

Contents lists available at [ScienceDirect](http://www.sciencedirect.com/science/journal/13858947)

Chemical Engineering Journal

Chemical Engineering Journal

journal homepage: www.elsevier.com/locate/cej

Computational fluid dynamics study of heat transfer in a microchannel reactor for low-temperature Fischer–Tropsch synthesis

G. Arzamendi^a, P.M. Diéguez^a, M. Montes^b, J.A. Odriozola^c, E. Falabella Sousa-Aguiar^d, L.M. Gandía^{a,∗}

a Departamento de Química Aplicada, Edificio de los Acebos, Universidad Pública de Navarra, Campus de Arrosadía s/n, E-31006 Pamplona, Navarra, Spain

^b Departamento de Química Aplicada, Facultad de Ciencias Químicas de San Sebastián, Universidad del País Vasco, P[∞] Manuel de Lardizábal 3, E-20018, San Sebastián, Spain

^c Instituto de Ciencia de Materiales de Sevilla, Centro Mixto CSIC-Universidad de Sevilla, Avda. Américo Vespucio 49, 41092 Sevilla, Spain

^d CENPES/PDEDS/Petrobras, Av. Horácio Macedo, 950 - Ilha do Fundão CEP 21941-915 Rio de Janeiro, Brazil

article info

Article history: Received 14 July 2009 Received in revised form 26 November 2009 Accepted 21 December 2009

Keywords: Microchannel reactor **Microreactor** Computational fluid dynamics (CFD) Fischer–Tropsch synthesis (FTS) Process intensification

ABSTRACT

A three-dimensional computational fluid dynamics (CFD) study of heat transfer in a microchannel reactor for the low-temperature Fischer–Tropsch synthesis (FTS) is presented. The microreactor studied is a steel block with 80 square microchannels of 1 mm of side arranged in cross-flow configuration for the transport of syngas and cooling water. Syngas space velocities in the 5000–30,000 h⁻¹ (STP) range have been considered. The microreactor exhibited good isothermicity under most simulated conditions. The FTS can be conducted with very low-temperature change between 483 and 523 K within a wide range of CO conversions using boiling water as coolant. To this end the pressure has to be set at the appropriate value between about 5 and 35 atm. The pressure would have to be reduced as the CO conversion increases which might have a negative effect on the FTS selectivity to middle distillates. However, adjusting the cooling water flow rate in the range $0.25-250$ g min⁻¹ allows maintaining the FTS temperature at suitable values while avoiding the use of low pressures. Relatively high values of the overall heat transfer coefficient in the 20–320 W m⁻² K⁻¹ range have been obtained. A significant effect of the buoyancy forces on the thermal performance of the microreactor has been found.

© 2009 Elsevier B.V. All rights reserved.

1. Introduction

The Fischer–Tropsch synthesis (FTS) is a key step in the conversion of natural gas and solid feedstocks such as coal or biomass into liquid fuels (synfuels) through the so-called gas-to-liquids (GTL) and coal/biomass-to-liquids (CTL/BTL) processes. Among them, GTL is particularly attractive from the point of view of operating costs, carbon and thermal efficiencies as well as environmental impact [\[1,2\]. T](#page-6-0)he FTS is the catalytic conversion of syngas into a complex mixture of linear paraffins and α -olefins, and water. The commercial FTS plants have utilized either Fe or Co catalysts although now the trend is towards using low-temperature FTS with Co catalysts to increase the middle distillates (gasoline and diesel) yields [\[3,4\].](#page-6-0) The FTS can be viewed as a polymerization reaction where chain growth is the basic feature. Each growth step increases linearly by one the number of carbon atoms of the active hydrocarbon chain. Termination to paraffins by hydrogenation is irreversible whereas termination leading to the formation of olefins is reversible so that these species, especially the heaviest ones, can be readsorbed

to continue growing or hydrogenated to paraffins. The probability of growth (α) strongly depends on the operating conditions (temperature, pressure, H_2/CO ratio and residence time) as well as on the catalyst properties [\[5,6\]. T](#page-6-0)he FT reactors used commercially can be classified into two broad categories: high temperature (HTFT, 593–623 K) and low-temperature (LTFT, 493–523 K) reactors [\[7\].](#page-6-0) The HTFT reactors include the fluidized and circulating fluidized bed reactors that are characterized by the absence of a liquid phase inside the reactor. In contrast, in the LTFT reactors which include the multitubular fixed-bed (Shell) and the slurry bubble column (Sasol), the catalyst is wet by a hydrocarbon liquid phase. All these reactors suffer from several drawbacks and the existence of conflicting requirements makes them the result of a nonoptimal compromise, as analyzed by de Deugd et al. [\[5\].](#page-6-0)

Microreaction technology can help to solve many of the problems of the conventional FT reactors. It should be noted that present FTS reactors productivity is limited by their heatremoval capacity since the synthesis reaction is largely exothermic $(\Delta H_R = -165 \text{ kJ/mol}_{\text{CO}})$. One of the outstanding characteristics of microchannel reactors is the beat transfer enhancement that microchannel reactors is the heat transfer enhancement that results from the increase of the heat transfer coefficients and the heat exchange surface area per unit volume with decreasing the channel hydraulic diameter. Therefore, higher reactants concen-

[∗] Corresponding author. Tel.: +34 948 169605; fax: +34 948 169606. E-mail address: lgandia@unavarra.es (L.M. Gandía).

^{1385-8947/\$ –} see front matter © 2009 Elsevier B.V. All rights reserved. doi:[10.1016/j.cej.2009.12.028](dx.doi.org/10.1016/j.cej.2009.12.028)

trations and catalyst loadings are possible for exothermic reactions thus improving productivity [\[8–10\].](#page-6-0) Moreover, it is possible to achieve the virtually isothermal operation thus preventing the formation of hot spots which means a gain in operational safety as well as in selectivity for middle distillates since the chain growth probability decreases as temperature increases. Selectivity is also favored by the very short diffusion lengths prevailing in microreactors thus preventing CO depletion which results in shorter chains. Like for monolithic reactors [\[5\], m](#page-6-0)icroreactors can be easily stacked which allows for staged feeding to compensate nonstoichiometric $H₂/CO$ ratios.

This paper reports on a computational fluid dynamics (CFD) study of heat transfer in a microchannel reactor for FTS coupling the exothermic Fischer–Tropsch synthesis with the partial boiling of water for heat removal. The aim of our study was to analyze the conditions under which the synthesis reaction could be conducted at a reasonably high CO conversion under close to isothermal conditions at temperatures between 483 and 513 K, which are typical of the LTFT reactors using cobalt catalysts. High syngas space velocities have been considered in order to explore the potential of the designed microreactor for FTS intensification [\[11\].](#page-6-0)

2. Microreactor model and simulation conditions

Three-dimensional (3D) simulations have been carried out using ANSYS CFX software. This code is based on the finite-volume method for spatial discretization of the conservation laws, the integral formulation of the Navier–Stokes equations. A fully coupled solver is used for flow velocity and pressure. This software tool has provided satisfactory results from the point of view of the consistency of the results and the computational speed for a variety of microfluidic problems [\[12–14\].](#page-6-0)

2.1. Microreactor geometry and grid characteristics

The simulated microreactor is a steel block 17 mm high, 21 mm width, and 21 mm long containing 80 microchannels arranged in cross-flow configuration with 40 microchannels in each direction for the transport of syngas-FTS products and cooling water, respectively. Fig. 1A and B illustrates some aspects of the microreactor geometry showing the fluidic and solid domains, respectively. The block can be viewed as the stacking in an alternate position of 8 steel plates 2 mm thick, 21 mm width, and 21 mm long; actually, the two outer plates are 2.5 mm thick. The plates have 10 parallel square microchannels of 1 mm of side and 21 mm long. The distance between adjacent channels is 1 mm in both directions whereas from each lateral side of the plates to the first channel the distance is 0.5 mm. The access to and the exit from the channels is through rectangular chambers 17 mm high, 21 mm width, and 10 mm long that are connected to circular pipes (7.2 mm internal diameter) by means of pyramidal-shaped flanges 10 mm long. Syngas and water are fed to the microreactor through the pipes.

The CFD model of the microreactor has three main physical domains, two of them are fluidic and the third is the solid block. These domains were meshed using combinations of tetrahedral, prismatic and pyramidal elements resulting in dense computational unstructured grids. In order to resolve the boundary layers accurately a mixed unstructured grid approach [\[15\]](#page-6-0) was applied inside the microchannels.

2.2. Simulations conditions

Simulations have been conducted under stationary conditions. It has been assumed that a very thin layer of an active catalyst has been uniformly deposited onto the walls of the microchannels. Gas hourly space velocities (GHSV) in the 5000–30,000 h⁻¹

Fig. 1. (A) The two fluidic domains of the microreactor geometry, syngas-FTS products (orange) and cooling water (blue). (B) Solid domain of the microreactor. The steel block is 17 mm high, 21 mm width and 21 mm long, and can be viewed as the stacking of 8 plates in alternate positions. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of the article.)

range at standard temperature and pressure (STP) have been considered for the syngas stream $(H₂/CO$ molar ratio = 2). These GHSV values are well above the ones typical of the FT synthesis conducted in commercial slurry and tubular fixed-bed reactors [\[16\].](#page-6-0) Taking into account that the available volume for the syngas stream in the microchannels is 0.84 cm^3 , the adopted GHSVs imply feeding the microreactor with 70–420 cm³ min⁻¹ (STP) of syngas. This results in a low contact time of 0.4–0.07 s that obviously requires very active FTS catalysts such as the ones developed by Oxford Catalysts plc [\[17,18\].](#page-6-0)

When included in the CFD codes, chemical kinetics is very computer time demanding, especially for a complex reaction scheme as the FTS [\[19\]. I](#page-6-0)n some simulation studies the complexity of the FTS chemistry has been reduced by using a set of global one-step mechanisms for selected reactions [\[20\]. T](#page-6-0)he aim of our work was to study the thermal performance of the microchannel reactor so the emphasis has been put on heat transfer. Therefore, our first approach in this paper has been to simulate the thermal effect of the exothermic FTS as an uniform heat source associated to the internal walls of the FTS microchannels, where the catalyst is located. This is of course an approximation because higher reaction and heat generation rates are expected at the microchannels entry. On the other hand, simulations have evidenced that the velocity of the fluid at the entry is almost identical for the several microchannels, so the residence times should be also very similar. For a given molar flow rate of CO fed to the microreactor ($F_{\text{CO},0}$, mol s⁻¹) and CO conversion at the reactor outlet (X_{CO}) the heat generated (Q_g) by the FTS synthesis has been calculated as follows:

$$
\dot{Q}_{g} \left[\text{kW m}^{-2} \right] = \frac{F_{\text{CO},0} X_{\text{CO}} (-\Delta H_R)}{40 \times (4 \times 1 \times 21) \times 10^{-6}} = 49,107 F_{\text{CO},0} X_{\text{CO}} \tag{1}
$$

As concerns the cooling microchannels it has been assumed that water enters the microreactor as liquid saturated at the reactor operating pressure. Water flow rates in the range between 0.25 and 250 g min−¹ have been considered. The microreactor block is assumed to be adiabatic, so heat absorbed by water generates steam. In consequence, the fluidic domain corresponding to the coolant has to be explicitly established in the CFD code as boiling flow involving a biphasic liquid water/steam heterogeneous system. Under these circumstances, buoyancy effects are obviously of importance, greatly conditioning the bubble dynamics and the coolant flow pattern. Therefore, buoyant flow has to be also explicitly taken into account when defining the flow model of the water/steam system in the CFD code. In this regard, the density of the continuous phase, in our case liquid water, is established as the reference density.

The validity of the continuum model and the Navier-Stokes equations for the cases under consideration in this work have been examined through the evaluation of the Knudsen number (Kn) which is defined as the molecular mean free path (λ) divided by the characteristic length (l) of the system. In our case the hydraulic diameter, that is, the side of the square channels $(l=0.001 \text{ m})$ has been adopted as the characteristic length. For an ideal gas in the framework of the kinetic theory, the Knudsen number can be also calculated as follows [\[21,22\]:](#page-6-0)

$$
Kn = \frac{\lambda}{l} = \sqrt{\frac{\pi \times \gamma}{2}} \times \frac{Ma}{Re}
$$
 (2)

where *Ma* is the Mach number, *Re* the Reynolds number and γ , the specific heat ratio $(c, (c))$ which can be taken as $7/5$ [22] Maxi specific heat ratio (c_p/c_v) , which can be taken as 7/5 [\[23\]. M](#page-7-0)aximum values of the Knudsen number were of the order of 2×10^{-5} which are much lower than 0.001 thus assuring the validity of the continuum model [\[22\].](#page-6-0)

Simulations were performed on a Dell Precision PWS690 workstation running MS Windows XP^{\circledast} \times 64 with an available RAM of 16.0 GB. Criteria of convergence were based on the residuals and the imbalance level of the conservation equations.

3. Results and discussion

3.1. Microreactor disposition and buoyancy effects

A first series of simulations was carried out to investigate possible effects associated to the disposition of the microreactor with respect to the gravity force as well as the influence of the buoyancy forces in the coolant domain, where bubbles are generated. Three dispositions have been considered that are shown in Fig. 2, where the buoyancy forces are represented by arrows. In disposition A both FTS and the water/steam streams flow perpendicularly to the direction of the gravity force. In disposition B, gravity helps the exit of the FTS products whereas the coolant flow is as in disposition A. Finally, in disposition C the coolant flows upward, in opposite direction to that of the gravity force. In order to evaluate the influence of the disposition on the thermal performance of the microreactor, simulations under 10 different sets of operating conditions have been carried out with the three dispositions shown in Fig. 2 as well as considering the coolant flow as non-buoyant, that is, in the absence of the gravity force. The simulations were performed setting the operating pressure at 20 atm and the syngas ($H_2/CO = 2$) inlet temperature at 523 K. Other conditions as syngas GHSV, CO conversion and water mass flow rate are compiled in [Table 1. T](#page-3-0)he thermal performance of the microreactor has been evaluated in terms of the mean temperature at the FTS stream exit ($T_{FTS,out}$) and

Fig. 2. Microreactor dispositions considered to investigate the effect of buoyancy forces in the coolant domain. Red arrows represent the magnitude of buoyancy forces. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of the article.)

the overall heat transfer coefficient (U) . In this regard, the microreactor has been analyzed as a single-pass cross-flow heat exchanger with both fluids unmixed; accordingly, U has been calculated as follows:

$$
U = \frac{q}{A \times F \times \Delta T_{lm}}\tag{3}
$$

where A is the heat exchange surface area, which in this case is the same for both the hot and cold sides $(A=0.00336 \,\mathrm{m}^2)$. The correction factor F is 1 because water vaporization takes place and

Table 1
Conditions of the simulations performed to study the effect of the microreactor disposition and buoyancy forces^a.

^a Operating pressure was set at 20 atm and the syngas temperature at the reactor inlet was 523 K in all cases.
^b Pesults are the mean starm centert at the misrographer sutlet when operating under disposition A

^b Results are the mean steam content at the microreactor outlet when operating under disposition A.

then, there is no change in the water temperature $(T_w = 486.1 \text{ K})$. The heat transfer rate (q) can be easily calculated as latent heat from the data of steam production. Finally, the temperature difference is calculated as the logarithmic mean for a counterflow heat exchanger [\[24\]. T](#page-7-0)he results are shown in Fig. 3A and B. It can be seen that, as far as the coolant is concerned, the thermal performance of the microreactor does not depend significantly on the disposition with respect to the gravity. Results obtained with dispositions A and B are almost identical as expected from the fact that in both cases the water/steam stream moves perpendicularly to the gravity force. These dispositions are more efficient (lower FTS outlet temperatures are obtained) than disposition C, with the coolant flowing in opposite direction to that of gravity, thus leading to slightly higher values of U (see Fig. 3B). This can be interpreted as one effect of the direction of the buoyancy force on the flow pattern, which is more markedly affected when the direction of the flow does not coincide with that of the buoyancy force. Indeed, when the coolant flow in disposition C is reversed, that is, water moves downward, the resulting performance is very close to that of dispositions A and B because now buoyancy and flow have opposite directions. Although the thermal conductivity of steam is much lower than that of liquid water (about 19 times at 500 K) the instabilities introduced in the flow by the steam bubbles have a positive effect in the heat transfer characteristics. As a matter of fact in absence of buoyancy forces, U significantly decreases, which results in high values of the FTS stream outlet temperature. Indeed, for simulations 6, 7 and 8 under non-buoyant flow the FTS product exits the reactor at 557, 579 and 538 K, respectively, which are well above the inlet temperature of 523 K. Obviously, this would have a very negative effect on the FTS selectivity to middle distillates. To illustrate the effect of the buoyancy force, the magnitude and direction on the velocity in the coolant domain (disposition A) is shown in [Fig. 4](#page-4-0) under the same conditions (simulation 8 in Table 1) with and without buoyancy effects. In absence of gravity the flow is uniform with parallel streamlines; the fluid is accelerated in the microchannels due to the reduced pass cross-sectional area as well as by bubbles formation, then the flow becomes slower to go out of the reactor. In contrast, under the action of gravity the flow is turbulent, eddies being present in the rectangular chambers. Furthermore, fluid recirculation is established in such a way that the flow in just half the microchannels rows (the lower ones) has an opposite direction to that in the upper rows. Obviously, these conditions greatly improve the heat transfer capacity. Turbulence is due to the effect of buoyancy forces on the system when sufficient steam is present. In the cases shown in [Fig. 4](#page-4-0) the mean steam content at the microreactor outlet was 16.6% (Table 1). When the steam content is much lower, as for conditions of simulation 10 (0.2%), the instability of the flow is greatly reduced in spite of using a coolant flow rate 100 times higher (results not shown).

Fig. 3. Mean temperature of the FTS stream at the reactor outlet (A) and overall heat transfer coefficient (B) resulting when the simulation conditions compiled in Table 1 are applied to different microreactor dispositions, including non-buoyant flow.

Fig. 4. Velocity in the coolant domain for disposition A. Simulations correspond to case 8 in [Table 1.](#page-3-0)

Simulation conditions considered in this section (see [Table 1\)](#page-3-0) can be divided into two groups according to the syngas GHSV, 5000 and 30,000 h−1. Maximum FTS stream mean outlet temperatures under normal operation (buoyant flow) are 498 and 521 K, respectively [\(Fig. 3A](#page-3-0)), and correspond to the simulations with the highest CO conversion (95%) and then, highest thermal power, 2.7 and 16.1 W_t. These temperatures are within the limits suitable for lowtemperature FTS. As concerns the overall heat transfer coefficient, it can be seen ([Fig. 3B](#page-3-0)) that it increases with the steam content, as can be deduced from the comparison of simulations 1, 2, 3 on the one hand and 5, 6, 7 on the other. However, U is more sensible to the stream flow rates from both the hot and cold sides than to the vapor fraction. The highest value of U obtained in this series of simulations corresponds to case 10, with GHSV of 30,000 h⁻¹ and water mass flow rate of 250 g min−1. Under these conditions the coolant flow regime is still laminar inside the microchannels (maximum Re of 1042) but becomes turbulent in the rectangular chambers (maximum Re of 7400). The fact that the flow regime in the channels is laminar explains the very low drop pressures obtained in the simulations that were always below 100 Pa.

3.2. Control of the FTS temperature

The aim of this study was to analyze the conditions under which the FTS could be conducted in a microchannel reactor at a reasonably high CO conversion under close to isothermal conditions at any desired reaction temperature between 483 and 513 K. To this end, a series of CFD simulations have been carried out in which

Fig. 5. Distribution of temperatures in the solid block (A) and in a plane of the coolant domain (B) for a CFD simulation corresponding to case 9 in [Table 1.](#page-3-0)

the effect of the system pressure and coolant flow rate have been examined at different levels of CO conversion: 25, 75 and 95%. In all cases the adopted disposition has been B in [Fig. 2, w](#page-2-0)ith gravity helping the exit of the FTS products. Syngas $(H₂/CO$ molar ratio of 2) GHSV has been set at 30,000 h⁻¹ which, taking into account that the volume of process channels, corresponds to a relatively high feed flow rate of 420 cm³ min⁻¹ (STP) relevant for FTS intensification.

A significant result from this simulation study has been the isothermicity exhibited by the microreactor block. As an example, Fig. 5A shows the distribution of temperatures in the steel block at steady state for a simulation conducted under conditions of case 9 in [Table 1. H](#page-3-0)eat removal was carried out with 25 g min⁻¹ of liquid water saturated at 486.1 K. As can be seen, the maximum difference of temperature inside the block is lower than 3 K, and the mean temperature of the solid is about 490.2 K, close to that of the coolant. As concerns the syngas stream, the distribution of temperatures in a central plane parallel to the flow direction is shown in Fig. 5B. In this case the variation is from 523.15 K at the entry to 491.4 K at the outlet. Interestingly, the temperature of the fluid inside the microchannels, where the reaction takes place, is almost constant at about 498 K that is well-suited temperature to low-temperature FTS over cobalt catalysts. These results evidence a very efficient heat exchange performance of the microreactor. As mentioned previously the simulations were conducted assuming uniform heat generation along the walls of the FTS microchannels. In order to evaluate the impact of this approximation on the results, a conversion profile was created to describe amore intense heat generation at themicrochannels entry, where the reaction rate is higher, but maintaining constant the total heat involved (case 9 in [Table 1,](#page-3-0) syngas GHSV 30,000 h⁻¹). This profile included null conversion at the microchannels inlet, 55% conversion at half channel length and 75% CO conversion at the exit. The results indicated that the maximum difference of temperature inside the solid block increased from 3 to 4 K only. Regarding the syngas, the temperature inside the microchannels decreased from about 505 K at the entry to 488 K at the exit. This is in contrast with the almost isothermal behaviour shown in Fig. 5B under uniform heat generation conditions. Nevertheless, the temperature still remains between the limits suitable for the low-temperature FTS. The main effects of increasing the syngas GHSV are more pronounced temperature differences in the fluid due to higher heat generation rate as well as higher overall heat transfer coefficients due to lower heat transfer resistance in the FTS microchannels.

It should be noted that the reaction temperature can be controlled with the system pressure, provided that saturated liquid water is used as coolant fluid. Indeed, as shown in Fig. 6 it is possible to maintain the FTS temperature between 483 and 513 K within a wide range of CO conversions (25–95%) working at pressures between 5 and 30 atm. This is the result of the efficient performance of the microreactor as heat exchanger and the fact that the saturation temperature of water in that range of pressures falls within the range of values suitable for low-temperature FTS operation. The maximum change of temperature of the FTS stream inside the block from the entry to the exit is about 5–6 K. Therefore, almost isothermal FTS can be achieved by setting the operating pressure at a value at which the saturation temperature of liquid water is slightly below the temperature at which the FT synthesis has to be carried. The pressure has to be reduced as the CO conversion increases to lower the boiling point and increase the heat-removal capacity. However, in the range of conditions considered the chain

Fig. 6. Effect of the pressure on the mean FTS temperature at different levels of CO conversion.

growth probability and the selectivity to middle distillates both decrease as the operating pressure is reduced. A series of numerical simulations were conducted to illustrate the effect of pressure on the FTS selectivity assuming plug-flow as reactor model. The reaction scheme and kinetics developed by Visconti et al. [19] for the low-temperature FTS over a cobalt on alumina state-of-art catalyst were implemented in the model. The results show that at 508 K and $H₂/CO$ molar ratio in the feed of 2, the chain growth probability decreases from 0.86 to 0.81 and 0.73 as the operating pressure decreases from 20 to 10 and 5 atm, respectively. This is equivalent to a decrease of the C_{5+} hydrocarbons mass fraction from 84.5 to 76 and 61%, respectively.

An alternative to use relatively low pressures is to increase the coolant flow rate. This can be seen in Fig. 7A where the mean FTS temperature is depicted for a series of simulations conducted at 20 atm with CO conversion of 75%. Increasing the water mass flow rate from 1.5 to 250 g min⁻¹ the FTS temperature can be maintained in the 516–495 K range. As regards the overall heat transfer coefficient it can be seen in Fig. 7B that U clearly increases with the

Fig. 7. Effect of the coolant fluid mass flow rate on the mean FTS temperature and steam fraction (A) and the overall heat transfer coefficient (B) for a series of CFD simulations carried out at 20 atm, syngas GHSV of 30,000 h−¹ and CO conversion of 75%.

coolant flow rate attaining values close to 300 W m⁻² K⁻¹ at the highest water flows, which can be considered typical for flow boiling heat transfer in microchannels at the heat fluxes in the range between 0.5 and 4 kW m−² considered in this study [\[25\].](#page-7-0)

4. Conclusions

Computational fluid dynamics (CFD) simulations pointed to the effectiveness of microchannel reactor technology for process intensification, in this case in relation to heat transfer rate enhancement. In this study, simulation conditions relevant for the low-temperature Fischer–Tropsch synthesis (FTS) have been selected, using high syngas GHSVs and saturated liquid water in cross-flow arrangement as coolant fluid. The results indicated that when processing up to 30,000 h⁻¹ of syngas (H₂/CO molar ratio of 2) FTS operation with low-temperature change in the 483–513 K range can be achieved setting the pressure at the appropriate value between about 5 and 35 atm and adjusting the cooling water flow rate in the range 0.25–250 g min⁻¹. An important role of the buoyancy effects on the thermal performance of the microreactor has been found. In this regard, very low steam content (1%) in the coolant stream is sufficient to improve the heat exchange effectiveness.

The hydraulic diameter of the microchannels considered in this study (1 mm) falls within the category of "minichannels" in the context of flow boiling in microdevices. This is a relevant consideration because under these conditions it is very likely that phenomena such as liquid superheat are not significant [\[26\].](#page-7-0)

Acknowledgements

We gratefully acknowledge financial support of this work by Petróleo Brasileiro S.A.-PETROBRAS and the Spanish Ministry of Science and Innovation (MAT2006-12386-C05).

References

- [1] C.H. Bartholomew, R.J. Farrauto, Fundamentals of Industrial Catalytic Processes, John Wiley & Sons, Inc. – AIChE, Hoboken, NJ, 2006, p. 398.
- [2] M.E. Dry, P. Steynberg, Stud. Surf. Sci. Catal. 152 (2004) 406.
- [3] B.H. Davis, Ind. Eng. Chem. Res. 46 (2007) 8938.
- [4] T. Riedel, G. Schaub, Topics Catal, 26 (2003) 145.
- [5] R.M. de Deugd, F. Kapteijn, J.A. Moulijn, Topics Catal. 26 (2003) 29.
- [6] H. Schulz, Topics Catal. 26 (2003) 73.
- [7] P. Steynberg, M.E. Dry, B.H. Davis, B.B. Breman, Stud. Surf. Sci. Catal. 152 (2004) 64.
- [8] V. Hessel, S. Hardt, H. Löwe, Chemical Micro Process Engineering, Wiley-VCH, Weinheim, 2004
- [9] G. Kolb, V. Hessel, Chem. Eng. J. 98 (2004) 1.
- [10] X. Ouyang, R.S. Besser, Catal. Today 84 (2003) 33.
- [11] K.T. Jarosch, A.L.Y. Tonkovich, S.T. Perry, D. Kuhlmann, Y. Wang, Microchannel Reactors for Intensifying Gas-to-Liquid Technology, in: Y. Wang, J.D. Holladay (Eds.), Microreactor Technology and Process Intensification, ACS Symposium Series 914, Washington, 2005, p. 258.
- [12] T. Glatzel, C. Litterst, C. Cupelli, T. Lindermann, C. Moosmann, R. Niekrawietz, W. Streule, R. Zengerle, P. Koltay, Comput. Fluids 37 (2008) 218.
- [13] G. Arzamendi, P.M. Diéguez, M. Montes, M.A. Centeno, J.A. Odriozola, L.M. Gandía, Catal. Today 143 (2009) 25.
- [14] G. Arzamendi, P.M. Diéguez, M. Montes, J.A. Odriozola, E. Falabella Sousa-Aguiar, L.M. Gandía, Chem. Eng. J. 154 (2009) 168.
- [15] J. Blazek, Computational Fluid Dynamics: Principles and Applications, Elsevier, Amsterdam, 2005.
- <http://www.compactgtl.com/download/> (last accessed June 28, 2009).
- [17] Y. Wang, A.L. Tonkovich, T. Mazanec, F.P. Daly, D. VaderWiel, J. Hu, C. Cao, C. Kibby, X.S. Li, M.D. Briscoe, N. Gano, Y.-H. Chin, Fischer–Tropsch Synthesis using Microchannel Technology and Novel Catalyst and Microchannel Reactor. US Patent No.: 7,084,180 B2 (2006).
- [18] <http://www.velocys.com/news/patent.php> (last accessed June 28, 2009).
- [19] G.C. Visconti, E. Tronconi, L. Lietti, R. Zennaro, P. Forzatti, Chem. Eng. Sci. 62 (2007) 5338.
- [20] K. Jarosch, B. Yang, S. Fitzgerald, R. Taha, T. Mazanec, A.L. Tonkovich, Prep. Pap. -Am. Chem. Soc., Div. Fuel Chem. 53 (2008) 90.
- [21] A.A. Rostami, A.S. Mujumdar, N. Saniei, Heat Mass Transf. 38 (2002) 359.
- [22] M. Wang, X. Lan, Z. Li, Int. J. Heat Mass Transf. 51 (2008) 3630.
- [23] G.A. Bird, Molecular Gas Dynamics and the Direct Simulation of Gas Flows, Oxford University Press Inc., New York, 2003.
- [24] F.P. Incropera, D.P. De Witt, Fundamentals of Heat and Mass Transfer, John Wiley & Sons, New York, 2002.
- [25] J.R. Thome, M. Groll, R. Mertz, Boiling and evaporation, in: G.F. Hewitt, G.P. Celata (Eds.), Heat Transfer and Fluid Flow in Microchannels, Begell House,
- Inc., New York, 2004, pp. 60–68. [26] S.G. Kandlikar, Exp. Thermal Fluid Sci. 26 (2002) 3893.