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Integration of methanol steam reforming and combustion in a microchannel reactor for H_2 production: A CFD simulation study

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ABSTRACT

A computational fluid dynamics (CFD) study of the thermal integration of the steam reforming of methanol (SRM) and the combustion of methanol in a catalytic microchannel reactor is presented. This issue is of interest for in situ H_2 production for portable power units based on low-temperature PEM fuel cells. Three-dimensional simulations have been carried out under relevant conditions for the SRM reaction that have shown that microreactors allow achieving complete methanol reforming and combustion at space velocities as high as 50,000 h^{-1}, with selectivities for H_2 above 99% at relatively low temperatures in the 270–290 °C range.

1. Introduction

There is an increasing interest in methanol as a fuel for power units based on low-temperature small size fuel cells, mainly of the proton-exchange-membrane (PEMFC) type. Main applications of these systems are the replacement of batteries in portable electronics as well as auxiliary power units [1]. Another important application of fuel cells will be in the transportation sector; in this regard, methanol can be used also as a fuel for onboard production of the hydrogen to be fed to the fuel cells of the vehicles driven by electric engines [2]. The advantages of using methanol for hydrogen production can be summarized as follows [1,3]: (i) high hydrogen to carbon ratio (4, like methane); (ii) it is liquid at ambient conditions thus overcoming the problems of hydrogen distribution and storage; (iii) is miscible with water so both methanol and water can be premixed in fuel cartridges; (iv) is biodegradable and free of sulfur; (v) the absence of C–C bonds and its reactivity allows conversion to hydrogen (reforming) at lower temperatures (200–350 °C) than for most other hydrocarbon fuels (above 500–600 °C); (vi) low temperature reforming with selective catalysts leads to low levels of CO formation so secondary conversion such as the water gas shift (WGS) reaction is generally unnecessary in the case of methanol; (vii) its net energy content is comparable to that of gasoline on a well-to-wheel basis; (viii) the theoretical energy input required (145 J/kg of usable H_2) for the steam reforming of methanol (SRM) is about the same that for other fuels. Of course, there are also some drawbacks: methanol is toxic, being ingestion the main concern, and the H_2 yield is relatively low (18.9 g H_2 per 100 g of steam-reformed methanol) compared with other fuels (50.3 g H_2 per 100 g of steam-reformed CH_4).

As concerns the use of fuel cells for portable applications, one of the most important challenges is the availability of a compact and light unit of H_2 supply. Catalytic microreactors can contribute to solve this technological problem [1,4–6]. Microreactors are very compact, have a high surface to volume ratio, exhibit enhanced heat and mass transfer rates, produce extremely low pressure drop and allow easy thermal integration of the processes involved.

Within this context, the aim of this computational fluid dynamics (CFD) simulation study is to guide the design of an unit based on catalytic microchannel reactors for the production of hydrogen from methanol. This work forms part of a joint project with the final goal of constructing the fuel microprocessor including both the primary conversion of methanol and the CO mitigation stages and put it into operation. This paper is only concerned with the initial conversion unit and the idea is simple: to couple in the same device the endothermic ($\Delta H^\circ_{250\,^\circ C} = 59.5$ kJ/mol) steam reforming of methanol (SRM) with the exothermic combustion of methanol ($\Delta H^\circ_{250\,^\circ C} = -673.2$ kJ/mol) in air for heating purposes. The SRM reaction has been extensively studied; it is catalyzed by a variety of compounds mainly based on copper or palladium and the state of the art on this subject has been updated and can be consulted in excellent reviews [1,2,7].

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2. CFD model

2.1. Microreactor geometry, grid characteristics and flow characterization

Three-dimensional (3D) simulations have been carried out with the commercial software package ANSYS CFX that is based in the finite volume method for spatial discretization of the governing Navier–Stokes equations [8,9]. Our approach of the CFD simulation study of the methanol reformer has been using two physical models of increasing complexity. A representative example of the first model is shown in Fig. 1. As can be seen it includes a solid block of 20 mm of length made of steel with 4 square parallel microchannels. In order to investigate the effect of the channels size, microchannels with 0.35, 0.70 and 1.40 mm of side (d) have been considered. This model has been used to integrate the kinetics of the chemical reactions involved into the CFD codes and to investigate the effect of some of the main process variables such as the space velocity of the reforming and combustible streams and the microchannels size. This simple model has been scaled up to a geometry closer to that of the real microreactor that is now being fabricated. It consists in 2 superposed steel sheets with 20 microchannels in order to investigate the effect of the flow arrangement: parallel, counter flow and cross flow (see Fig. 2). The dimensions of each sheet are 20 mm of width and length and 1 mm of depth. Each sheet has 10 square parallel microchannels of 0.70 mm of side and 20 mm of length and separated by 0.30 mm fins. The geometries were designed with the CAD-type software incorporated by the ANSYS CFX package and included one solid domain, the block made of stainless steel, and a number of fluidic domains coinciding with the microchannels. After the generation of these geometries, their physical space was divided into an unstructured mesh [10] with a number of control volumes where the governing equations are solved iteratively until the established criteria of convergence are fulfilled. The number of elements depends on the complexity of the system and ranged from 44,700 total elements (36,700 prisms and 8,000 hexahedrons) for the 4-channels system to 2,160,155 total elements (1,756,118 tetrahedrons, 379,877 prisms and 32,000 hexahedrons) for the 2 sheets superposed in cross flow arrangement. It can be appreciated in Fig. 1 that a dense meshing has been applied in the fluidic regions near the channels walls to suitably take into account boundary layer phenomena.

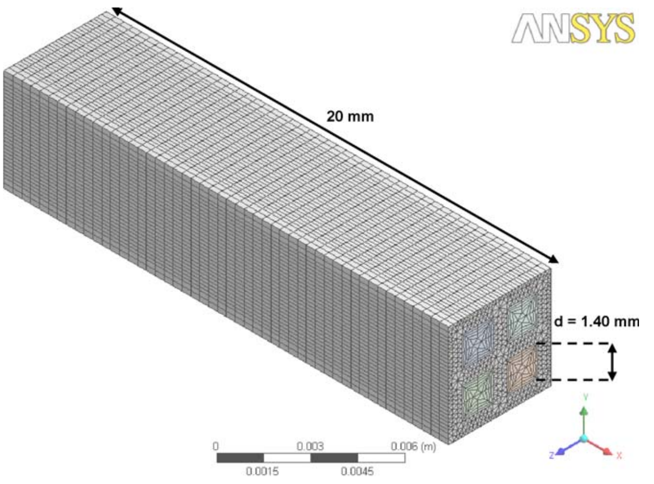

Fig. 1. Example of the CFD geometry of a system formed by 4 square parallel channels showing the unstructured meshing applied. Dimensions of the channels are 20 mm of length and 1.4 mm of side (in this case).

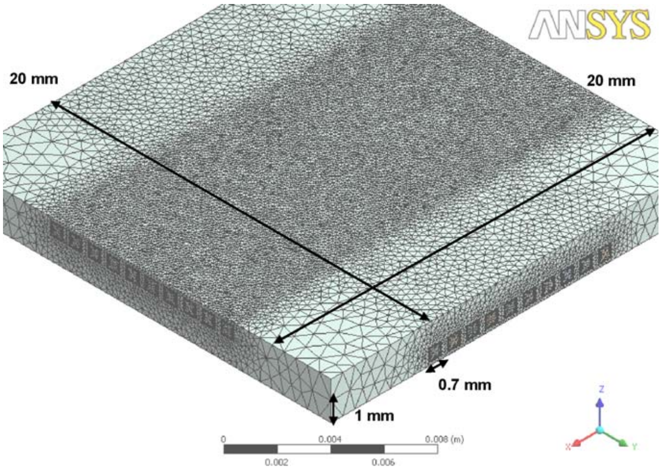

Fig. 2. Example of the CFD geometry of a system formed by 2 superposed sheets in a cross flow arrangement showing the unstructured meshing applied. Dimensions of the sheets are 20 mm of length and width and 1 mm of depth. Each sheet has 10 square parallel channels of 20 mm of length and 0.70 mm of side.

When working in micro-fluidics it is very important to check the validity of the continuum model and evaluate possible rarefied gas flow effects [11]. To this end, the Knudsen number (Kn) has been evaluated

$$Kn = \frac{\lambda}{l} \tag{1}$$

This number compares the molecular mean free path (λ) with the characteristic geometric dimension (l) of the system. The molecular mean free path has been evaluated according to Bird [12] for both the SRM and combustion gases in the 250–350 °C range resulting values between 93 and 115 nm. Taking into account that in our case the characteristic dimension is the channel side (d) and that the most unfavourable situation is for the smallest channel ($l = d = 0.35$ mm $= 3.5 \times 10^5$ nm), the Knudsen numbers are between 2.6×10^{-4} and 3.3×10^{-4}. These values are lower than 0.001 [11] which assures the validity of the continuum model and the Navier–Stokes equations for the systems considered in this work. The Reynolds number is another important parameter to characterize the flow. Maximum values of this number have been 105 and 50 for the SRM and the methanol combustion streams, respectively, so the flow regime of the gases is clearly laminar in our case which means that viscous forces play a dominant role. Finally, the characteristic radial diffusion time-scale (t_D) has been also calculated [13]:

$$t_D = \frac{d^2}{4D_{AB}} \tag{2}$$

The diffusion coefficient (D_{AB}) for the methanol–water system was estimated according to the Chapman–Enskog kinetic theory for low-density gases as described by Bird et al. [14]. Calculations were performed at 1 atm and 300 °C, which can be considered as representative conditions, due to the system isothermicity. A diffusivity of 7.8×10^{-5} m^2 s^{-1} was obtained, resulting in a low-radial diffusion time-scale of 1.6×10^{-3} s according to Eq. (2) for the channel of intermediate size ($d = 7 \times 10^{-4}$ m). The mean residence time (τ) of the gaseous streams in the simulations that have been carried out ranged between 0.07 and 0.6 s. When comparing these time-scales a ratio τ/t_D in the 44–375 range is obtained; that is, the diffusion time is very low compared with the residence time which suggests that radial profiles of the flow properties can develop. An analysis of the velocity profiles has shown that, from the combustion side, the laminar regime is rapidly well developed. In the case of the reforming channels there is a clear velocity profile only in the second half of the channel.

2.2. Chemical kinetics and simulations conditions

A state-of-art $Cu/ZnO/Al_2O_3$ catalyst has been adopted for both SRM and methanol combustion reactions. It has been assumed that a thin and homogeneous layer of 1 mg/cm^2 of this catalyst has been uniformly deposited onto the channels walls. This is a reasonable catalyst loading that can be reached for microreactor applications by several preparation methods [15]. As concerns the kinetics over $Cu/ZnO/Al_2O_3$, the rate equations have been taken from the literature. In the case of the SRM channels, the rate expressions reported by Jiang et al. [16] for the steam reforming of methanol and Choi and Stenger [17] for the water gas shift reaction have been selected. The rate of methanol combustion has been evaluated according to Reitz et al. [18]. The kinetic equations are incorporated in the CFD codes in a per cm^2 of catalyst basis and the reactions are modelled considering the microchannel walls as sources of products and sinks of reactants obeying the appropriate stoichiometry and rate.

Other simulation conditions have been: steady state, adiabatic external walls and constant total pressure of 1 atm at the channels outlet. Criteria of convergence were based on the residuals defined as the normalized root mean square of the difference between the latest solution and the running arithmetic average of the variables as well as on the imbalance level of the conservation equations. In order to consider valid the results of a simulation, the maximum values of the residuals and the imbalances were set at 10^{-4} and 5–10%, respectively [19]. All the simulations were performed on a Dell Precision PWS690 workstation running MS Windows XP® × 64 with an available RAM of 16.0 GB. The duration of the simulations varied between 4 and 20 h depending on the complexity of the geometry.

3. Results and discussion

3.1. Four channels system

This simple model has been used to investigate the effects of the gas streams flow rate and the microchannel size. Two channels are fed with a vapour mixture of methanol and water for the SRM and the other two channels are fed in a parallel flow arrangement with a methanol stream diluted in air to perform the combustion reaction. The inlet temperature and composition of the gases have been fixed at typical values [20]. Thus, the inlet temperature to the reforming channels has been set at 150 °C. Preliminary simulations showed a relatively weak effect of the water vapour excess on the SRM reaction. Therefore, the inlet molar H_2O/methanol ratio has been set at 1, and more frequently 1.25, which is within the optimum steam to carbon ratio of 1.2–1.5 [3]. In the case of the combustion channels the inlet composition has been established at 2% (vol.) methanol in air and the temperature at 200 °C.

3.1.1. Effect of the combustible space velocity

This part of the study has been carried out with the microchannels of intermediate size (d = 0.70 mm). To investigate the effect of this important system variable for the thermal integration of the system, the space velocity of the SRM channels was set at gas hourly space velocity (GHSV) of 6,000 h^{-1} (STP) which is equivalent to a weight hourly space velocity (WHSV) of 117 h^{-1}. This means that each reforming microchannel is fed with 0.98 cm^3/min (STP) of gas with a molar H_2O/methanol ratio of 1. The combustible gas flow rate has been varied from 1.6 to 3.2 cm^3/min (STP) per channel; that is, GHSVs between 10,000 and 20,000 h^{-1} and WHSVs between 225 and 450 h^{-1}. The conversion of the steam reforming of methanol and the mean temperature at the SRM channels outlet are shown in Fig. 3. In all cases complete combustion of methanol was achieved; therefore, for a given SRM space velocity, the outlet temperature and the reforming conversion increase with the combustible flow rate. In this case, it is required to achieve al least 270 °C (combustible WHSV = 360 h^{-1}) to reach complete methanol reforming conversion. The results of the selectivity for H_2 expressed as moles of H_2 obtained per mol of steam reformed methanol as well as moles of methanol reformed to H_2 per mol of methanol converted are depicted in Fig. 4. As can be seen, for combustible WHSVs below 360 h^{-1}, that is, outlet reforming temperatures below 270 °C, the selectivity for hydrogen is very high: more than 2.9 mol of H_2 per mol of steam reformed methanol and above 0.995 mol of methanol reformed to H_2 per mol of methanol converted. However, above 360 h^{-1} there is an excess of combustible giving rise to a rapid increase of the temperature above 270 °C and a rapid decrease of the selectivity for H_2 due to an enhanced production of CO through the reverse water gas shift (RWGS) reaction [21]. Therefore, for a given SRM space velocity there is an optimum combustible flow rate that allows obtaining complete methanol reforming conversion with high selectivity for

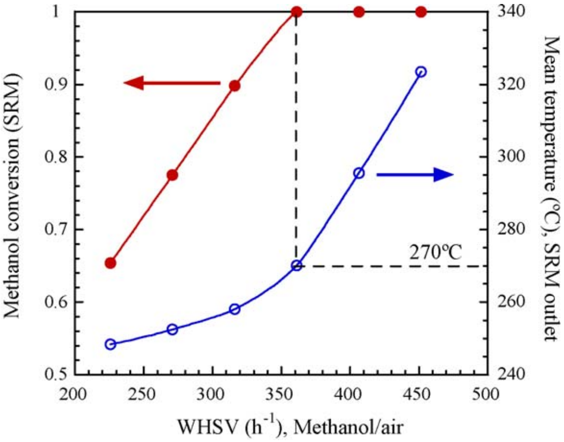

Fig. 3. Methanol steam reforming conversion (closed symbols) and mean temperature at the SMR channels outlet (open symbols) as a function of the combustible weight hourly space velocity in a 4 channels system (d = 0.70 mm) with parallel flow arrangement. Reforming WHSV = 117 h^{-1}.

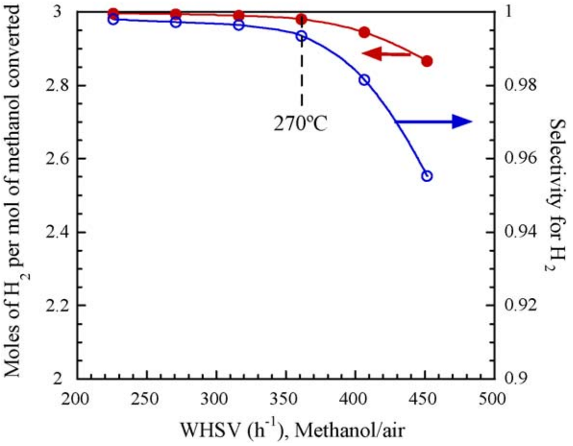

Fig. 4. Selectivity for H_2 expressed as moles of H_2 obtained per mol of reformed methanol (closed symbols) and moles of methanol reformed to H_2 per mol of methanol converted (open symbols) as a function of the combustible weight hourly space velocity in a 4 channels system (d = 0.70 mm) with parallel flow arrangement. Reforming WHSV = 117 h^{-1}.

hydrogen. In the case of the example presented in this section a suitable value of the combustible space velocity is WHSV of 360 h^{-1}, or equivalently, GHSV of 16,000 h^{-1}, which means that 2.6 cm^3/min (STP) of the methanol/air mixture are fed to each combustion microchannel. This also means that 9.4 mol of methanol can be selectively reformed to H_2 per mol of methanol combusted. This proportion can be compared with 11.3 mol of methanol that could be theoretically reformed if one takes into account only the heat of reaction. Obviously, more methanol has to be combusted to reach and sustain the reforming temperature. This can be also achieved by increasing the methanol concentration in the combustion channels feed; however, a relatively lean mixture with 2 vol.% methanol in air has been selected in this study because, for safety reasons, it is considered more suitable for practical applications.

A more detailed analysis of this case is presented in Figs. 5 and 6. Fig. 5A shows the distribution of temperatures in the solid block. Note that the full colour scale is equivalent to a maximum temperature change of less than 1 °C, so it has to be emphasized the remarkable isothermicity of the solid block, especially taking into account that the two streams exit the reactor with complete conversion. As concerns the fluids temperature, Fig. 5B shows the distribution of temperatures in a central plane of a SRM and a methanol combustion channel. Both streams experience a much higher temperature increase than the solid block but this change is almost restricted to a very short distance at the reactor entry. The combustible enters the reactor at 200 °C, rapidly reaches the maximum temperature of 272 °C and then slowly cools down to the exit temperature of 270 °C. The reforming gas enters at 150 °C and rapidly reaches a temperature of about 268 °C at the reactor entry; then, the temperature slowly increases to the exit value of 270 °C. After the entry section, the maximum variation of the temperature of both gases along the microchannel is of only 2 °C, so the flow of the fluids is practically isothermal. Fig. 6A shows the evolution of the methanol conversion along a central plane in a SRM and combustion channel. It is clear that the combustion of methanol is more rapid than the steam reforming; therefore, the combustion reaction is controlling the SRM by heat transfer. Complete combustion of methanol is achieved at about middle channel length, and complete methanol reforming at about 70% of the reactor length. Obviously, this case is not optimized with respect to the H_2 production since it would be possible to reform a greater methanol flow rate. As concerns the gas composition, Fig. 6B shows the evolution of the H_2 and CO mass fractions in a central plane of a reforming channel. The H_2 mass fraction increases more rapidly at the reactor entry, where the methanol concentration is high. In fact, the H_2 mass fraction is about 10% at middle channel length, and increases only up to 12% at the reactor outlet, although this implies a very high selectivity for H_2 of above 99%. In contrast, the formation of CO is favoured at the reactor exit where the H_2 concentration and temperature are higher. It can be seen that in the second half of the channel the CO mass fraction increases from 0.1 to 0.36%. Therefore, an important conclusion is that in order to reduce the formation of CO the flow rates of both gases have to be carefully adjusted to avoid unnecessary overheating and achieve complete SRM conversion just at the microreactor exit.

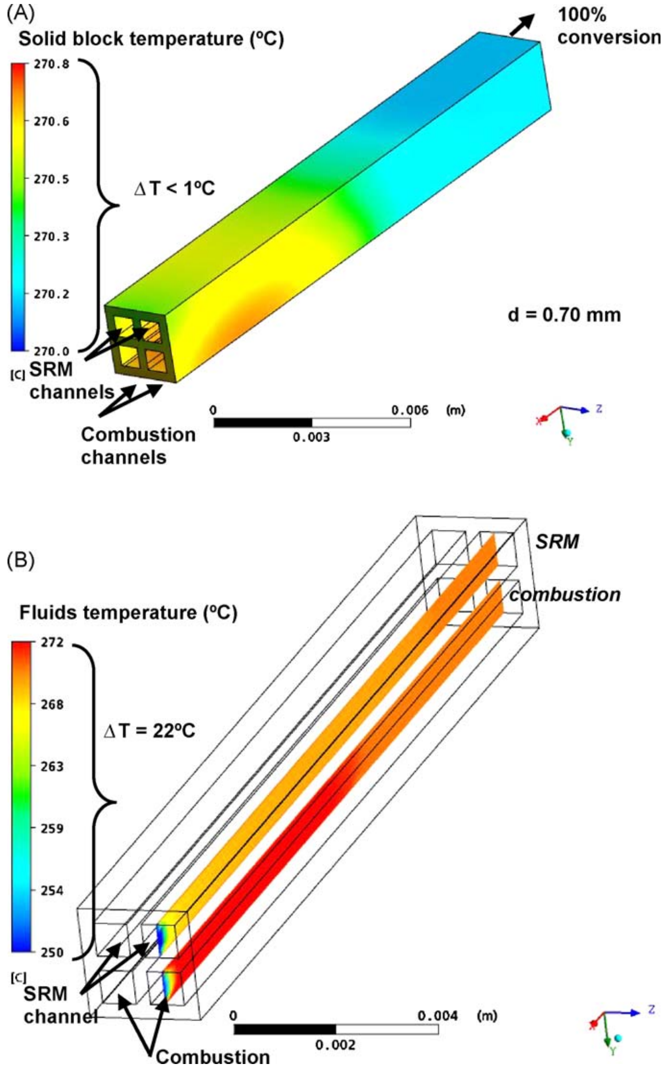

Fig. 5. Distributions of the solid block temperature (A) and the temperature of the fluids in a central plane of a reforming and a combustion channel (B) in a 4 channels system (d = 0.70 mm) with parallel flow arrangement. Reforming WHSV = 117 h^{-1} and combustible WHSV = 360 h^{-1}.

3.1.2. Effect of the SRM space velocity and microchannel size

To perform this study, the steam to carbon ratio was set at 1.25 and the GHSV of the SRM stream was varied between 770 and 74,000 h^{-1} whereas the combustible flow rate was adjusted to maintain constant at the microreactor entry a ratio of 9.4 mol of methanol fed to the reforming channels per mol of methanol fed to the combustion channels. The evolution of the steam reforming methanol conversion and mean outlet temperature as a function of the SRM gas hourly space velocity is depicted in Fig. 7 for the systems with microchannels side of 0.35, 0.70 and 1.40 mm. As can be seen, as the feed flow rate increases the reactor temperature for a given reactor size has to increase in order to maintain complete methanol conversion. Nevertheless, above a certain space velocity the reactor capacity is not high enough and the methanol conversion starts to decline in spite of the fact that the temperature continues increasing because methanol combustion is still complete. Interestingly, the smallest reactor (d = 0.35 mm) is the most effective since it allows obtaining complete SRM conversion at space velocities as high as 50,000 h^{-1} and relatively low temperature of 290 °C. Under the same conditions, the intermediate reactor gives about 80% methanol conversion, and a much lower value can be estimated for the reactor with channels of 1.40 mm of side (see Fig. 7). This illustrates the interest of using microreactors for chemical processes intensification. It should be noted that the catalyst is located on the walls; therefore, the reason of the different behavior of the microreactors is their different area to volume ratio, which varies with the inverse of the channel side (l/d), and then, is higher for the smallest reactor. As illustrated in Fig. 8, this is confirmed by the fact that when the results are normalized with respect to the amount of catalyst through the

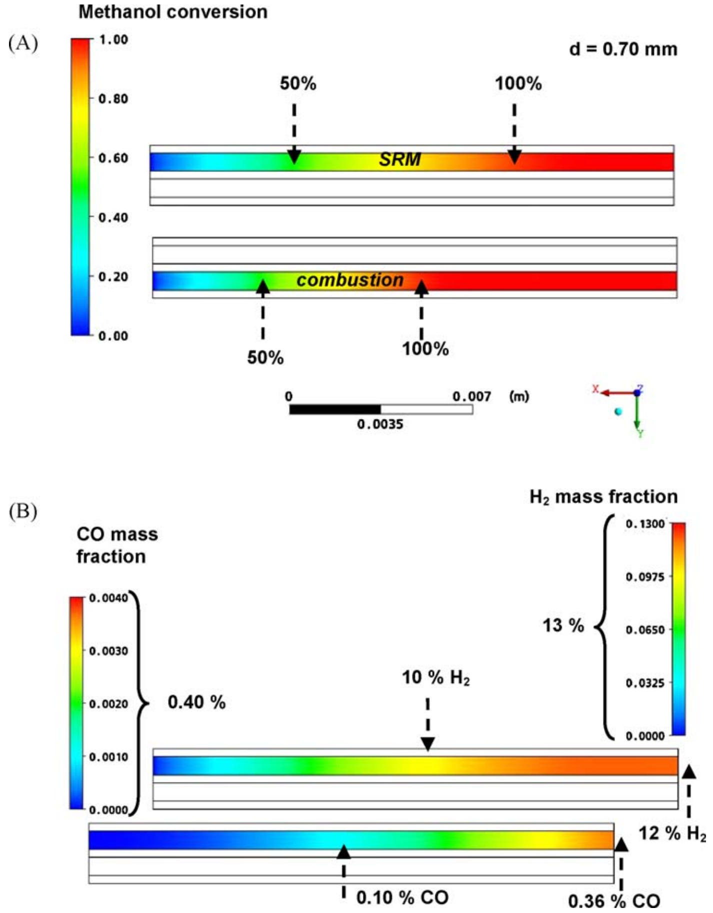

Fig. 6. Distributions of the methanol conversion (A) and the H_2 and CO mass fractions (B) in a central plane of a reforming and a combustion channel in a 4 channels system (d = 0.70 mm) with parallel flow arrangement. Reforming WHSV = 117 h^{-1} and combustible WHSV = 360 h^{-1}.

WHSV the differences almost disappear. The effect of the feed flow rate and microchannel size on the reforming selectivity is negligible at high space velocities. Only at very low space velocities, the relative overheating due to the high microreactors effectiveness gives rise to a loss of selectivity for hydrogen through the RWGS reaction, especially with the smallest channels.

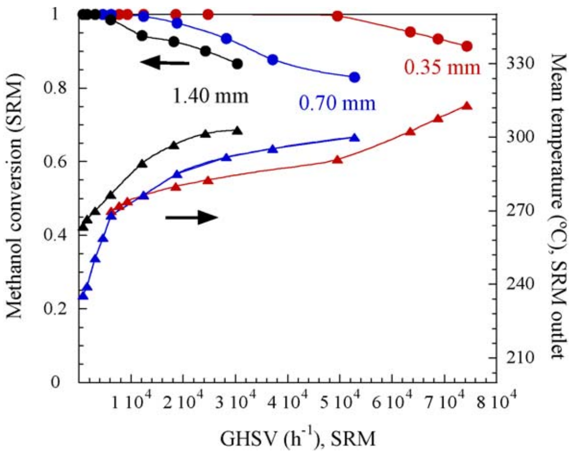

Fig. 7. Methanol steam reforming conversion (circles) and mean temperature at the SMR channels outlet (triangles) as a function of the reforming gas hourly space velocity (GHSV) in a 4 channels system with parallel flow arrangement. Microchannel size: 0.35 mm (red symbols), 0.70 mm (blue symbols) and 1.40 mm (black symbols). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of the article.)

3.2. Two sheets system

Passing from 4 channels to 2 superposed sheets with a total of 20 channels supposes an important increase in the number of volume elements and therefore in the computation time. One of the sheets is fed with the vapour mixture of methanol and water

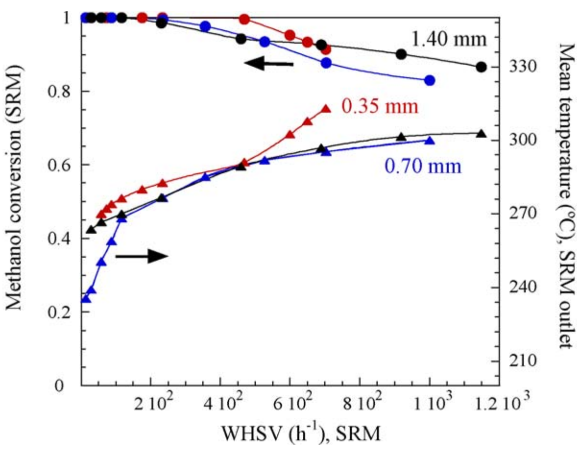

Fig. 8. Methanol steam reforming conversion (circles) and mean temperature at the SMR channels outlet (triangles) as a function of the reforming WHSV in a 4 channels system with parallel flow arrangement. Microchannel size: 0.35 mm (red symbols), 0.70 mm (blue symbols) and 1.40 mm (black symbols). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of the article.)

for the SRM and the other with a methanol/air stream to perform the combustion reaction. A first series of simulations were performed with the two sheets in parallel flow arrangement to compare the performance of the two systems under the same inlet conditions and microchannel side of 0.70 mm. Very high gas hourly space velocities were considered: 28,224 and 75,263 h^{-1} for the SRM and methanol combustion reactions, respectively. The results showed a reasonable scalability although in the 2 sheets system the SRM reaches exit temperatures (298 °C) slightly higher than in the 4 channels geometry (292 °C). At the very high space velocities considered these temperature differences were sufficient to give different methanol conversions. As a result, complete reforming conversion was obtained only with the 2 sheets system although the conversion achieved with the 4 channels was also high, above 98%. The conversion of the methanol combustion was complete in all cases.

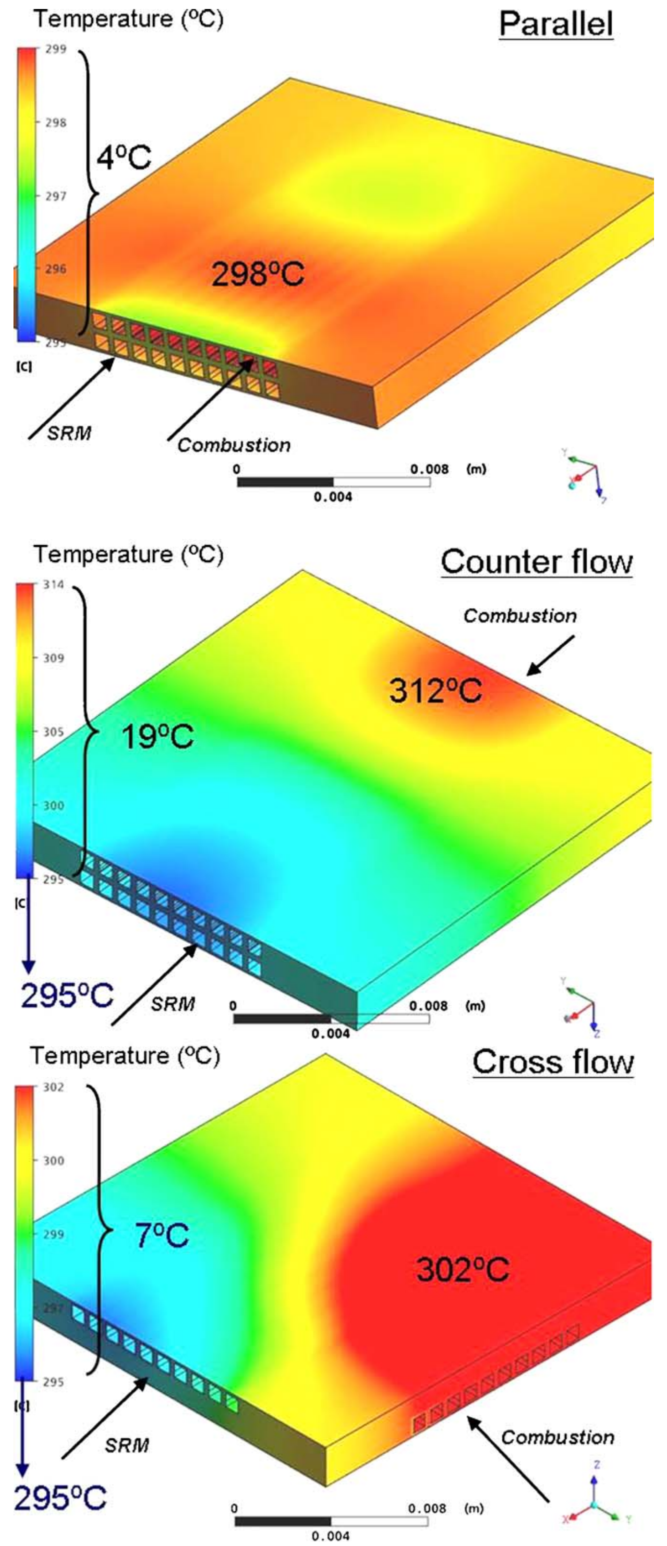

Fig. 9. Distribution of temperatures in the steel block of 2 superposed sheets in parallel, counter flow and cross flow arrangement (d = 0.70 mm). Reforming GHSV = 28,224 h^{-1} and combustible GHSV = 75,263 h^{-1}.

The 2 sheets system allowed studying the effects of the flow arrangement. To this end, simulations were carried out at the above-mentioned space velocities, obtaining complete SRM and methanol combustion conversions, with selectivity for H_2 above 99%. The main differences corresponded to the distribution of temperatures in the block as can be appreciated in Fig. 9. The parallel flow arrangement gives the minor variation of temperature in the block, only 4 °C, with a maximum temperature of 298 °C. In contrast, the counter flow arrangement exhibits the largest temperature change, being the SRM entry the coolest zone (295 °C) and the combustion entry the hottest region (312 °C). In the case of the cross flow arrangement the maximum temperature change is low, 7 °C; however, there is a wide relatively hot zone (302 °C) from the side of the combustible entry. According to these results there is no definitive reason based on performance criteria for selecting one of the flow arrangements as the most suitable. From the point of view of the thermal stress the most favourable situation is for the parallel flow arrangement. On the other hand, the cross flow arrangement allows an easier feed streams distribution and assembly of the connectors and tube fittings. This is the arrangement that has been selected for the micro-reformer that is now under construction.

4. Conclusions

A CFD model has been developed that allows studying the thermal integration of the methanol steam reforming, including WGS, with the combustion of methanol in catalytic microchannels containing a state-of-art $Cu/ZnO/Al_2O_3$ catalyst. The model has allowed to determine the most suitable ratio between the combustible and SRM flow rates for the particular case considered. This is an important system variable to ensure complete SRM conversion while avoiding overheating that increases the formation of CO through RWGS. The model has shown the advantages of using microreactors for process intensification due to the short diffusion distances and the increase of the area to volume ratio. Experimental validation is still required although the model is in general accordance with experimental results reported in the literature [20,21]. The approach of the simulation study based on the use of a first simple physical model including 4 parallel microchannels for investigating the effects of the relevant system variables, and a second, more complex model closer to that of the real microreactor including 2 superposed steel sheets with 20 microchannels, has been found useful to guide the design of the microreactor that is now being fabricated.

Acknowledgements

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