie Chen*

Department of Energy and Power Engineering, School of Mechanical and Power Engineering, Henan Polytechnic University, Jiaozuo, Henan, 454000, P.R. China

* Corresponding author, E-mail: cjjmmm@163.com

Abstract

Endothermic reactions performed in thermally integrated microchannel reactors are driven using heat from an external source. However, the temperature of the gas stream providing the heat is limited by constraints imposed by the materials of construction. This study relates to a thermochemical process for producing hydrogen by the catalytic endothermic reaction of methanol with steam in a thermally integrated microchannel reforming reactor. Computational fluid dynamics simulations are conducted to better understand the consumption, generation, and exchange of thermal energy between endothermic and exothermic processes in the reactor. The effects of wall heat conduction properties on heat transfer characteristics and reactor performance are investigated. Processes of conducting reactions in integrated combustion reactors are described and the results are presented. Particular reactor designs are also described. The results indicate that asymmetric operation requires spatial distribution of the feed for the exothermic reaction in order to prevent excess temperatures and to ensure stable operation. The peak reaction heat flux increases with the channel dimensions while maintaining the flow rates. The change in specific enthalpy is positive for the exothermic reaction and negative for the endothermic reaction. The change in specific sensible enthalpy is always positive. The thermal conductivity of the channel walls is fundamentally important. Materials with high thermal conductivity are preferred for the channel walls. Thermally conductive ceramics and metals are well-suited. The application of autothermal reactor concepts can be extended to endothermic high temperature reactions. Advantages are the compact design which allows fast start-up and load changes. Drawbacks include the dilution of the reforming product with nitrogen if air is used as oxidant.

Keywords: Transport phenomena; Autothermal reactors; Endothermic reactions; Exothermic reactions; Thermal conductivity; Thermodynamic systems

1. Introduction

In engineering, physics and chemistry, the study of transport phenomena concerns the exchange of mass, energy, charge, momentum and angular momentum between observed and studied systems [1, 2]. While it draws from fields as diverse as continuum mechanics and thermodynamics, it places a heavy emphasis on the commonalities between the topics covered. Mass, momentum, and heat transport all share a very similar mathematical framework [3, 4], and the parallels between them are exploited in the study of transport phenomena to draw deep mathematical connections that often provide very useful tools in the analysis of one field that are directly derived from the others. The fundamental analysis in all three subfields of mass, heat, and momentum transfer are often grounded in the simple principle that the sum of the quantities being studied must be conserved by the system and its environment [5, 6]. Consequently, the different phenomena that lead to transport are each considered individually with the knowledge that the sum of their contributions must equal zero [7, 8]. This principle is useful for computing many relevant quantities [9, 10]. For example, in fluid mechanics, a common use of transport analysis is to determine the velocity profile of a fluid flowing through a rigid volume.
In physics, transport phenomena are all irreversible processes of statistical nature stemming from the random continuous motion of molecules, mostly observed in fluids \[11, 12\]. Every aspect of transport phenomena is grounded in two primary concepts: the conservation laws, and the constitutive equations. The conservation laws, which in the context of transport phenomena are formulated as continuity equations, describe how the quantity being studied must be conserved \[13, 14\]. The constitutive equations describe how the quantity in question responds to various stimuli via transport \[15, 16\]. Examples of transport processes include heat conduction, fluid flow, molecular diffusion, and radiation \[17, 18\]. Transport phenomena have wide application \[19, 20\]. For example, in solid state physics, the motion and interaction of electrons, holes and phonons are studied under "transport phenomena". In chemical engineering, transport phenomena are studied in reactor design, analysis of molecular or diffusive transport mechanisms, and metallurgy.

Transport phenomena are ubiquitous throughout the engineering disciplines. Some of the most common examples of transport analysis in engineering are found in the fields of process, chemical, and mechanical engineering, but the subject is a fundamental component of the curriculum in all disciplines involved in any way with fluid mechanics, heat transfer, and mass transfer \[21, 22\]. It is now considered to be a part of the engineering discipline as much as thermodynamics, mechanics, and electromagnetism \[23, 24\]. Recently, a thermally integrated microchannel chemical reactor has been developed for simultaneously conducting exothermic and endothermic reactions \[25, 26\]. There is a continuing effort to perform steam reforming reactions in thermally integrated microchannel chemical reactors \[27, 28\]. However, the mechanisms for the effects of design factors on heat transfer characteristics are still not fully understood.

The present study relates to a thermochemical process for producing hydrogen by the catalytic endothermic reaction of methanol with steam in a thermally integrated microchannel reforming reactor. Computational fluid dynamics simulations are conducted to better understand the consumption, generation, and exchange of thermal energy between endothermic and exothermic processes in the reactor. The effects of wall heat conduction properties on heat transport characteristics and reactor performance are investigated. The objective of this study is to gain insight into the fundamental characteristics of heat transfer in thermally integrated microchannel reforming reaction systems. Particular emphasis is placed on the dependence of heat transfer characteristics on wall heat conduction properties in various situations, with an attempt to improve the distribution of thermal energy for use in microchannel reforming reaction systems.

2. Computational methods

2.1. Description of the reactor

The present study relates to a thermally integrated microchannel methanol reforming reactor. The reactor consists of a set of combustion channels and a set of reforming channels in an alternating arrangement. The thermally integrated microchannel reactor is depicted schematically in Figure 1. The straight channels can be configured and manifolded for simultaneous passage of different process reactant streams with flow paths in counter-current, cross-flow, or co-current flow modes. In the present study, the reactor is configured to operate in a co-current flow mode, and each channel contains a layer of catalyst, as depicted schematically in Figure 1. A reactant stream of methanol and air is introduced into the combustion channels and a reactant stream of methanol and steam is introduced into the reforming channels. The flow paths are configured in the reactor to thermally contact exothermic and endothermic reactant streams in adjacent channels.
Figure 1. Schematic illustration of the thermally integrated microchannel methanol reforming reactor used to simultaneously conduct exothermic and endothermic reactions. The channel walls are not depicted for clarity.

A high temperature exothermic reaction takes place in the combustion channels and the reforming process reactant stream simultaneously undergoes an endothermic reaction in the reforming channels. No flame combustion is involved in the process. The catalyst layers in each channel are designed in an opposed relationship such that the exothermic heat of reaction taking place within the catalyst layers of the first set of flow channels can be transferred conductively directly through the channel walls to the catalyst layers of the second set of flow channels. The catalytically active surface area or catalyst loading can be balanced between the two sets of channels. In this context, the heat released by the exothermic reaction could be entirely consumed by the endothermic reaction, thereby avoiding heat imbalances within the thermally integrated microchannel methanol reforming reactor or reducing the likelihood of the formation of hot spots within the catalyst layers, which could sinter or deactivate if exposed to high temperatures. Although the combustion may have both homogeneous and heterogeneous contributions, catalytic combustion in a microchannel, or a channel with a minimum open dimension less than or slightly greater than the quench diameter, will reduce the contribution of homogeneous reactions and favor heterogeneous combustion. This will also further enhance safety by reducing gas phase reactions that might otherwise take the combustion mixture well above the safe operating temperature limit of the material. Inhibition of gas phase combustion grows stronger with decreasing channel minimum dimension and with increasing catalytic surface area.

The temperature of the reactant streams is 373 K at the flow inlets, with a pressure of 2.0 MPa. The equivalence ratio of fuel to air is 0.8 and the steam-to-carbon molar ratio is 1.4. The velocity of the process reactant stream and the combustible reactant stream is 2.0 and 0.6 m/s, respectively, at the flow inlets. The cross-sectional shape of the channels is square, with a side length of 0.7 mm. The channels are 50.0 mm in length. The catalyst layers and the channel walls are 0.1 and 0.7 mm, respectively, in
thickness. At room temperature, the thermal conductivity, which indicates the ability to conduct heat, of the channel walls is 200 W/(m·K). An integrated combustor can use the high surface area of reactor microchannels to remove heat as it is produced, thus keeping microreactor components from exceeding material temperature constraints while combusting with much less excess air than would be necessary for an external combustor. The exothermic reaction chamber comprises at least one exothermic reaction chamber wall that is adjacent at least one endothermic reaction chamber. The endothermic reaction chamber comprises an endothermic reaction catalyst in contact with at least the at least one endothermic reaction chamber wall that is adjacent at least one exothermic reaction chamber, and transferring heat from the at least one exothermic reaction chamber into the at least one endothermic reaction chamber.

2.2. Mathematical model

The model consists of channel walls with the adjacent combustion and reforming half-channels in a co-current flow configuration. The mathematical model is solved and implemented in ANSYS FLUENT to obtain the problem solution. ANSYS FLUENT permits multi-dimensional modeling of physical and chemical phenomena in the processes, and various modes of heat transfer can be modeled. In chemical engineering, diffusion is responsible for mass transfer. Three different patterns of diffusion are responsible in this process: ordinary diffusion, thermal diffusion, and pressure diffusion. Theory of diffusion primarily focuses on the mass-flux vector and its relation to concentration gradients and diffusion coefficients. These diffusion coefficients have to be estimated to make computations of practical interest. There are numerous ways of expressing concentration in diffusion problems, the most important for the purposes being mass density, molar density, mass fraction, and mole fraction.

The continuity equation is given by

\[
\frac{\partial (\rho u_x)}{\partial x} + \frac{\partial (\rho u_y)}{\partial y} + \frac{\partial (\rho u_z)}{\partial z} = 0,
\]

where \(x, y,\) and \(z\) are coordinate variables, \(\rho\) is the density, and \(u\) is the velocity.

The momentum conservation equations can be written as

\[
\frac{\partial p}{\partial x} + \frac{\partial }{\partial x}\left[\frac{2}{3} \mu \left(\frac{\partial u_x}{\partial x} + \frac{\partial u_y}{\partial y} + \frac{\partial u_z}{\partial z}\right)\right] + \frac{\partial }{\partial y}\left[\mu \left(\frac{\partial u_x}{\partial x} + \frac{\partial u_y}{\partial y}\right)\right] + \frac{\partial }{\partial z}\left[\mu \left(\frac{\partial u_x}{\partial x} + \frac{\partial u_z}{\partial z}\right)\right] = 0,
\]

(2)

(3)

(4)

where \(p\) is the pressure, and \(\mu\) is the dynamic viscosity.

The energy conservation equation is given by
\[
\frac{\partial (\rho u, h)}{\partial x} + \frac{\partial (\rho u, h)}{\partial y} + \frac{\partial (\rho u, h)}{\partial z} + \frac{\partial \left( \rho \sum_{k=1}^{\gamma} w_k h_k V_{k,z} - k_g \frac{\partial T}{\partial x} \right)}{\partial x} + \frac{\partial \left( \rho \sum_{k=1}^{\gamma} w_k h_k V_{k,y} - k_g \frac{\partial T}{\partial y} \right)}{\partial y} + \frac{\partial \left( \rho \sum_{k=1}^{\gamma} w_k h_k V_{k,z} - k_g \frac{\partial T}{\partial z} \right)}{\partial z} = 0,
\]

where \( h \) is the enthalpy, \( k \) is the thermal conductivity, \( T \) is the temperature, \( \gamma \) is the total number of gaseous species, \( w \) is the mass fraction, and \( V \) is the diffusion velocity. The subscripts \( k \) and \( g \) denote gaseous species \( k \) and the gas mixture, respectively.

The species conservation equation can be written as

\[
\frac{\partial (\rho u, w_k)}{\partial x} + \frac{\partial (\rho u, w_k)}{\partial y} + \frac{\partial (\rho u, w_k)}{\partial z} + \frac{\partial (\rho w_k V_{k,z})}{\partial x} + \frac{\partial (\rho w_k V_{k,y})}{\partial y} + \frac{\partial (\rho w_k V_{k,z})}{\partial z} - \dot{\xi}_k W_k = 0,
\]

\( k = 1, \ldots, K_g \)

where \( W \) is the molecular mass, and \( \dot{\xi}_k \) is the rate of production by gas-phase reaction.

The surface species conservation equation is given by

\[
\theta_n \dot{\xi}_m \Gamma^{-1} = 0, \quad \omega = \gamma + 1, \ldots, \gamma + \delta,
\]

where \( \theta \) is the coverage, \( \omega \) and \( \delta \) are the total number of chemical species and surface species, respectively, \( \Gamma \) is the active site density, and \( \dot{\xi}_k \) is the rate of production by surface reaction. The subscript \( m \) denotes surface species \( m \).

The energy conservation equation of the solid phase can be written as

\[
\frac{\partial \left( k_s \frac{\partial T}{\partial x} \right)}{\partial x} + \frac{\partial \left( k_s \frac{\partial T}{\partial y} \right)}{\partial y} + \frac{\partial \left( k_s \frac{\partial T}{\partial z} \right)}{\partial z} = 0.
\]

where the subscript \( s \) denotes the solid walls.

Equilibrium conversion is defined in the classical manner, where the maximum attainable conversion is a function of the reactor temperature, pressure, and feed composition. For the case of steam reforming reactions, the equilibrium conversion increases with increasing temperature and decreases with increasing pressure.

Reaction chamber volume is the internal volume of a reaction chamber. This volume includes the volume of the catalyst, the open flow volume and metal support ribs or fins within the reaction chamber volume. This volume does not include the reaction chamber walls. The reaction chamber volume must contain a catalyst somewhere within its cross-section and must be directly adjacent another reaction chamber for heat transport. This volume is used for computations of endothermic reaction chamber volumetric heat flux, area heat flux, and endothermic reaction contact time.

Heat exchanger flux is defined as the total heat transferred to the cold streams divided by the heat exchanger core volume.

Heat exchanger core volume is defined as the total heat exchanger volume inclusive of microchannels, ribs between microchannels, and the walls separating microchannels for all fluid streams transferring heat. The heat exchanger volume is inclusive of the heat exchanger region described for the reactor. The heat exchanger core volume does not include the perimeter metal or manifolds or headers. The heat exchanger core volume does not include the endothermic reaction chamber nor any volume that could be included within any plane that bisects the endothermic reaction chamber orthogonal to the direction of flow.

Average area heat flux is defined as the endothermic reaction heat duty divided by the area of the
endothermic reaction chamber heat transfer surface. The endothermic heat transfer surface is defined by a planar area, which may be intermittent in the case of ribs or other structures in the endothermic reaction chamber, above which there is area for flow of reactants and below which there is a wall that separates the endothermic reaction chamber and the exothermic reaction chamber. This area is the path for heat transfer from the exothermic reaction chamber to the endothermic reaction chamber.

2.3. Numerical algorithms

The computational domain is divided into discrete control volumes using a computational grid. The typical mesh consists of about 600,000 nodes in total. The governing equations are integrated on the individual control volumes to construct algebraic equations for the discrete dependent variables such as temperature, pressure, velocities, and conserved scalars. The discretized equations are linearized and the resultant linear equation system is solved to yield updated values of the dependent variables. The constraint of mass conservation of the velocity field is achieved by solving a pressure equation. The pressure equation is derived from the mass and momentum conservation equations in such a way that the velocity field, corrected by the pressure, satisfies the continuity. The second-order upwind spatial discretization scheme is used for the convection terms of each governing equation. Pressure-velocity coupling is achieved by using the standard SIMPLE algorithm. The under-relaxation parameters are reduced for all variables. Convergence is judged by examining residual levels.

2.4. Validation of the model

To verify the accuracy of the model, the predictions are compared with the data obtained from experimental measurements [29, 30]. The cross-sectional shape of the channels is rectangular. The channels have a height of 0.6 mm, a width of 0.5 mm, and a length of 33.0 mm. The reaction temperature varies from 473 to 533 K. The steam-to-carbon molar ratio is 1.1 for the reforming process. The reaction chamber wall is thermally conductive. The methanol conversion is plotted in Figure 2 against temperature. Methanol conversion is determined by measuring the outlet product composition and the outlet flowrate of methanol reforming reaction products. The predictions are in satisfactory agreement with the data obtained from experimental measurements.

![Figure 2. Methanol conversion at different reaction temperatures. The experimental data are included for comparison. The cross-sectional shape of the channels is rectangular.](image-url)
4. Results and discussion

The reaction heat fluxes are investigated to better understand the thermal coupling between the endothermic and exothermic streams. The results are presented in Figure 3, in which the endothermic and exothermic reaction heat fluxes are plotted against the streamwise distance. The channels are 0.7 mm in width. The exothermic catalytic combustion reaction provides the necessary heat flux to increase the temperature of the reactants in both channels such that the endothermic reaction will occur. Heat flux is a vector quantity, and therefore the heat flux is negative for the endothermic steam reforming reaction. The exothermic heat flux is greater than the absolute value of the endothermic heat flux. The peak exothermic heat flux is located upstream of the peak endothermic heat flux. An un-uniform catalyst distribution could be employed for the reactor so as to provide optimum synchronization of the reaction fluxes of heat consumption and generation in the endothermic reforming and exothermic combustion channels, respectively. The contact time for the steam reforming reaction may be up to about one second. The microchannel reactor may comprise a plurality of plates in a stack [31, 32], the steam reforming reaction being conducted for at least about thousands of hours without metal dusting pits forming on surfaces of the plates. The microchannel reactor comprises an endothermic process layer and an exothermic heat exchange layer. The reactor core volume is defined as the reaction chamber volume and all combustion chamber volume and the metal webs that separate the two chambers. The combustion chamber volume is defined as the chamber volume in which the exothermic heat generating reaction occurs and is adjacent to the reaction chamber volume. Perimeter metal is not included in reactor core volume. The reactor core volume does not include any preheat exchanger region volume that may or may not be attached to the reactor core volume. The preheat exchanger region may be attached to the reactor but does not contain an endothermic reaction catalyst along any plane that bisects the device orthogonal to the direction of flow.

![Figure 3. Endothermic and exothermic reaction heat fluxes as a function of the streamwise distance for the thermally integrated microchannel methanol reforming reactor. The channels are 0.7 mm in width. The effect of wall heat conduction properties on the temperature field within the thermally integrated microchannel methanol reforming reactor is investigated. The results are presented in Figure 4, in which the two-dimensional contour plots of temperature are illustrated for the thermally integrated...](image-url)
microchannel methanol reforming reactor. The thermal conductivity of the channel walls varies from 0.2 to 200 W/(m·K). The temperature increases with decreasing the wall thermal conductivity. For the thermally integrated microchannel methanol reforming reactor, the desired reaction temperatures can influence the choice of channel wall material. For example, when chosen for the channel walls, the material should not impede on the transport of thermal energy between the endothermic and exothermic streams within the thermally integrated microchannel methanol reforming reactor, in addition to a suitable melting point. Within the channel walls, a substantially uniform temperature profile is achieved in the case of a high thermal conductivity of 200 W/(m·K). For example, the excellent heat conduction properties enable a more uniform distribution of temperature along the streamwise direction. This causes a reduction of peak temperature within the reactor, thereby ensuring the structural integrity of the reaction system and prolonging the life of the catalytically active materials. Therefore, the channel walls of the thermally integrated microchannel methanol reforming reactor must be formed using materials with excellent heat conduction properties. In this context, thermally conductive ceramics and metals are well-suited, since materials with high thermal conductivity are preferred for the channel walls. The plates may be aligned horizontally and stacked one above another, aligned vertically and positioned side-by-side, or they may be aligned at an angle to the horizontal [33, 34]. The process layers and heat exchange layers may be aligned in alternating sequence with a process layer adjacent to a heat exchange layer, which in turn is adjacent to another process layer, which in turn is adjacent to another heat exchange layer.

Figure 4. Two-dimensional contour plots of temperature for the thermally integrated microchannel methanol reforming reactor. The thermal conductivity of the channel walls varies from 0.2 to 200 W/(m·K). A high temperature exothermic reaction takes place in the combustion channels and the reforming process reactant stream simultaneously undergoes an endothermic reaction in the reforming channels.

The thermal energy released from the combustion channels is conducted through the channel walls to reforming channels, thereby supporting the endothermic conversion reaction. The thermal conductivity of the channel walls is high so as to facilitate the efficient transfer of

![Figure 4](image-url)

860 K
373 K
677 K
373 K
596 K
373 K
557 K
373 K

Figure 5 illustrates the contour plot of temperature for the thermally integrated microchannel methanol reforming reactor. The thermal energy released from the combustion channels is conducted through the channel walls to reforming channels, thereby supporting the endothermic conversion reaction. The thermal conductivity of the channel walls is high so as to facilitate the efficient transfer of
thermal energy from the combustion channels to the reforming channels, as illustrated in Figure 5. To enhance heat transfer within the thermally integrated microchannel methanol reforming reactor by dramatically increasing heat transfer area, the flow channels could contain internal, function fins, for example, castellated walls, saw tooth walls, or any other type of walls, such as grooved, serpentine or any other design. The geometry and dimensions of the flow channels may vary depending upon the design parameters of the reaction system. The temperature rises very quickly in the thermally integrated microchannel methanol reforming reactor, as illustrated in Figure 5, reaching about 560 K at which the structural integrity of the thermally integrated microchannel methanol reforming reactor might be compromised. High temperatures would potentially destroy or deactivate the catalyst layers of the thermally integrated microchannel methanol reforming reactor and may pose a risk to the structural integrity of the thermally integrated microchannel methanol reforming reactor. Within the channel walls, a substantially uniform temperature profile is achieved, as illustrated in Figure 5, because of the excellent heat conduction properties of the channel walls, which can improve the performance of the reaction system with increased conversion due to their high thermal conductivity. The common wall may vary in thickness. However, adjacent channels may not be separated by an intervening channel that interferes with heat transfer between the channels [35, 36]. One channel may be adjacent to another channel over only part of the channel. However, asymmetric operation requires spatial distribution of the feed for the exothermic reaction in order to prevent excess temperatures and to ensure stable operation. Advantages are the compact design which allows fast start-up and load changes. Drawbacks include the dilution of the reforming product with nitrogen if air is used as oxidant.

![Contour plots of temperature for the thermally integrated microchannel methanol reforming reactor.](image)

**Figure 5.** Contour plots of temperature for the thermally integrated microchannel methanol reforming reactor. At room temperature, the thermal conductivity of the channel walls is 200 W/(m·K). The channels are square in cross section.

The contour plots of enthalpy and sensible enthalpy are illustrated in Figure 5 for the thermally integrated microchannel methanol reforming reactor. Enthalpy is a state function used in many measurements in chemical and physical systems at a constant pressure, which is conveniently provided by the large ambient atmosphere [37, 38]. Instead of temperature, a change in enthalpy or sensible enthalpy can be used as the state variable to account for simplifying the description of heat transfer. For the mixtures, the enthalpy correlates to their thermal energy. The change in enthalpy for the reforming process is the heat absorbed by the endothermic reactant stream. The change in enthalpy for the combustion process is the heat released by the exothermic reactant stream. There is a significant change in specific enthalpy or specific sensible enthalpy along the streamwise direction, as illustrated in Figure 5.
6, especially near the channel inlets. For the exothermic catalytic combustion reaction, the change in total enthalpy is negative, since the total enthalpy of combustion products is smaller than that of the reactants of the reaction. The change in total enthalpy is equal to the heat released by the exothermic reaction. For the endothermic steam reforming reaction, the change in total enthalpy is positive, since the total enthalpy of reforming products is larger than that of the reactants of the reaction. The change in total enthalpy is equal to the heat absorbed by the endothermic reaction. However, these results can be applied only to total enthalpy. When applied to specific enthalpy, the change in specific enthalpy is positive for the exothermic catalytic combustion reaction and the change in specific enthalpy is negative for the endothermic steam reforming reaction, as illustrated in Figure 6. However, the change in specific sensible enthalpy is always positive, especially for the exothermic process. This is because the temperature of the streams will continue to rise along the streamwise direction due to the heat released by the combustion reaction.

Figure 6. Contour plots of specific enthalpy and specific sensible enthalpy for the thermally integrated microchannel methanol reforming reactor. At room temperature, the thermal conductivity of the channel walls is 200 W/(m·K). The channels are square in cross section.

6. Conclusions

Computational fluid dynamics simulations are conducted to better understand the consumption, generation, and exchange of thermal energy between endothermic and exothermic processes in a thermally integrated microchannel reforming reactor. The effects of wall heat conduction properties on heat transfer characteristics and reactor performance are investigated.

The results indicate that asymmetric operation requires spatial distribution of the feed for the exothermic reaction in order to prevent excess temperatures and to ensure stable operation. The application of autothermal reactor concepts can be extended to endothermic high temperature reactions...
if the endothermic reactions are coupled with an auxiliary exothermic reaction, such that the total process is weakly exothermic. The peak reaction heat flux increases with the channel dimensions while maintaining the flow rates. The change in specific enthalpy is positive for the exothermic reaction and negative for the endothermic reaction. The change in specific sensible enthalpy is always positive, especially for the exothermic process. The thermal conductivity of the channel walls is fundamentally important. Materials with low thermal conductivity pose a risk to the structural integrity of the reactor and reduce the life of the catalysts. Materials with high thermal conductivity are preferred for the channel walls. Thermally conductive ceramics and metals are well-suited. Advantages are the compact design which allows fast start-up and load changes. Drawbacks include the dilution of the reforming product with nitrogen if air is used as oxidant.

**Declaration of competing interest**

The authors declare that there is no conflict of interest.

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Figure 1

Schematic illustration of the thermally integrated microchannel methanol reforming reactor used to simultaneously conduct exothermic and endothermic reactions. The channel walls are not depicted for clarity.
Figure 2

Methanol conversion at different reaction temperatures. The experimental data are included for comparison. The cross-sectional shape of the channels is rectangular.

Figure 3

Endothermic and exothermic reaction heat fluxes as a function of the streamwise distance for the thermally integrated microchannel methanol reforming reactor. The channels are 0.7 mm in width.
Figure 4

Two-dimensional contour plots of temperature for the thermally integrated microchannel methanol reforming reactor. The thermal conductivity of the channel walls varies from 0.2 to 200 W/(m·K). A high temperature exothermic reaction takes place in the combustion channels and the reforming process reactant stream simultaneously undergoes an endothermic reaction in the reforming channels.
Contour plots of temperature for the thermally integrated microchannel methanol reforming reactor. At room temperature, the thermal conductivity of the channel walls is 200 W/(m·K). The channels are square in cross section.
Contour plots of specific enthalpy and specific sensible enthalpy for the thermally integrated microchannel methanol reforming reactor. At room temperature, the thermal conductivity of the channel walls is 200 W/(m·K). The channels are square in cross section.