



Microchannel design for thin-film catalyst: A model-based study

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ABSTRACT

This paper investigates microchannel design strategies for Fischer-Tropsch synthesis (FTS) process using a novel approach of thin-film catalysts by mathematical modelling. Due to the geometrical limitations of 2-dimensional films special attentions were paid to the effects of channel geometry and operation conditions on the backmixing and mass transport phenomena, and subsequently, FTS conversion level and selectivity. The simulation results suggest that a microchannel geometry with high length-to-width ratio L/W minimizes the backmixing effects under conditions of low catalytic activity and small gas flow rates, which is of special importance for measurements under kinetic conditions. However, under conditions of high catalytic activity and high gas flow rates the microchannel seems less preferable for productivity of long-chain hydrocarbons due to the inevitable mass transfer effects from microchannel boundaries. Ranges of design and operation parameters for axial Péclet number $Pe_L \geq 10$ and transverse Péclet number $Pe_d \leq 0.1$ are proposed for the FTS thin-film microchannels.

1. Introduction

Mitigating carbon dioxide emissions requires the replacement of fossil feedstock by renewable or recycled alternatives for chemicals, especially fuels (Ail and Dasappa, 2016). For instance, the aviation sector requires sustainable alternatives to fossil fuel with very high energy density. Thus, Fischer-Tropsch Synthesis (FTS) using renewable energy for the process and recycled CO₂ as feedstock becomes an attractive concept (Denzil Moodley, et al., 2024). On the other hand, just recently thin-film catalysts have emerged as a promising alternative to conventional catalysts due to several reasons: based on semiconductor, photovoltaic or microsystems technology, thin-film catalysts intrinsically own high potential for atomic-scale control, offering the advantage of tunable parameters (e.g., crystallographic properties such as grain-size or orientation, strain, addition of dopants, component gradients of active metals, microstructuring of bulk and surface materials, etc.), opening a pathway to tailor catalyst materials (Trinh et al., 2023; Li et al., 2024). The applications of thin-film catalysts on acetylene semi-hydrogenation (Trinh et al., 2023), methane dry reforming (Mohamad jafar Moradi et al., 2023), CO₂ hydrogenation (Shivam et al., 2025), and CO oxidation (Ates et al., 2013) have been already shown in literature, indicating a successful knowledge transfer of thin-film technology to thermocatalysts. To harvest the full potential of these thin-film catalysts,

a suitable reactor concept is highly demanded, since, morphologically different from powder catalysts, thin-film catalysts are characterized as a 2-dimensional (2D) catalyst with a few nano meters of metal atoms deposited on substrate support. Due to the ultra-low catalyst loading the productivity per reactor volume may be quite small, however, the catalytic activity per weight catalyst can match or even surpass traditional powder catalysts (Kunene et al., 2025). In view of this ultra-low catalyst loading, microreactors, where reactor dimensions are 10⁻²–10⁻¹ mm or even smaller (Wei et al., 2025), are envisioned for thin-film catalysts, and it also favors the concept of process intensification (Stankiewicz and Moulijn, 2000).

Two ideal models can mathematically describe the fluids passing through a vessel, i.e., plug flow reactor (PFR) and continuous stirred-tank reactor (CSTR). The first case indicates no mixing of earlier with later entering fluids, e.g. no backmixing, while the latter case suggests perfect backmixing within the whole vessel. Due to small reactor dimension, generally, microreactors are designed as microchannels and are also mathematically described as PFR (Wei et al., 2025; Dong et al., 2021). However, applying backmixing into microreactors has attracted increasing attention, e.g., (Trinh et al., 2023; Mohammad, et al., 2022; Holgado et al., 2001), since backmixing can provide an improved temperature uniformity and concentration homogeneity around inlet region or hot-spot region. Though design examples of microchannels, where catalysts are packed as powder particles in the channel or are attached as

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Nomenclature			
a	Reaction rate constant, [$\text{mol}\cdot\text{kg}^{-1}\cdot\text{s}^{-1}\cdot\text{bar}^{-2}$]	T	Temperature, [K]
a_0	Frequency factor for reaction rate constant, [$\text{mol}\cdot\text{kg}^{-1}\cdot\text{s}^{-1}\cdot\text{bar}^{-2}$]	$\mathbf{u}$ or u	Velocity vector or velocity, [$\text{m}\cdot\text{s}^{-1}$]
A_s	Active metal surface, [$\text{m}^2\cdot\text{kg}_{\text{cat}}^{-1}$]	$\dot{v}$	Flow rate, [$\text{m}^3\cdot\text{s}^{-1}$]
b	Absorption constant, [bar^{-1}]	ν	Stoichiometric coefficient, [-]
b_0	Frequency factor for absorption constant, [bar^{-1}]	ν	Kinematic viscosity, [$\text{m}^2\cdot\text{s}^{-1}$]
C	Concentration, [$\text{mol}\cdot\text{m}^{-3}$]	V	Volume, [m^3]
d	Hydraulic diameter, [m]	W	Width, [cm]
D	Diffusivity, [$\text{m}^2\cdot\text{s}^{-1}$]	x	Distance in length direction, [m]
Da_i	First Damköhler number, [-]	X	Conversion, [-]
Da_{ii}	Second Damköhler number, [-]	y	Distance in width direction, [m]
E_A	Active energy, [$\text{kJ}\cdot\text{mol}^{-1}$]	<i>Greek Letters</i>	
E	E function for RTD, [s^{-1}]	α	Chain growth probability, [-]
E_θ	E_θ function for RTD, [-]	ρ	Gas density, [$\text{kg}\cdot\text{m}^{-3}$]
F	Activity factor, [-]	μ	Dynamics viscosity, [Pa·s]
H	Height, [cm]	ω	Mass fraction, [-]
I	Identity matrix, [-]	γ	Termination probability factor, [-]
j	Mass flux, [$\text{kg}\cdot\text{m}^{-2}\cdot\text{s}^{-1}$]	<i>Subscripts</i>	
k_α	Selectivity coefficient, [-]	0	Initial or inlet condition
L	Length, [cm]	d	Calculated by hydraulic diameter
n	Carbon number, [-]	C1	Methane
$\dot{n}$	Mole flux, [$\text{mol}\cdot\text{s}^{-1}$]	Cn	Hydrocarbon with carbon number n
P	Partial pressure, [bar] or [Pa]	H	Calculated by height
Pe	Péclet number, [-]	L	Calculated by length
$\mathbf{q}$	Particle position based on massless model, [m]	i or j	Number of gas species
r	Reaction rate, [$\text{mol}\cdot\text{kg}_{\text{cat}}^{-1}\cdot\text{s}^{-1}$] or [$\text{mol}\cdot\text{m}^{-2}\cdot\text{s}^{-1}$]	in	Inlet
R	Ideal gas constant, [$\text{J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$]	out	Outlet
Re	Reynolds number, [-]	p	Product
S	Selectivity, [-]	r	Reactor
t	Time, [s]	S	Surface reaction

porous particle layers on the channel walls via wash-coating, exist in the literature, yet the effects of backmixing on the reaction performance in the microchannel reactors, and general design criteria and principles of microchannel reactors for thin-film catalysts are seldom investigated. Previously, it is observed in our recent study (Kunene et al., 2025) that a cobalt-based thin-film catalyst exhibited significant performance for FTS, and it is suggested that thin-film catalysts might be an interesting approach in FTS catalyst development. Thus, there is an immediate need for a comprehensive design strategy for the thin-film-based FTS process.

In this study, design strategies for channel geometry, catalyst area and operation conditions for thin-film microchannel are preliminarily investigated. For this, ideal models, namely PFR and CSTR, are first mathematically studied to compare for the effects of backmixing on the FTS performance. Next, two geometries, i.e. small and large length to width (L/W) ratio, with a fixed catalyst area under two extreme operation conditions, low catalytic activity and small gas flow rates as well as high catalytic activity and large gas flow rates, are compared based on Multiphysics modelling with considerations of fluid hydrodynamics, mass transfer and reaction kinetics. Finally, primary design rules for thin-film microchannels are proposed.

2. Problem statement

Due to the low total catalyst loading related to small surface area, thin-film catalysts exhibit generally low volumetric productivity (Kunene et al., 2025; Abbas et al., 2025). Thus, low syngas flow rates are required to achieve significant CO conversion levels, and the reaction is usually governed by the reaction kinetics. Furthermore, a parabolic velocity profile is usually formed due to the laminar flow pattern, and the fluid velocity near reactor wall is almost stagnant. Subsequently, the

gaseous reactants must diffuse from the bulk flow to the catalyst surface at the reactor wall through very slow fluid layers, and the products from the surface back to the bulk flow. This feature under low catalytic activity and small flow rates makes the operation pattern for thin-film reactors quite different from powder catalysts, for which higher flow rates are normally adapted owing to quite larger catalyst loading. As such, though external- and internal-mass-transfer phenomena also exist in powder systems, the flow patterns are greatly governed by turbulences and fluctuations in packing cavities and boundary layers are thinned.

However, the catalytic activity of thin-film catalysts is not limited to the geometric surface area. Specially favored from thin-film technology (e.g., micro structuring technologies (Shivam et al., 2025; Rossnagel, 2003)) the catalytic activity is able to be increased in several magnitudes via micro-structuring to enhance active-site exposure while the catalyst sample size remains unchanged. For this, larger flow rates should be then applied to keep the contact time comparable, though the reactor volume might only be changed slightly. Therefore, sound design instructions for thin film reactors are of interest, where both 'low catalytic activity – small flow rate' and 'high catalytic activity – large flow rate' should be considered with a given catalyst sample area.

Amongst many catalytic reactions, FTS remains attractive due to its versatile nature providing a wide product spectrum of hydrocarbons (n -alkanes, n -alkenes) and oxygenates, depending on reaction conditions and applied catalytic systems. The chain growth probability, α , which is based on ideal Anderson–Schulz–Flory (ASF) distribution, is commonly used to describe the product distribution of Fischer–Tropsch reactions. Fig. 1 displays the reaction rate as a function of CO concentration and α as a function of H_2/CO ratio, based on intrinsic reaction kinetics (Becker et al., 2016; Becker et al., 2019; Vervloet et al., 2012; Yates and

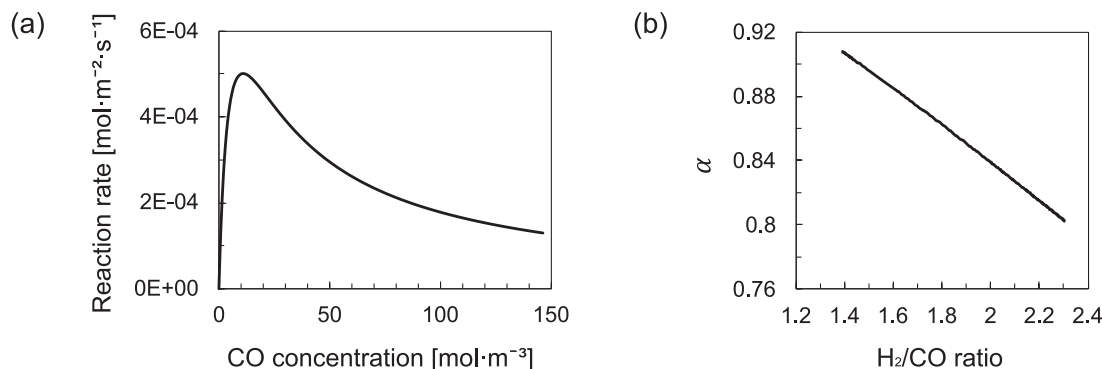


Fig. 1. FTS kinetics and selectivity. (a) Calculated reaction rate as a function of CO concentration based on the intrinsic reaction rate of powder-based catalysts (Becker et al., 2016; Becker et al., 2019; Yates and Satterfield, 1991); total pressure 20 bar, operational temperature 220 °C, initial H_2/CO 2:1. (b) Calculated α as a function of H_2/CO based on ASF-distribution with modifications (Vervloet, 2012; Förtsch et al., 2015).

Satterfield, 1991; Förtsch et al., 2015). As seen, based on mass-transfer-free effects and the Langmuir-Hinshelwood-type equations (see Appendix A.1), a decrease of CO concentration may counterintuitively result in higher reaction rates. This is also observed and discussed in some simulation works (Becker et al., 2016; Becker et al., 2019; Vervloet et al., 2012) and experiments with wash-coated catalysts (Ibáñez et al., 2021). As presented in Fig. 1 (b), low CO concentration or high H_2/CO ratio could result in a decrease of α , indicating lower long-chain hydrocarbons or C_{5+} selectivity in the FTS process. Next to the reaction, the local concentrations of H_2 and CO are affected by many factors (e.g. flow dynamics, temperature inhomogeneities, backmixing, liquid film formations, etc.) where especially diffusion plays a significant role, with the diffusivity of H_2 being 6 times larger than of CO in the gas phase and 2.7 times in liquid hydrocarbons at reaction temperatures (Wang et al., 2001). As such, the CO consumption, selectivity of products and their productivity become a complex interlacing. To harvest high productivity and selectivity of the FTS process all these factors should be taken into account during the reactor design.

Before diving into simulation and predictions, it is practical to clarify design variables and dimensionless numbers, which are involved in this paper.

Firstly, hydraulic diameter d , as presented in Equation (1), is a characteristic dimension of cross section for a rectangle channel.

$$d = \frac{4WH}{2W + 2H} \quad (1)$$

where W is width and H height of channel cross section. Furthermore, to describe flow hydrodynamics, Reynolds number (Re), Péclet number (Pe) as well as residence time distribution (RTD) are commonly applied. Re number is defined in Equation (2).

$$Re = \frac{ud}{\nu} \quad (2)$$

where u is velocity [$\text{m} \cdot \text{s}^{-1}$] and ν is kinematic viscosity [$\text{m}^2 \cdot \text{s}^{-1}$].

Pe number compares the advection rate and diffusion rate. However, in the literature, there exist several definitions of Péclet numbers (Lopes et al., 2011; Balakotaiah and West, 2002; West et al., 2003; Aubin et al., 2009). Their main differences derive from the definition of the diffusion length. Since the diffusion of reactants is isotropic. Thus, diffusion length can be channel length (L), width (W) and height (H). Three characteristic times can be defined as

$$t_L = \frac{L^2}{D}, \quad t_H = \frac{H^2}{D}, \quad t_d = \frac{d^2}{D} \quad (3)$$

where D is diffusivity [$\text{m}^2 \cdot \text{s}^{-1}$]. Accordingly, these three characteristic times lead to three dimensionless groups of Pe number:

$$Pe_L = \frac{t_L}{L/u} = \frac{uL}{D}, \quad Pe_H = \frac{t_H}{L/u} = \frac{uH^2}{DL}, \quad Pe_d = \frac{t_d}{L/u} = \frac{ud^2}{DL} \quad (4)$$

where Pe_L is the axial Péclet number (which indicates the backmixing in the length direction), Pe_H is the height Péclet number (where diffusion from channel center to the flat catalyst surface is focused), and Pe_d is the transverse Péclet number (which is an overall description with consideration of hydraulic diameter d). With a given reactor volume, flow rate and channel height, Pe_H may be same, but Pe_L and Pe_d can differ by a few magnitudes for different L/W ratio. Therefore, specifying the definition of the Péclet number when designing the microchannel for thin film catalysts is quite important.

Apart from Pe , RTD is usually applied to describe temporal inhomogeneities in the flow. Typically, laminar flow patterns with parabolic velocity profile across the reactor cross section are translated into broad RTD, which most often result in a decrease of selectivity. RTD is usually described via E_θ curve:

$$E_\theta = \bar{t}E \quad (5)$$

$$\bar{t} = \int_0^\infty tE(t)dt = \frac{V}{\dot{V}} \quad (6)$$

where $\bar{t}$ represents the mean residence time [s], V is the total volume of a reactor [m^3] and $\dot{V}$ the gas flow rate [$\text{m}^3 \cdot \text{s}^{-1}$]. To relate chemical reactions with reactor design, the Damköhler number (Da) is usually applied, which translates the ratio between reaction rate (here based on the catalyst surface area) and transport rate within the overall reactor is defined as:

$$Da_i = \frac{r_s A_s}{C\dot{V}} \quad (7)$$

where Da_i is the first Damköhler number, r_s is surface reaction rate [$\text{mol} \cdot \text{m}^{-2} \cdot \text{s}^{-1}$], A_s is active surface area [m^2] and C is reactant concentration [$\text{mol} \cdot \text{m}^{-3}$]. It should be noted that, when no micro structuring is involved on catalyst surface, active surface area A_s is equal to catalyst sample size A . A Da_i number of 10^0 – 10^1 is usually aimed when scaling a reactor with significant conversion (Wei et al., 2025), through which catalyst loading and gas feed rate can be determined for a given catalytic activity. With a given catalyst surface area (i.e., catalyst sample size), the geometry of the thin-film catalyst is designed through L/W , namely length-to-width ratio.

Contrary to conventional powder catalysts, for which Thiele modulus, for instance, is usually applied to estimate the effects of pore diffusion (Mandić et al., 2017; Aguirre et al., 2020) and/or Mears criterion the effects of external mass transfer limitation (Mears, 1971), thin-film catalyst is characterized with its 2-D feature (Shivam et al., 2025), thus, the second Damköhler number (Da_{ii}) is applied here, which

corresponds to the ratio between reaction rate on the catalyst surface and transport rate to the catalyst wall, i.e., cross-sectional diffusion, and can be calculated as:

$$Da_{ii} = PeDa_i \quad (8)$$

where Pe can be calculated with Pe_H or Pe_d , depending on the cross-sectional geometry of the microchannel reactor. And it can be seen from equations above that Re , Da_{ii} and Pe are dependent parameters of Da_i , L/W and H for given catalyst activity or surface area. A range of $Da_{ii} \leq 10^{-3}$ is generally esteemed as mass-transfer-limitation-free or reaction-rate-controlled, while $Da_{ii} \geq 10^{-1}$ mass-transfer-limited or diffusion-controlled (Bošković, 2019).

With these short introductions, the investigations in this paper concentrate on two microchannel geometries with a small or large L/W ratio, whose height is fixed to be same for sake of comparison, as given in Fig. 2 and Table 1. These two geometries imply two design considerations: a microchannel with small L/W ratio has a larger cross-sectional area and is likely to allow for more backmixing (i.e., close to CSTR), while a microchannel with large L/W ratio tends to behave similar as a PFR. Thus, comparison of these two geometries on FTS selectivity and productivity under large operational ranges (i.e., low catalytic activity and small flow rate as well as high catalytic activity and large flow rate) is of interest to obtain insights into microchannel design strategies for FTS thin-film catalysts.

3. Mathematical modelling

3.1. FTS reaction

To date, there is insufficient experimental data for catalytic performance of thin-film catalysts and no comprehensive kinetic model has yet been established that convincingly describes the reaction mechanism. Thus, we adapt the kinetics models from the literature under the framework of powder catalysts (Becker et al., 2016; Becker et al., 2019; Yates and Satterfield, 1991) (see Appendix A.1) to this work based on several assumptions (yet, further measurements and investigations are indeed necessary): i) FTS kinetics based on powder catalysts can reveal the intrinsic reaction mechanism regardless the catalyst morphology, and thin-film catalysts with a few nanometers thickness follow the same intrinsic kinetics as the powder catalysts tested, wherein this assumption is even strengthened with temperature-gradient-free and internal-mass-limitation-free features of thin-film catalysts; ii) cobalt-based catalyst is considered, based on previous experimental work (Kunene et al., 2025), which has low water-gas shift (WGS) activity, and the FTS reaction is given in Eq. (A1); iii) catalytic activity per weight catalyst can be related to its exposed catalyst surface area, which indicates the exposed active sites. Therefore, the surface reaction rate r_s [$\text{mol}\cdot\text{m}^{-2}\cdot\text{s}^{-1}$] can be rewritten:

$$r_s = \frac{Fr_{\text{H}_2+\text{CO}}}{A_s} \quad (9)$$

Table 1

Dimensions of two microchannel configurations.

	Small L/W ratio	Large L/W ratio
Width [cm]	2	0.5 ^a
Length [cm]	2.75	11 ^b
Height [cm]	0.2	0.2
Hydraulic diameter [m]	0.0036	0.0029
L/W	1.4	22

^a Compared to small L/W ratio, $W/4$.

^b Compared to small L/W ratio, $L \times 4$.

where F is an additional activity factor (see Table A1 of Appendix A.1), $r_{\text{H}_2+\text{CO}}$ is the rate of disappearance of either hydrogen plus carbon monoxide or carbon monoxide from powder catalysts [$\text{mol}\cdot\text{kg}_{\text{cat}}^{-1}\cdot\text{s}^{-1}$] (c. f. Equation (A9) of Appendix A.1) and A_s is active metal surface [$\text{m}^2\cdot\text{kg}_{\text{cat}}^{-1}$]. CO conversion (X_{CO}) and C_n (hydrocarbon with carbon number n) selectivity (S_{Cn}) are defined as:

$$X_{\text{CO}} = \frac{\dot{n}_{\text{CO},\text{in}} - \dot{n}_{\text{CO},\text{out}}}{\dot{n}_{\text{CO},\text{in}}} \quad (10)$$

$$S_{Cn} = \frac{\sum_j^n j\dot{n}_{Cj}}{\dot{n}_{\text{CO},\text{in}} - \dot{n}_{\text{CO},\text{out}}} \quad (11)$$

where $\dot{n}$ is mole flux [$\text{mol}\cdot\text{s}^{-1}$]. It should be noted that S_{Cn} in Equation (11) is distinguished from Equations (A3) and (A4) in the appendix, since S_{Cn} in Equation (11) describes the selectivity results from the a reactor and will be presented in the following sections while S_{C1} and S_{Cn} in Equations (A3) and (A4) are calculated selectivity based on chain growth probability α for calculating stoichiometric coefficients in FTS reaction (see Equation (A1) of Appendix A.1).

The value of α depends on H_2/CO ratio and temperature, based on a modified ASF-distribution (see Equation (A2) of Appendix A.1). To investigate the influence of concentration gradients, local $\alpha_x(y)$ values are analyzed by comparing the weighted average α along the channel width (α_W) and weighted average α along the channel length (α_L), which are defined as:

$$\alpha_W = \frac{\int_0^W r_{s,x}(y) \cdot \alpha_x(y) dy}{\int_0^W r_{s,x}(y) dy} \quad (12)$$

$$\alpha_L = \frac{\int_0^L r_{s,y}(x) \cdot \alpha_w(x) dx}{\int_0^L r_{s,y}(x) dx} \quad (13)$$

where x represents the distance in length direction and y the distance in width direction.

Contrary to $\alpha_x(y)$, α_W and α_L are weighted by the local surface reaction rate (r_s) along the respective dimension, thus, can quantify the contribution of local selectivity on overall productivity, and furthermore, α_W is able to highlight the effects of boundaries.

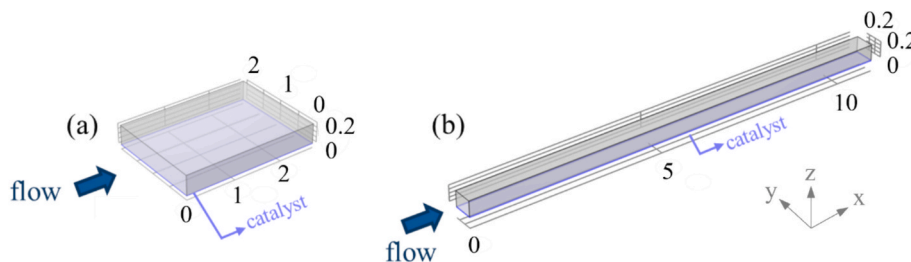


Fig. 2. Configurations of microchannels with one thin-film catalyst at bottom channel wall (unit: cm). (a) Small L/W channel; (b) Large L/W channel. The area of catalyst sample is same in both configurations. z direction is scaled to twice for clarification.

3.2. PFR and CSTR models

Two ideal reactor models, i.e. PFR and CSTR, are first used to compare the effects of backmixing on FTS performance, where intrinsic kinetics are applied without mass and heat transfer phenomena.

PFR:

$$dc_i = \frac{Wr_s}{\sum \dot{v}_{i,0} + \dot{v}_p} dx \quad (14)$$

CSTR:

$$V \frac{dc_i}{dt} = \dot{v}_{i,0} c_{i,0} - \left(\sum \dot{v}_{i,0} + \dot{v}_p \right) c_i + A_s r_s \quad (15)$$

where c is the concentration of reactant species i and '0' indicates the initial or inlet condition. Due to the consumption of reactants and production of products, the change in the flow rate $\dot{v}_p$ [$\text{m}^3 \cdot \text{s}^{-1}$] is calculated as:

$$\dot{v}_p = \frac{RT}{P} A_s r_s \sum v_i \quad (16)$$

where T and P are temperature and pressure, set by the typical FTS condition (see details in Table 2).

3.3. Multiphysics simulation

The formulations of mass and momentum balance and species transport are described as in Appendix A.2. A Lagrangian particle tracking method is applied to determine the RTDs. Instead of solving for the particle velocity or momentum, massless fluid particles are assumed to simply follow the fluid velocity streamlines, as presented in Equation (A16) of the appendix, which avoids the introduction of numerical diffusion, interaction between the individual particles and molecular diffusion.

3.4. Assumptions and conditions

The microchannel is assumed to be filled with gaseous reactants and products, and it is governed by ideal gas law; thus, no fluid formation is considered at this current stage, which is validated in Ref. (Becker et al., 2019), for preliminary investigations. Hydrocarbons with carbon numbers up to C_{10} are calculated for FT reaction (see Equation (A1)) based on ASF-distribution (see Equations (A3)–(A9)), and high-chain n -alkanes are lumped in one single $C_{19}H_{40}$. Details are c.f. Appendix A.1. Besides, a few nano-meter active metals are deposited on highly conductive substrates for thin-film catalysts, thus, with respect to thermal and mass transport, internal mass transport as well as heat transfer resistance of the catalyst is excluded; finally, catalyst deactivation is not

considered. Both ideal models (PFR and CSTR) and Multiphysics models are assumed to be isothermal (for this, an adapted Mears' criterion is checked, as presented in Appendix A.3).

The dimension and geometry of two microchannel objects for Multiphysics simulation are given in Table 1. A height of 2 mm, which is the upper limit of a common range of microchannel height in the literature for powder catalysts (Wei et al., 2025), is assigned for preliminary-stage investigation here. As seen in Table 1 and Fig. 2, the microchannel with small L/W ratio has a larger width and smaller length, while the width of the one with large L/W ratio is 4 times smaller and length 4 times larger, suggesting two design directions, i.e., wide-short and narrow-long geometries. Thus, the cross section from the small L/W ratio microchannel is larger and is also likely to allow more backmixing, especially at very small flow rates. To observe the backmixing and avoid complex effects of boundary conditions, virtual extensions before and after microchannel with thin-film catalyst are added (not drawn in Fig. 2).

Typical low-temperature FTS conditions for cobalt-based catalysts are applied, as outlined in Table 2. In order to compare the effects of channel geometries on FTS performance under large operational ranges while keeping Da_i constant, a low flow rate of 5 sccm (Kunene et al., 2025) is chosen and a large flow rate with 100-time increase is set as the contrary extreme. Correspondingly, for these two cases, catalyst activity changes differently, as seen in Table 2, however, Da_i remains constant for comparison between the two geometries as well as two extreme operation conditions. Therefore, a Da_i number at 5 sccm without catalytic activity enhancement is distinguished as Da_i^* , and correspondingly, the increase of catalytic activity is represented by Da_i/Da_i^* in the following sections.

3.5. Computation

The calculation of the 1-dimensional (1D) PFR model is conducted through MATLAB R2023a, and the 0-dimensional (0D) CSTR model is calculated via *Reaction Engineering* module for CSTR (constant volume) module in COMSOL Multiphysics 6.1. Microchannels (see Fig. 2) are built as 3D model in COMSOL Multiphysics 6.1: computational fluid dynamics (CFD) based on finite volume scheme for flow pattern as well as velocity and pressure distribution, mass transfer and chemical reaction model (*Transport of Concentrated Species*) based on surface rate equations and selectivity models. Upon the computation of the velocity field has been computed, the *Particle Tracing Module* is coupled and 10^5 weightless particles that are randomly distributed over the section of the microchannel inlet are released into the flows. To eliminate the particle tracers that are trapped near the walls due to a velocity close to zero, a restitution coefficient of unity is applied for RTDs.

The mesh is generated using the Physics-Controlled Mesh Method in COMSOL Multiphysics 6.1 with boundary-layer meshing at the catalyst surface (see Appendix A.4).

4. Results and discussions

4.1. Results of PFR and CSTR simulations

Fig. 3 presents the CO conversion, C_1 and C_{5+} selectivity as function of catalytic activity (Da_i/Da_i^*) for PFR (perfect repression) and CSTR (perfect backmixing) cases. The ideal models assume that diffusion coefficient D is 0 for PFR and ∞ for CSTR, thus, the effects of dimension are omitted. It can be seen that CO conversion and C_{5+} selectivity increase as the rise of catalytic activity, while C_1 selectivity decreases. FTS performance (i.e., X_{CO} and $S_{C_{5+}}$) in the PFR reaches a plateau at around an activity factor of 20 and further increase in catalytic activity does not further improve conversion or selectivity, it is rather a waste of the (expensive) catalysts. The reason for this is that H_2 is completely consumed in the PFR (see Fig. A3 in the appendix), since the stoichiometric coefficient for H_2 (ν_{H_2} in Equation (A7) of appendix) is larger than the feeding ratio of 2. For the CSTR case, however, the backmixing

Table 2
FTS conditions.

Parameter	Value	Unit
P	20	bar
T	220	°C
$CO/H_2/$ N_2	30:60:10	%
$A_{s,0}$	14.4 (van de Loosdrecht et al., 2014; van de Loosdrecht et al., 2003)	$\text{m}^2 \cdot \text{g}_{\text{cat}}^{-1}$
$\dot{v}$	5 ^a , 500 ^b	sccm
Da_i^*	0.072	—
$A_s/A_{s,0}$ ^c	1 ~ 100 ^a , 100 ~ 10000 ^b	—
Da_i	0.072 ~ 7.2 ^a , 0.072 ~ 7.2 ^b	—
Da_i/Da_i^*	1 ~ 100	—

^a 'Low catalytic activity – small flow rate' case.

^b 'High catalytic activity – large flow rate' case, but the range of Da_i is same as case in ^a.

^c Increase catalytic activity through increasing active catalyst surface area.

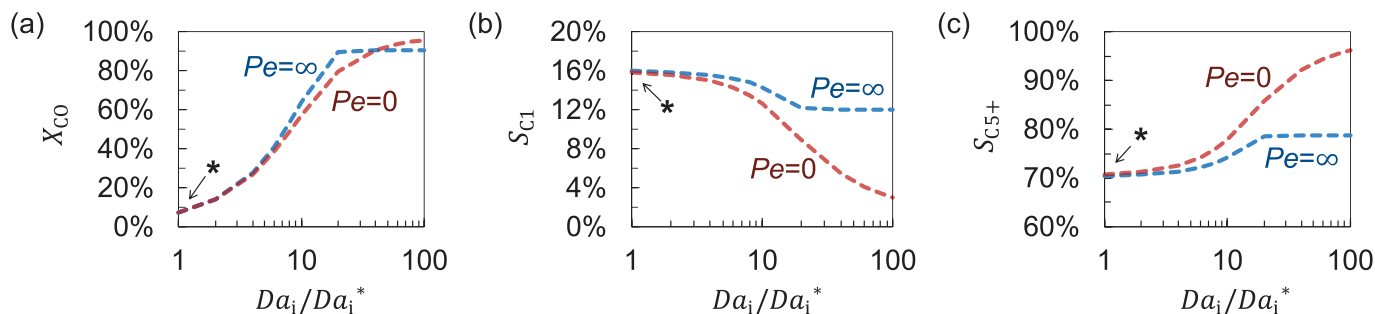


Fig. 3. (a) CO conversion level, (b) C_1 and (c) C_{5+} selectivity as function of catalyst activity within ideal PFR ($Pe = \infty$) and CSTR ($Pe = 0$) with consideration of only intrinsic kinetics. ‘*’ marks the condition under low flow rate without catalytic activity enhancement and its corresponding Da_i^* is given in Table 2.

causes a decrease in the CO conversion compared to the PFR case for an activity factor below 20, as seen in Fig. 3 (a). This is consistent with findings in the literature that backmixing in slurry beds (SB, behaving similar as CSTR) leads to significant decreases of conversion per pass (Maretto and Krishna, 1999; Hooshyar et al., 2012). However, as the catalyst activity further increases, the CO conversion levels in the CSTR can exceed the PFR at comparable mean residence time, because, in contrast to the PFR, H_2 is not fully consumed (see Fig. A3). On the other hand, as presented in Figures (b) and (c), backmixing seems to favor C_{5+} selectivity, i.e., lower C_1 selectivity and higher C_{5+} selectivity in the CSTR. These ‘positive’ effects on selectivity are even promoted with increase of catalyst activity, based on the here applied selectivity model, which seems counterintuitive, since backmixing is usually avoided (Hooshyar et al., 2012; Yang et al., 2009). FTS resembles polymerization reactions, and large extent of backmixing may dilutes the reactants and products, decreases the reaction driving forces and even could promote the side reactions (Alvaré and Al-Dahhan, 2006). As such, large amounts of backmixing are usually deemed detrimental in SBs for FTS. However, in the current selectivity model (see Appendix A.1), where chain growth probability α is independent of chain length, only effects of temperature and H_2/CO ratio on ASF-distribution are considered (Vervloet et al., 2012), and therefore, the propagation and termination reactions at the active sites on the catalyst are simplified. Eventually, the C_1 and C_{5+} selectivity of the CSTR seems more preferable than that in the PFR. This suggests that the current selectivity model might fall short to describe FTS product selectivity with large extent of backmixing at the high CO conversion levels and more comprehensive selectivity model for FTS process is demanded. However, the model has extensively been validated by packed-bed reactor (Kruit et al., 2013; Visconti et al., 2011), proved to be informative for powder particles in fixed beds (FB) (Vervloet et al., 2012; Förtsch et al., 2015) and been applied in cross-flow-structured packed beds for FTS (Kaskes et al., 2016), where the flow pattern is a combination of PFR and CSTR, and thus, we believe that the selectivity model together with the intrinsic kinetics models can be applied to Multiphysics simulation for the 3D microchannels (presenting mixed performance of PFR and CSTR, as seen follows) in this paper to predict the H_2/CO distribution in the channel and to preliminarily investigate the effects of channel design on FTS performance.

4.2. Results of multiphysics simulation for two geometries

As stated before, the Péclet number is applied to describe the backmixing or mass transport extent in the reactor. The values of Pe_L , Pe_H and Pe_d under small and large flow rates (defined by Re) for the two microchannel geometries are presented in Table 3. As seen from the magnitude of Re , the flow pattern in both microchannels can typically be considered as laminar flow ($Re \leq 2300$). However, the values of Pe_L , Pe_H and Pe_d differ in several magnitudes, regardless of Pe_L and Pe_d , Pe_H stays constant for two geometries. Therefore, in the following sections, ‘low catalytic activity – small flow rate’ is signified by ‘ $Pe_H \sim 10^{-3}$, $Da_{ii} \sim 10^{-3}$ ’, and ‘high catalytic activity – large flow rate’ ‘ $Pe_H \sim 10^{-1}$, $Da_{ii} \sim$

Table 3

Values of dimensionless numbers of the two channel geometries in two operation regimes.

	Small L/W ratio Low catalytic activity – small flow rate	High catalytic activity – large flow rate	Large L/W ratio Low catalytic activity – small flow rate	High catalytic activity – large flow rate
Re	0.17	17	0.53	53
Pe_L	1.7	1.7×10^2	27	2.7×10^3
Pe_H	8.8×10^{-3}	8.8×10^{-1}	8.8×10^{-3}	8.8×10^{-1}
Pe_d	0.029	2.9	0.018	1.8
Da_{ii}	6.3×10^{-3}	6.3	6.3×10^{-3}	6.3

[†] Calculated by Eq. (8) with Pe_H and Da_i/Da_i^* of 10.

10^{-1} , corresponding to two extreme cases. Besides, as determined in Fig. 3, FTS reaction reaches full conversion at Da_i/Da_i^* of 20. Thus, results within Da_i/Da_i^* of 10 are presented in the following sections (i.e., CO conversion level 50 ~ 60 %), yet the overall results can be found in Appendix A.5.

CO conversion level of two ideal reactor models as well as two geometries under two extreme conditions within Da_i/Da_i^* of 10 is presented in Fig. 4, and the corresponding C_1 and C_{5+} selectivity is presented in Fig. 5.

As seen in Fig. 4 (a), within Da_i/Da_i^* of 5, the difference in CO conversion levels for all cases is quite small. This suggests a degree of freedom in choosing reactor types, geometries and even operation conditions when CO conversion level is lower than ~ 20 %. A clear distinguishment is shown for X_{CO} larger than 50 %, as displayed in Fig. 4 (b). Though the influence on CO conversion is not severe, the influence of geometry and operation conditions on product selectivity is quite remarkable, as displayed in Fig. 5. Thus, the results of two geometries under two extreme cases are discussed separately as follows.

For the ‘low catalytic activity – small flow rate’ ($Pe_H \sim 10^{-3}$, $Da_{ii} \sim 10^{-3}$) condition, the CO conversion level of the two geometries lies between the ideal reactor models, as displayed in Fig. 4: the microchannel with small L/W ratio behaves quite similar as a CSTR, indicating a large degree of backmixing, while the one with large L/W ratio lies between PFR and CSTR. It is consistent when kinetic control governs the reaction with a positive reaction order, the backmixing decreases the reaction rate and thus conversion level. However, C_1 and C_{5+} selectivity does not necessarily follow the same trend. As seen in Fig. 5, the microchannel with small L/W ratio yields less methane selectivity and higher selectivity for long-chain hydrocarbons, while the one with large L/W ratio lies between PFR and CSTR. This seems a bit deviated from the convention in literature, since a majority of microchannels are designed to be large L/W (Wei et al., 2025).

On the other hand, for the ‘high catalytic activity – large flow rate’ ($Pe_H \sim 10^{-1}$, $Da_{ii} \sim 10^{-1}$) condition, the two microchannel geometries perform very similarly in terms of CO conversion and C_1 and C_{5+} selectivity. However, their CO conversion levels are slightly larger than

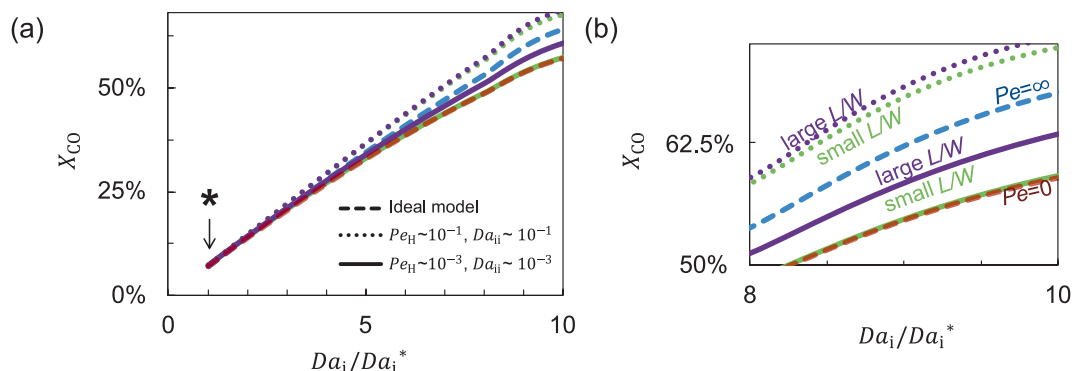


Fig. 4. (a) CO conversion level as function of catalyst activity within two microchannels (i.e., large and small L/W ratio for purple and green colors, correspondingly) under ‘low catalytic activity – small flow rate’ ($Pe_H \sim 10^{-3}$, $Da_{ii} \sim 10^{-3}$) and ‘high catalytic activity – large flow rate’ ($Pe_H \sim 10^{-1}$, $Da_{ii} \sim 10^{-1}$) conditions. ‘*’ marks the condition under low flow rate without catalytic activity enhancement and its corresponding Da_i^* is given in Table 2. (b) The enlarged graph of (a) at CO conversion level larger than 50 %.

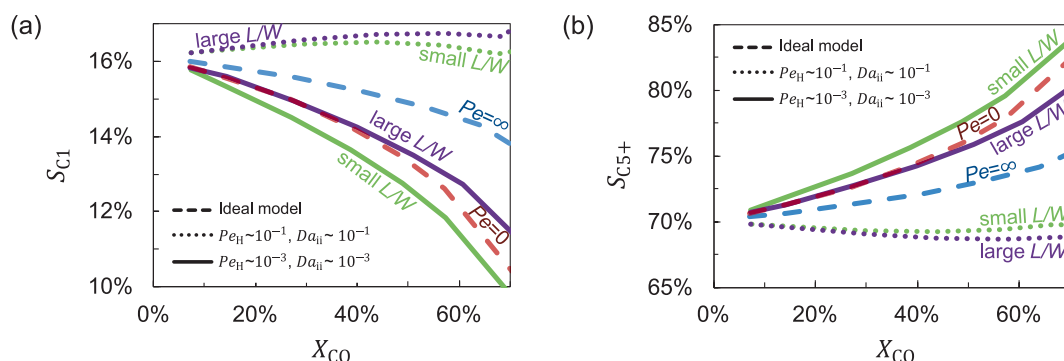


Fig. 5. (a) C_1 and (b) C_{5+} selectivity as a function of CO conversion level within two microchannels (i.e., large and small L/W ratio for purple and green colors, correspondingly) under ‘low catalytic activity – small flow rate’ ($Pe_H \sim 10^{-3}$, $Da_{ii} \sim 10^{-3}$) and ‘high catalytic activity – large flow rate’ ($Pe_H \sim 10^{-1}$, $Da_{ii} \sim 10^{-1}$) conditions.

two ideal reactors, as seen in Fig. 4. As a relatively large Da_{ii} implies emerging mass transfer limitation, this can change the distribution of H_2 and CO across the whole channel volume due to their quite different diffusivities and subsequently result in results beyond the ideal models.

At this point the observed results are out of expectations, and thus, in-depth analysis of effects of mass-transport phenomena and back-mixing on the reaction performance is discussed in the following sections.

4.3. Effects of backmixing

The CO and H_2 mole fractions and H_2/CO ratio along the length of the two microchannel geometries under two extreme conditions are presented in Fig. 6. In Figures (a, c, e), the region with catalysts in the microchannel is marked with gray color, and before and after catalyst region is the virtual extensions; comparison between the two geometries with the PFR is presented in the enlarged Figures (b, d, f). The corresponding reaction rates on catalyst surface of Fig. 6 are presented in Fig. 7.

The backmixing effects can be directly seen by the CO and H_2 distribution before the catalyst region (starting at $x/L = 0$). Since no catalyst is presented here, under ideal conditions the CO and H_2 mole fraction should remain constant and equal to the value of the feed at the channel inlet. And after reaction starts at the front edge of the catalyst region on the microchannel wall, CO and H_2 mole fraction changes along the channel length; the reaction terminates at the end edge of the catalyst region, and CO and H_2 mole fraction remains again invariant in the later section. This feature is well captured under ‘high catalytic activity – large flow rate’ ($Pe_H \sim 10^{-1}$, $Da_{ii} \sim 10^{-1}$) condition, as shown by

the dotted lines in Figures (a and c), indicating the minor effects of backmixing. However, under ‘ $Pe_H \sim 10^{-3}$, $Da_{ii} \sim 10^{-3}$ ’ condition, the backmixing effects lead to a significant deviation of the original CO and H_2 distribution, especially in the microchannel with small L/W ratio.

As seen in Fig. 6 (a), in the ‘ $Pe_H \sim 10^{-3}$, $Da_{ii} \sim 10^{-3}$ ’ case, before the catalyst region the CO mole fraction is larger than 0.3, which is the initial mole fraction of the feed at the channel inlet. And accordingly, H_2 mole fraction is smaller than 0.6, as seen in Fig. 6 (c). However, the rise of CO and decline of H_2 mole fraction before the catalyst region is less pronounced for the microchannel with large L/W ratio and large virtual extension is not necessary. Such backmixing effects derive mainly from the low gas velocity due to the large cross section (see Table 1) and the large difference in H_2 and CO diffusivity, i.e., H_2 diffusivity is almost 6 times faster than CO (Wang et al., 2001). Thus, before catalyst region, CO and H_2 are redistributed, wherein H_2 travels faster to the microchannel region and catalyst surface, and this is even promoted by the concentration gradient induced by the H_2 and CO consumption of the FT reaction, while CO becomes likely lagging behind. However, for the microchannel with large L/W ratio, whose cross-sectional area is relatively smaller (see Table 1) and thus flow velocity is higher, such backmixing phenomena from diffusive effects are alleviated due to higher convective velocity. This also confirms that the backmixing effects due to gaseous diffusion is even negligible for the $Pe_H \sim 10^{-1}$, $Da_{ii} \sim 10^{-1}$ condition.

The redistribution of CO and H_2 before the catalyst region leads to a significant change of the H_2/CO ratio in the microchannel, as displayed in Fig. 6 (e and f), and thus a change of α as well as reaction rate on the catalyst surface, as displayed in Fig. 7. As seen in Fig. 6 (e), due to the complex backmixing effects the H_2/CO ratio in the microchannel

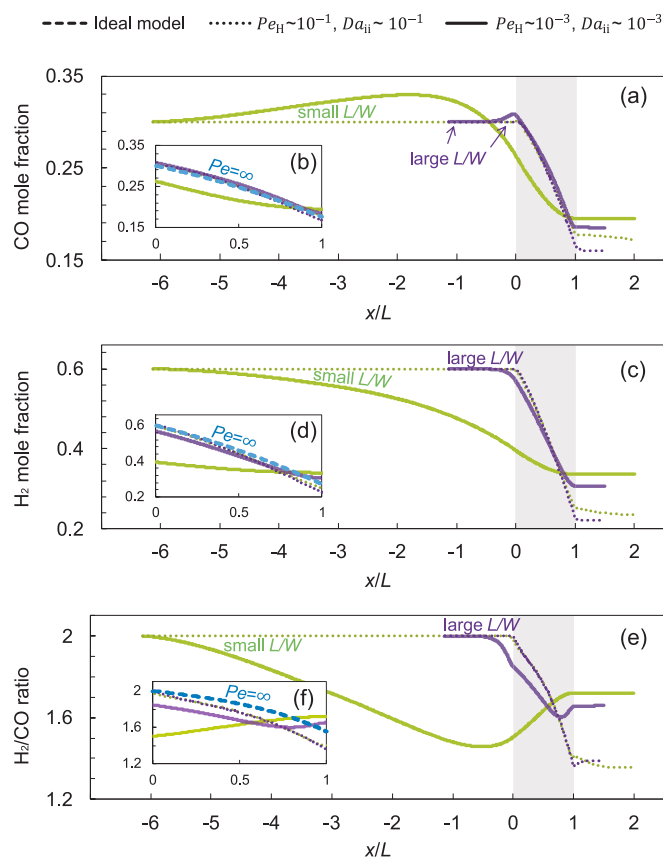


Fig. 6. CO and H₂ mole fraction and H₂/CO ratio along length of the two microchannel geometries (i.e., large and small L/W ratio for purple and green colors, correspondingly) under ‘low catalytic activity – small flow rate’ ($Pe_H \sim 10^{-3}$, $Da_{II} \sim 10^{-3}$) and ‘high catalytic activity – large flow rate’ ($Pe_H \sim 10^{-1}$, $Da_{II} \sim 10^{-1}$) conditions. Results are abstracted from channel center line. Da_I/Da_{II}^* is fixed in all cases to be 10. Region with catalyst is marked with gray color, before and after the marked region are the virtual extensions. The ideal model (dash curve $Pe = \infty$) is compared in the enlarged graphs (b, d, f).

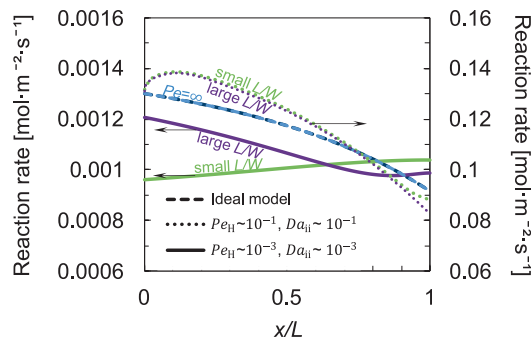


Fig. 7. Reaction rates at central line of catalyst surface along dimensionless length. Curves of PFR ($Pe = \infty$) for ‘ $Pe_H \sim 10^{-3}$, $Da_{II} \sim 10^{-3}$ ’ and ‘ $Pe_H \sim 10^{-1}$, $Da_{II} \sim 10^{-1}$ ’ conditions are overlapped.

deviates greatly from the feed value at the inlet of 2. Additionally, as shown in Fig. 6 (f), the H₂/CO ratio even increases within the catalyst region for the small- L/W channel, compared to the ideal reactor and the large L/W one. Based on the selectivity model, the smaller H₂/CO ratio for the microchannel geometry of small L/W ratio results in a larger α (see Fig. 1 (b)), indicating less C₁ selectivity and more C₅₊ selectivity, and subsequently explains the positive effects of backmixing on the selectivity in Fig. 5 above. Furthermore, these effects lower the reaction rate on the catalyst surface compared to the PFR (see Fig. 7) and

eventually decrease the CO conversion levels (see Fig. 4). These findings are of relevance for reactor design with 2D catalyst or ultra-low catalyst loading where very small flow rates are applied to obtain measurable catalytic performance (Ates et al., 2013; Kunene et al., 2025; Abbas et al., 2025). Even though the validity of the current selectivity model on CSTR-type or backmixing-rich reactors is lacking, the deviations of H₂/CO ratio derive intrinsically from the diffusivity differences of reactants. And such backmixing effects must not be overseen when the reactor geometry has a larger cross section. The measured reaction kinetics based on the feed composition as well as reactor downstream may not reveal the true kinetics of the catalyst. Thus, it is reasonable that such adverse effects should first be evaluated when designing channel dimensions and geometry as well as selecting operating conditions.

4.4. Effects of mass transport

Based on results from the channel central line in Fig. 6, the difference of the CO and H₂ distribution between the ideal reactor and the two microchannel L/W ratios under $Pe_H \sim 10^{-1}$, $Da_{II} \sim 10^{-1}$ condition is small, thus, the reaction rates should be similar. However, a notable difference in reaction rate on the catalyst surface is displayed in Fig. 7. Thus, a non-uniformity of H₂ and CO distribution due to the mass-transport phenomena is assumed. Distinguished from backmixing, which describes the axial mass transfer in this paper, the mass transport phenomena here refer to the corner/wall effects at ‘high catalytic activity – large flow rate’ condition, which normally occurs due to large velocity gradients from the reactor wall to the center of the bulk. Fig. 8 (a) presents the H₂/CO ratio abstracted from channel central, catalyst surface central and corner lines, and Figure (b) displays the corresponding weighted average α along width (α_W) and weighted average α along length (α_L) on the catalyst surface for two microchannels, as defined on Equations (12)–(13).

As seen in Fig. 8 (a), the H₂/CO ratio starts from 2 at the inlet and diverges across the reactor: the H₂/CO ratio in the channel center (red curves) keeps decreasing due to the catalytic reaction, which is similar as in the PFR, as shown in Fig. 6; however, the H₂/CO ratios at the catalyst surface central line (blue curves) and corner (green curves) is overall larger than that in the channel center, and more precisely, it first rises and then drops. The rise of the H₂/CO ratio suggests a local increase of H₂ and decrease of CO. Since the Pe_L number under the current condition is 10^2 – 10^3 (see Table 3) while no-slip wall is set as boundary conditions, the velocity in the channel center is much larger than that at channel walls and corners, where flows are almost stagnant (see Fig. 9 (a) and (b)). However, due to a Re number of $\sim 10^1$, the laminar pattern is dominating. Therefore, fluid layers with steep-velocity gradients from channel walls or corners to the channel center are formed and the gas reactants must diffuse through these fluid layers and react on the catalyst surface. Similarly, the products also diffuse from very slow fluid layers to the bulk center. As discussed above, H₂ diffuses almost 6 times faster than CO, and thus, the H₂ mole fraction is higher around the cross-sectional boundaries. Besides, as reaction proceeds, products are formed as a stagnate layer due to this mass transport phenomena, and this further decreases the CO mole fraction near walls and corners. Accordingly, an overall increase of H₂/CO ratio on catalyst surface and channel corners compared to channel center is observed, and the H₂/CO ratio rises first and later decreases. This also confirms that $Da_{II} \geq 10^{-1}$ usually states mass-transfer-limited or diffusion-limited.

As discussed in Fig. 1 (b), a rise of H₂/CO ratio results in a reduction of the α value, meaning a higher local α is unfavorable for the C₅₊ selectivity, while favoring methane formation. As presented in Fig. 8 (a), in the small L/W geometry the local H₂/CO ratio mostly exceeds those of the large L/W one, especially in the corners, while at the same time showing a higher selectivity (as compared in Fig. 5). To rationalize this, the rate weighted average α along width (α_W) and length (α_L) were introduced and their results are presented in Fig. 8 (b). As shown by the α_W curve, due the effects of transport phenomena near channel walls and

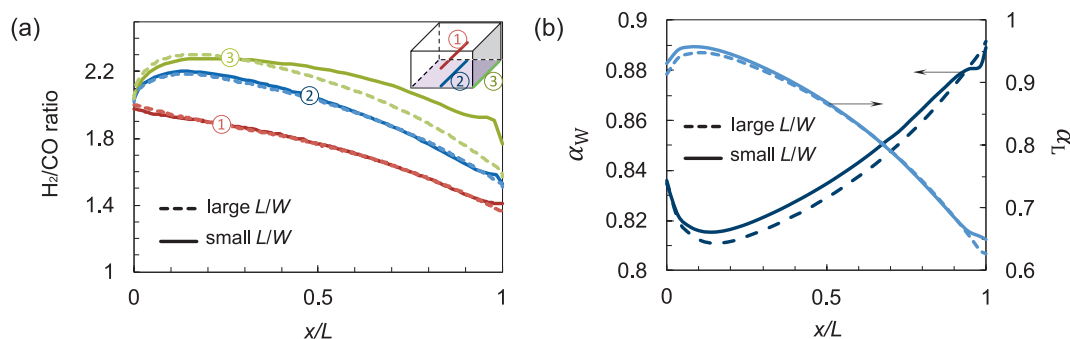


Fig. 8. (a) H_2/CO ratio at channel central (red marked line ①), catalyst surface central (blue marked line ②) and corner lines (green marked line ③) along dimensionless length. (b) Weighted average α along width (α_w with dark blue color) and weighted average α along length (α_L with light blue color) along dimensionless length. Both figures are under ‘high catalytic activity – large flow rate’ ($Pe_H \sim 10^{-1}$, $Da_{ii} \sim 10^{-1}$) condition. Da_i/Da_i^* is fixed to be 10.

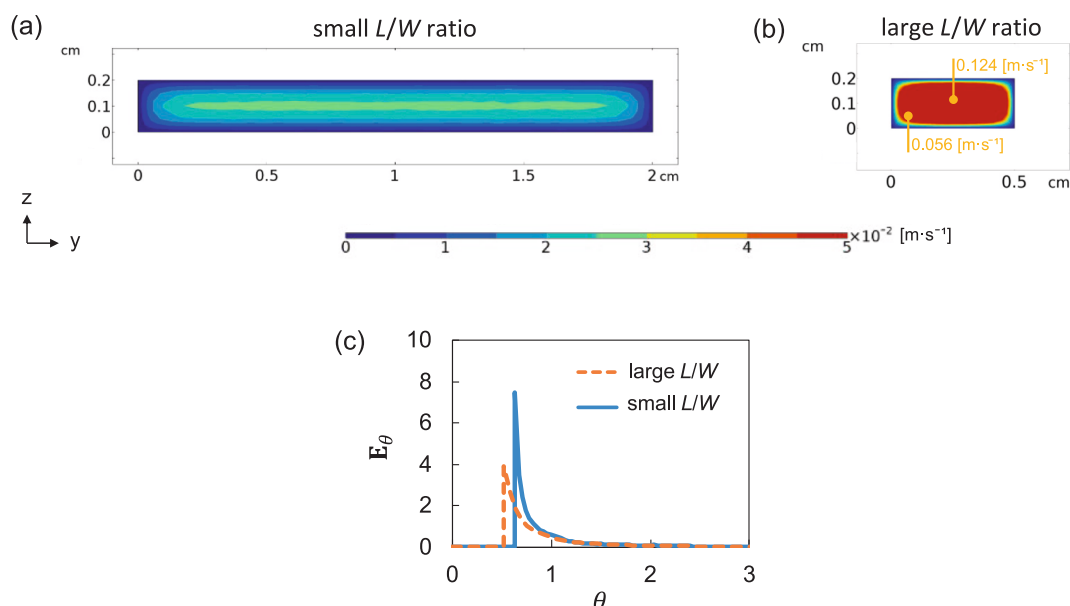


Fig. 9. (a) Cross-sectional velocity profiles of the microchannel with small L/W ratio and (b) with large L/W ratio; (c) RTD profiles of two microchannels under ‘low catalytic activity – small flow rate’ ($Pe_H \sim 10^{-1}$, $Da_{ii} \sim 10^{-1}$) condition. Da_i/Da_i^* is fixed to be 10.

corners, the α_w value drops first and later rises. The value of α_w for the large L/W drops more strongly than that of the small L/W one. This suggests that geometries with large L/W ratio suffer more from the wall/corner effects due to a higher total contribution of corner effects on the overall performance. However, the difference of the overall α_L for two geometries becomes again minor. This explains the quite similar CO conversion and C_1 / C_{5+} selectivity in Fig. 4 and Fig. 5. The decreasing difference in overall α_L is assumed to primarily result from the flow patterns, which is presented in Fig. 9.

The cross-sectional velocity profiles of two microchannels are displayed in Fig. 9 (a and b) and the RTDs for the overall channel volume are displayed in Figure (c). As displayed in Figure (a and b), it is obvious that the overall velocity in the microchannel with a small L/W ratio is lower than with a large L/W ratio, since the small L/W design exhibits a larger cross section (see Table 1). Besides, the velocity gradient in the microchannel with small L/W ratio is much smaller compared to the large L/W ratio. This is also expressed in the RTD curves in Fig. 9 (c). Since the two geometries own same volume and are operated under identical flow rates, the mean residence times ($\bar{t}$) are equal, and within θ ($t/\bar{t} = 1$) the residence time of tracers in the microchannel with larger L/W ratio has broader distribution. Compared to the case with the small L/W ratio, as shown in Fig. 9 (b), the steep-velocity gradient in the microchannel with larger L/W ratio leads to ‘thinner slow-velocity’

layers. This is especially beneficial for efficient transport of products upon the catalyst surfaces. Subsequently, the negative wall/corner effects could be compensated, resulting in comparable overall performance with the small L/W ratio. Such inherent differences in flow patterns between two geometries might inspire even more interesting discussions on, e.g., paraffin/olefin ratio, than plain chain growth probability or overall C_{5+} selectivity. As seen in Fig. 8 (b), both geometries have comparable overall α_L (relating to same $\bar{t}$), however, it can still be postulated that FTS product distribution might look different due to α -olefin re-adsorption (Iglesia et al., 1991) (relating to distinguished RTD and velocity gradient). But unfortunately, as discussed in Section 4.1, the current selectivity model (see Appendix A.1) has simplified the complex propagation and termination reactions to an empirical process-condition-dependent model. And further investigations are indeed demanded. It should also be noted that in this paper no liquid (i.e., long-chain hydrocarbons from low-temperature FTS process) is considered, the steep-velocity gradient and thin slow-velocity layers are preferable when liquid is formed upon the catalyst surface with respect to efficient evaporation and drainage to mitigate fouling.

To short, as presented in Fig. 5, it is obvious that, the significant mass-transport effects are unfavorable in terms of C_1 and C_{5+} selectivity when applying one single microchannel for this ‘high catalytic activity – large flow rate’ condition. This supports the idea of process scale-up

through numbering up (e.g., integrated, compact lab-scale kinetic-measurement setups as well as offshore and remote production facilities) (Wei et al., 2025; Dong et al., 2021): instead of a single microchannel with highly active catalyst and large flow rate, the pilot-scale FTS setups usually consist of multi parallel but identical microchannels with distributed, moderate catalytic activity. Nevertheless, due to its “thin-film” and (almost) zero-pore properties (Shivam et al., 2025) the thin-film catalysts still own the potential to alleviate pore-diffusion-induced deactivation (e.g., wax accumulation in powder catalysts (Pöhlmann et al., 2016) and to improve thermal management (Trinh et al., 2023) even at ‘high catalytic activity – large flow rate’ condition.

4.5. Microchannel design

In summary, for the ‘low catalytic activity – small flow rate’ ($Pe_H \sim 10^{-3}$, $Da_{ii} \sim 10^{-3}$) conditions, microchannels with a larger cross section (small L/W ratio) suffer more from backmixing, which leads to a decrease of CO conversion levels. Special attention must be paid when the microchannel is designed with such large cross sections for kinetic investigations, since the pronounced backmixing may lead to misinterpretation of obtained data assuming PFR behavior. On the other hand, for the ‘high catalytic activity – large flow rate’ ($Pe_H \sim 10^{-1}$, $Da_{ii} \sim 10^{-1}$) condition, microchannel concept seems not favorable for effective FTS selectivity due to the negative effects of mass transport between channel center and boundaries. Therefore, proper design strategies and boundaries have to be discussed.

As introduced in Equations (3) and (4), Pe_L describes the backmixing in the axial direction of the channel. A large Pe_L indicates high convection rates, and subsequently, the diffusive effects in the axial direction become negligible. On the other hand, the Pe_d number compares the mass transport between radial and axial directions. Here, a small Pe_d number indicates perfect mixing across the channel cross section, meaning the mass transport resistance across the cross section is negligible. With a fixed Re number, Pe_L is proportional to L/d (i.e., $Pe_L = uL/D = (L/D)(Re/d)$), while Pe_d is proportional to d/L (i.e., $Pe_d = ud^2/DL = Re(\nu/D)(d/L)$). This allows a mapping of Pe_L and Pe_d within $Re = 10^{-2} \sim 10^3$ and $L/d = 10^{-1} \sim 10^3$, which is most relevant for microchannel design. This map is calculated in Fig. 10. The microchannel

geometries considered in this paper as well as design examples from experiments in literature are added to the figure for comparison.

As can be seen in Fig. 10, increasing both Re (i.e., large flow rate) and L/d (i.e., narrow-long geometry) can increase Pe_L , i.e., reduce axial backmixing and mitigate detrimental effects from reactor geometries when intrinsic kinetics are tested. Based on the FTS experimental study from Mohammad et al. (Mohammad et al., 2022; Mohammad et al., 2019; Mohammad et al., 2020), microchannel reactors with a square geometry ($d = 500 \sim 1000$ [μm]) with an activity range of ~ 0.7 [mol·m⁻³·s⁻¹] were used for kinetics measurement (mass-transfer-limitation-free condition was assumed but not confirmed). In their cases Pe_d was $0.01 \sim 0.1$; Pe_L was > 10 , which is similar as the large L/W geometry at the ‘low catalytic activity – small flow rate’ ($Pe_H \sim 10^{-3}$, $Da_{ii} \sim 10^{-3}$) condition in this paper, as compared in Fig. 10.

On the other hand, with a fixed, desired Da_i (i.e., flow rates and catalytic activity increase/decrease parallelly), an increase of Re also implies the increase of Pe_d and Da_{ii} , as shown by arrows in Fig. 10. And herein, the mass transport limitations across the reactor cross section are increased, which is the least favorable for FTS selectivity. According to another FTS experimental results from Walter et al. (St. Walter et al., 2005), a microchannel reactor with circular geometry ($d = 280$ [μm]) with high reaction rate ($r_s = 10^{-4} \sim 10^{-1}$ [mol·m⁻²·s⁻¹]) was found to be mass-transfer-limited. The Pe_d value in their case was ~ 10 , indicating inevitable mass transfer effects. This is also consistent with our observations on both geometries under the ‘high catalytic activity – large flow rate’ ($Pe_H \sim 10^{-1}$, $Da_{ii} \sim 10^{-1}$) condition.

Based on the discussions above, therefore, to avoid wrong data interpretation due to backmixing effects for low catalyst activities, $L/d \geq 10^2$ and $Pe_L \geq 10$ might be required. However, highly active catalysts, coupled with high flow rates ($Re > 10^2$), seem not recommendable to be applied in microchannels (meaning $Da_{ii} \geq 0.1$) due to several reasons: FTS selectivity might reduce because of the mass transfer phenomena; L/d might need to be $> 10^3$ to obtain $Pe_d \leq 0.1$, resulting in very tiny cross section, which may tremendously increase pressure drop and risk of blockage when liquid is formed.

Therefore, a region of $Pe_L \geq 10$ and $Pe_d \leq 0.1$ in Fig. 10 seems suitable for the current thin-film catalyst with moderate FTS activity (i.e., $Da_i/Da_i^* < 20$) and a Re of $1 \sim 100$. And accordingly, microchannel geometry L/d ranges of roughly $50 \sim 500$.

5. Conclusions

In this paper, design strategies for geometry, dimension and operation conditions for Fischer-Tropsch synthesis are preliminarily investigated. Aside from computational fluid dynamics, a chemical reaction model was developed and adapted to thin-film catalysts to investigate conversion and product selectivity. We discuss the effects of backmixing on the catalytic performance via theoretical models of plug flow reactor (PFR) and continuously stirred-tank reactor (CSTR), and mass transport phenomena are further studied through Multiphysics simulation of microchannels with wide-short and narrow-long geometries under low/high catalytic activity and small/large flow rates. The key findings of the simulations can be summarized accordingly:

- Backmixing derived from gas diffusivity differences was observed at especially small flow rates and could lead to a notable change of the H₂/CO ratio in the microchannel,
- thus, it could lead to significant deviations in interpretation of kinetic measurements, and it is sound to first check these effects when designing channel dimensions and geometry as well as choosing operating conditions. Special attention should be also given to selecting proper inlet boundary conditions and to creating a simulation model for each reactor section.
- Catalysts with high activities, requiring high feed rates, seem not recommended to be applied in one single microchannels for FTS due to the significant mass-transport effects. Instead, numbering-

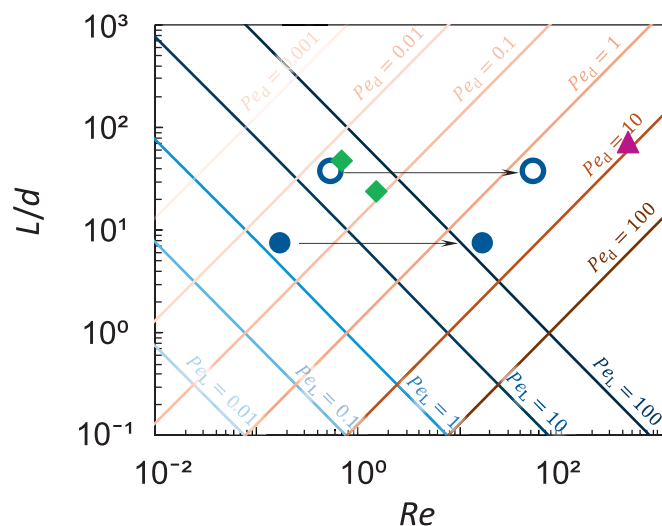


Fig. 10. Microchannel design parameter (L/d) as a function of operation parameter (Re) at $Pe_L = 0.001 \sim 100$ and $Pe_d = 0.01 \sim 100$. Solid circles: microchannel with small L/W ratio in this paper; hollow circles: microchannel with large L/W ratio in this paper; solid diamonds: microchannels for wash-coated powder catalyst from ref. (Mohammad et al., 2022; Mohammad et al., 2019; Mohammad et al., 2020); solid triangle: microchannel for wash-coated powder catalyst from ref. (St. Walter et al., 2005). Arrows indicate conditions from $Pe_H \sim 10^{-3}$, $Da_{ii} \sim 10^{-3}$ to $Pe_H \sim 10^{-1}$, $Da_{ii} \sim 10^{-1}$.

up to multi parallel microchannels with distributed, moderate catalytic activity could be a better alternative.

- (iv). For the current thin-film catalysts with moderate FTS activity, $Re = 1 \sim 100$ and the ratio of length to cross section $L/d = 50 \sim 500$ seems to be suitable, fulfilling $Pe_L \geq 10$ and $Pe_d \leq 0.1$.

Though the models developed in the present work are based on several major assumptions and convincing experimental results on this subject are still lacking, the observed phenomena in the flow-by chamber of microchannel derive intrinsically from gas properties, e.g., diffusivity in Da_{ij} . We hope that the design strategies are relevant for microchannels with ultra-low catalyst loading, e.g., thin-film catalysts, and to raise special attention of engineers for designing or simulating a 2-D and/or pseudo-2D catalytic (i.e., conventional wash-coated catalysts, yet, with additional considerations of mass transfer in catalyst layer) microchannel reactors.

CRedit authorship contribution statement

Yangjun Wei: Writing – review & editing, Writing – original draft,

Visualization, Software, Methodology, Investigation, Formal analysis, Data curation, Conceptualization. **Lukas Thum:** Writing – review & editing, Writing – original draft, Methodology, Investigation. **Avela Kunene:** Writing – review & editing. **Rutger Schlatmann:** Supervision, Project administration, Funding acquisition. **Daniel Amkreutz:** Writing – review & editing, Supervision, Project administration.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix

A.1. FTS

(1) Reaction



(2) ASF-distribution

$$\alpha = \frac{1}{1 + \left(\frac{C_{\text{H}_2}}{C_{\text{CO}}}\right)^\beta k_a \exp\left[\frac{E_{A,a}}{R} \left(\frac{1}{T_{\text{ref}}} - \frac{1}{T}\right)\right]} \quad (\text{A2})$$

where α is chain growth probability, γ is termination probability factor. Accordingly, the stoichiometric coefficients ν are dividually calculated by the model selectivity for methane S_{C1} and all other hydrocarbons S_{Cn} :

$$S_{\text{C1}} = \frac{(1 - \alpha)[1 - \alpha(1 - \gamma)]}{1 - \gamma\alpha} \quad (\text{A3})$$

$$S_{\text{Cn}} = \frac{n(1 - \alpha)^2 \alpha^{n-1} (1 - \gamma)}{1 - \gamma\alpha} \quad (\text{A4})$$

$$\nu_{\text{CO}} = -S_{\text{C1}} + \sum_{n=2}^{\infty} S_{\text{Cn}}(-1) = -1 \quad (\text{A5})$$

$$\nu_{\text{H}_2\text{O}} = S_{\text{C1}} + \sum_{n=2}^{\infty} S_{\text{Cn}} = 1 \quad (\text{A6})$$

$$\nu_{\text{H}_2} = -3S_{\text{C1}} + \sum_{n=2}^{\infty} [S_{\text{Cn}} \bullet \left(-\frac{2n+1}{n}\right)] \quad (\text{A7})$$

$$\nu_{\text{C,n}} = S_{\text{Cn}} \bullet \frac{1}{n} \quad (\text{A8})$$

(3) Kinetics

$$-r_{\text{H}_2+\text{CO}} = \frac{aP_{\text{CO}}P_{\text{H}_2}}{(1 + bP_{\text{CO}})^2} \quad (\text{A9})$$

where P is pressure of gas species [bar], and temperature-dependent adsorption constants a and b are calculated as

$$a = a_0 \exp\left[\frac{E_{A,a}}{R} \left(\frac{1}{T_{\text{ref}}} - \frac{1}{T}\right)\right] \quad (\text{A10})$$

$$b = b_0 \exp\left[\frac{E_{A,b}}{R} \left(\frac{1}{T_{\text{ref}}} - \frac{1}{T}\right)\right] \quad (\text{A11})$$

Values of the kinetic parameters and selectivity models are summarized in Table A1. As seen in the Table A1, an additional, dimensionless activity factor F is assigned with 605, while it is usually in a range of 1–20 for powder catalysts in literature (Guettel and Turek, 2009). The large number of F in this paper derives from our previous observation of significant performance for FTS using thin-film catalysts (Kunene et al., 2025), where a catalyst sample (0.07 wt-% Co loading) with size of 2.75×2 [cm²] is tested at 5 ~ 40 sccm for FTS performance. A main assumption is made: mass transfer limitation is preliminarily omitted at high flow rates, and the CO consumption rate at 40 sccm for thin-film catalysts was compared to $r_{\text{H}_2+\text{CO}}$ (see Equation (A9)) with an active metal surface $A_{\text{S},0}$ 14.4 [m²·g_{cat}⁻¹] (see Table 2). Although model adaptation may bring in deviations to some extent and further kinetic studies are needed to validate such assumptions, we hope that the model can preliminarily serve as an analyzing methodology to predict the trending effects of microchannel design on FTS performance.

Table A1
Parameterizations of kinetics and selectivity models.

Parameter	Value	Unit
F	605	—
a_0	8.853×10^{-3}	mol·kg ⁻¹ ·bar ⁻² ·s ⁻¹
b_0	2.226	bar ⁻¹
k_a	0.0567	—
$E_{A,a}$	37.37	kJ·mol ⁻¹
$E_{A,b}$	-68.48	kJ·mol ⁻¹
$E_{A,a}$	120.4	kJ·mol ⁻¹
β	1.76	—
T_{ref}	493.15	K
γ	0.5	—

A.2. CFD

(1) Continuity equation

$$\nabla \bullet (\rho \mathbf{u}) = 0 \quad (\text{A12})$$

where ρ represents the density of gaseous mixture, $\mathbf{u}$ is the velocity vector.

(2) Momentum equation

$$\rho \mathbf{u} \nabla \mathbf{u} = -\nabla P + \nabla \cdot \left[\mu (\nabla \mathbf{u} + (\nabla \mathbf{u})^T) - \frac{2}{3} \mu (\nabla \cdot \mathbf{u}) \mathbf{I} \right] \quad (\text{A13})$$

where μ is the fluid viscosity.

(3) Species transport

$$\nabla \bullet (\rho \omega_i \mathbf{u}) = -\nabla \cdot \mathbf{j}_i + r_i \quad (\text{A14})$$

$$\mathbf{j}_i = -\rho D_i \nabla \omega_i \quad (\text{A15})$$

where ω represents the mass fraction and $\mathbf{j}$ is the mass flux calculated by Maxwell-Stefan equation for gas diffusivity D ; FTS reaction rate r contributes the main source term.

(5) Particle tracking

$$\frac{d\mathbf{q}}{dt} = \mathbf{u} \quad (\text{A16})$$

A.3. Absence of radial temperature gradients

Mears' criterion (Ibáñez et al., 2021; Mears, 1971) is applied to check the radial temperature gradient within the ranges investigated in this work.

$$\frac{|\Delta H|(-r_r)d^2}{k_e T} < \frac{0.4RT/E_A}{[1 + 8Bi(\delta/d)]} \quad (\text{A17})$$

where ΔH is reaction enthalpy: 165,000 [J·mol⁻¹]; r_r is reaction rate per unit reactor volume: 0.6 ~ 60 [mol·m⁻³·s⁻¹], calculated from surface reaction rate $1.2 \times 10^{-3} \sim 1.2 \times 10^{-1}$ [mol·m⁻²·s⁻¹], channel volume 1.1×10^{-6} [m³] and catalyst sample area 5.5×10^{-4} [m²]; d is assigned to be channel height: 0.002 [m]; k_e is effective thermal conductivity, which is mainly contributed from fluids, 0.3 [W·m⁻¹·K⁻¹]; T is temperature at reactor wall, which is assumed to be value controlled by reactor set-up, 220 [°C] (493.15 K); R is gas constant: 8.314 [J·mol⁻¹·K⁻¹]; E_A is active energy: 62,600 [J·mol⁻¹] (C₅₊ formation) and 110,200 [J·mol⁻¹] (C₁₋₄ formation); Bi is Biot number of reactor wall, where aluminum is applied as substrate in the experiment (Kunene et al., 2025), thus 0.1 is applied here; δ is assigned to be the thickness of the substrate: 0.0005 [m]. Based on given parameters, the right side of Equation (A17) is 0.12 ~ 0.22, and the left side is 0.002 ~ 0.27. One can see that, at 'low catalytic activity – small flow rate' condition, isothermal assumption is valid within the overall microchannel, while at 'high catalytic activity – large flow rate' condition the temperature gradient

may slightly enlarge, and subsequently, ‘isothermal’ assumption may result in deviation. However, heat removal from convection is not considered in Equation (A17), and in ‘high catalytic activity – large flow rate’ case the high fluid velocity could enlarge k_e greatly, and thus, the isothermal assumption is still valid.

A.4. Meshing and grid independence

Grid independence is carried out. The deviation between coarse and fine mesh is within 1.3 % and between fine and extra fine mesh is 1 %, as displayed in Fig. A 1. However, it takes more than 9 days to run one case with extra fine mesh. Thus, fine mesh is applied with refinement on boundary layers, resulting in 790,791 domains elements and 55,448 boundary elements, as shown in Fig. A2.

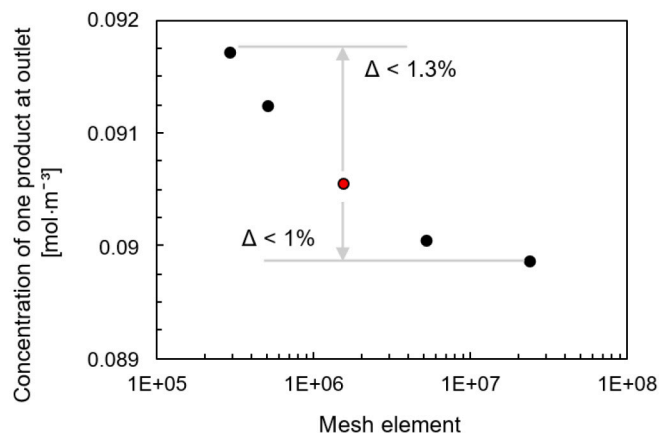


Fig. A1. Grid independence study.

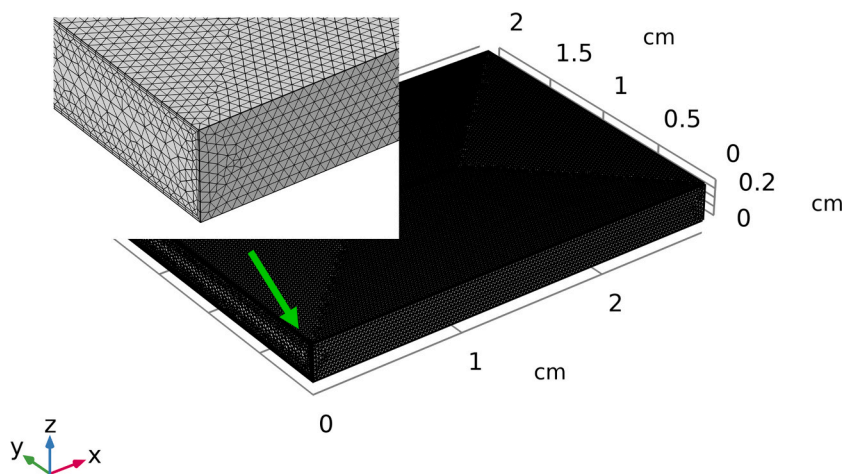


Fig. A2. Meshing and refinement on boundary layers.

A.5. Other simulation results

a) H₂ consumption

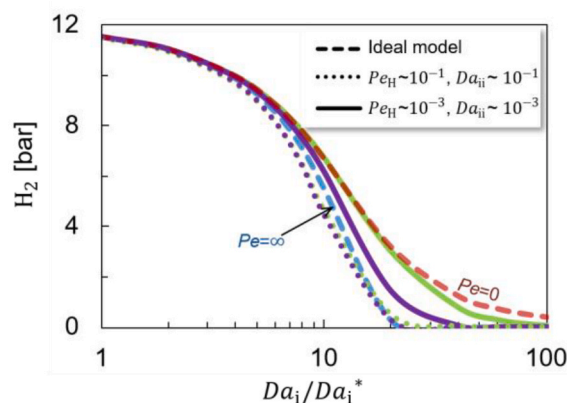


Fig. A3. H_2 partial pressure as a function of catalyst activity within two microchannels (i.e., large and small L/W ratio) under ‘low catalytic activity – small flow rate’ ($Pe_H \sim 10^{-3}$, $Da_{ii} \sim 10^{-3}$) and ‘high catalytic activity – large flow rate’ ($Pe_H \sim 10^{-1}$, $Da_{ii} \sim 10^{-1}$) conditions.

b) Overall CO conversion

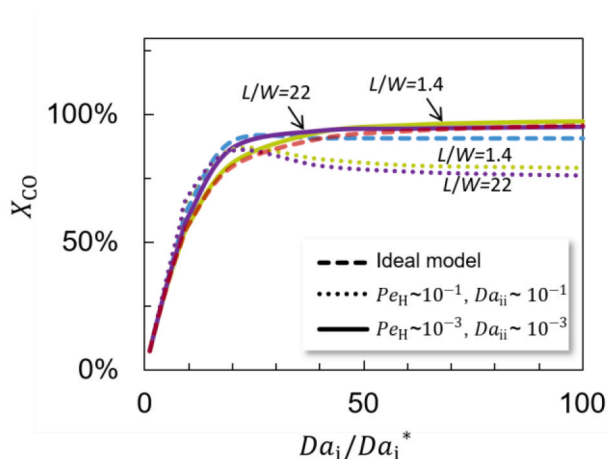


Fig. A4. Overall CO conversion results of Fig. 4.

Data availability

Data will be made available on request.

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