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## Research Article

**Keywords:** reaction kinetics, residence time distribution, flow chemistry, TPMS, CFD

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# Numerical investigation on the heat and mass transfer enhanced by Triply-Periodic-Minimal-Surface (TPMS) configuration in flow chemistry

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## Abstract

The continuous flow reaction technology has been widely recognized and developed due to its inherent safety, process control, reaction efficiency, etc. But the consistency of heat and mass transfer during the scale-up of continuous flow reactors remains a major challenge, and few reliable evaluation methods are currently available. In this work, a novel TPMS-based flow reactor is developed with characteristic length of 6mm, utilizing interconnected flow passages to enhance flow mixing and heat transfer. The flow pattern in the TPMS reactor is experimentally analyzed to exhibit near-ideal plug flow. Based on the decoupled CFD framework proposed in the present study, the flow, heat and mass transfer, and reaction kinetics in the TPMS reactor are numerically analyzed and compared with the traditional tubular flow reactors (diameters of 3mm and 6 mm). The TPMS reactor is demonstrated with superior heat transfer performance to maintain expected temperature and to achieve high selectivity. Under the condition of hypothetical pilot-scale extremely exothermic reaction, the advantages of the lab-scale TPMS reactor are further highlighted, especially for the increasing dominance of the side reactions. Therefore, the TPMS reactor is much potentially applied to nitration, lithiation, diazotization, etc., with few scale-up effects on the heat and mass transfer, and reaction performance. The numerical method provides a practical and effective solution for industrial scale-up design and optimization, with reasonable computational resources and efficiency.

**Keywords:** reaction kinetics; residence time distribution; flow chemistry; TPMS; CFD

## 1、 Introduction

Over the past decades, flow chemistry has evolved from an academic theory into an industrially recognized technology, especially in chemical and pharmaceutical fields <sup>[1]</sup>. Due to the dramatic advantages of inherent safety, process control, reaction efficiency, etc., many regulatory agencies,

including FDA, EMA, NMPA, etc. <sup>[2-3]</sup>, have actively introduced policies and guideline to encourage the adoption of continuous flow reactions. And flow chemistry was recognized by IUPAC as one of the 2019 top ten emerging technologies in chemistry <sup>[4]</sup>.

Based on the enhanced mass transfer and precise process control <sup>[5]</sup>, flow chemistry have been successfully used to synthesize active pharmaceutical ingredients (APIs), such as verubecestat (MK-8931) <sup>[6]</sup>, linezolid <sup>[7]</sup>, prexasertib monolactate monohydrate <sup>[8]</sup> and rufinamide <sup>[9]</sup>. Some high-risk reactions off limit in batch mode can be realized under flow mode. For example, various microfluidic reactors were developed for nitration <sup>[10-11]</sup> and organometallic-based reactions <sup>[12-13]</sup> to address the risks of thermal runaway and potential explosion. On-line quenching becomes significant for the reactions involving highly unstable intermediates and products <sup>[14]</sup>. Additionally, further applications of continuous flow reaction have been extended to photochemistry and electrochemistry <sup>[15-17]</sup>.

Although continuous flow reactions have been successfully conducted at the lab scale, reactor scale-up is widely recognized as a key challenge for industrial implementation <sup>[18-20]</sup>. In order to guarantee the consistency of heat and mass transfer under lab-environment, numbering up is one of scale-up strategies and widely adopted in scale-up of micro-reactors <sup>[21-22]</sup>. However, the fluid distribution is an urgent difficulty to achieve identical characteristics in massive parallel channels, restricting industrial production capacity.

Recently, Triply Periodic Minimal Surfaces (TPMS) have attracted extensive attention with the development of 3D printing technology <sup>[23-24]</sup>. The smooth curvature can reduce dead zone formation, and the large surface area greatly enhance heat transfer. According to the reported literatures, the TPMS-based structures are mainly used as heat exchangers <sup>[23-26]</sup>, with partial applications as static mixer in chemical field <sup>[27-28]</sup>. If TPMS topology is employed for flow reactor, accurate temperature control can be inevitably achieved for continuous flow reaction. The interconnected flow channels, analogous to vascular network, enable the fluid diverging and converging flow, dramatically enhancing flow mixing and mass transfer. Therefore, a flow reactor based on gyroid topology is developed in the present study, which potentially contributes to the consistency of heat and mass transfer during reactor scale-up.

The heat, mass, momentum transfer and reaction performance of flow reactors are generally assessed through cold model experiment <sup>[29-30]</sup>, heat transfer experiment <sup>[31-32]</sup>, Computation Fluid Dynamics (CFD) simulation <sup>[33-35]</sup>, chemical reaction kinetics <sup>[36-37]</sup>, chemical probe system <sup>[38-40]</sup>,

and real chemical reaction experiment <sup>[41-42]</sup>. The first three methods are used to analyze flow and heat transfer characteristics without the presence of chemical reactions. The forth method reveals the reaction mechanism and pathway, unable to derive quantitative results in complex reactions. The last two methods can generate reliable results under actual conditions. But the full-scale tests under various conditions result in unacceptable cost and safety risk. Recently, some researchers employed AI technology to autonomously discover the multi-physics mechanisms in chemical reactors <sup>[43-45]</sup>. But AI for chemical engineering still suffers from considerable challenges and requires long-term, in-depth exploration.

To date, a single approach is insufficient to fulfill the design and scale-up of chemical process. In this work, an integrated strategy is proposed, combining CFD simulation and chemical reaction kinetics. The CFD simulation is established to resolve the intra-reactor flow field, heat transfer and species concentration. And the chemical reaction kinetics is coupled to calculate mass transfer and temporal-spatial heat source. The integrated method is firstly validated by some chemical reaction experiments and then used to assess the performances of flow reactors. The heat, mass, momentum transfer and reaction performance of the novel Gyroid-based flow reactor is comprehensively analyzed and compared with the traditional tabular flow reactors. The present work potentially contributes to the scale-up consistency of flow chemistry process.

## 2、Design of flow reactors

Recently, TPMS-based heat exchangers have been extensively applied in the energy and aerospace engineering fields. The dominant topological configurations are mathematically described through the following equations.

$$\text{Primitive type:} \quad \cos\left(\frac{2\pi x}{L}\right) + \cos\left(\frac{2\pi y}{L}\right) + \cos\left(\frac{2\pi z}{L}\right) = c \quad (1)$$

$$\text{Gyroid type:} \quad \sin\left(\frac{2\pi x}{L}\right) \cdot \cos\left(\frac{2\pi y}{L}\right) + \sin\left(\frac{2\pi y}{L}\right) \cdot \cos\left(\frac{2\pi x}{L}\right) + \sin\left(\frac{2\pi z}{L}\right) \cdot \cos\left(\frac{2\pi x}{L}\right) = c \quad (2)$$

$$\text{Diamond type:} \quad \cos\left(\frac{2\pi x}{L}\right) \cdot \cos\left(\frac{2\pi y}{L}\right) \cdot \cos\left(\frac{2\pi z}{L}\right) - \sin\left(\frac{2\pi x}{L}\right) \cdot \sin\left(\frac{2\pi y}{L}\right) \cdot \sin\left(\frac{2\pi z}{L}\right) = c \quad (3)$$

where  $L$  and  $c$  denote unit cell size and offset value, respectively.

Given the superior heat transfer capability and interconnected flow passages, reactors designed with TPMS configurations probably exhibit remarkable superiority in flow chemistry, especially for mixing-sensitive reactions and strongly exothermic reactions. As shown in reported literatures <sup>[23-26]</sup>, the primitive-type and diamond-type configurations are analogous to many flow cavities

connected by multiple tributaries, possibly leading to local dead zones. Nevertheless, such undesired local small cavities are not distinct in gyroid-type topology, characterized by interconnected flow channels with smooth curvature. Therefore, the gyroid-type flow reactor is developed with the unit cell size of 6mm in this work, leveraging its recirculating mixing and plug flow. Figure 1 presents the domains of raw material, coolant and solid. The solid domain can be 3D-printed with metallic materials, silicon carbide and others, spatially separating the raw material domain and coolant domain. The enhanced flow mixing and mass transfer substantially accelerate target chemical reaction. The exothermic heat can be rapidly removed, finally resulting in a relatively stable temperature for the full-flow reaction.

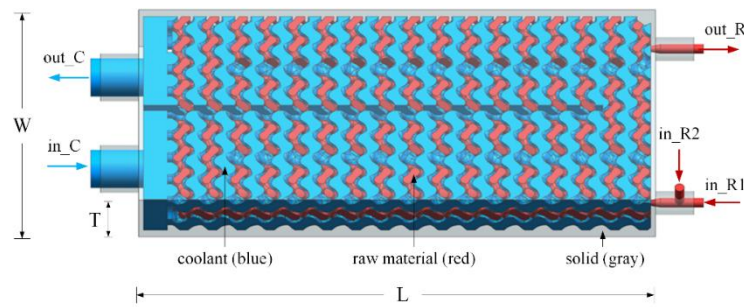


Figure 1 Domains of raw material, coolant and solid in TPMS reactor

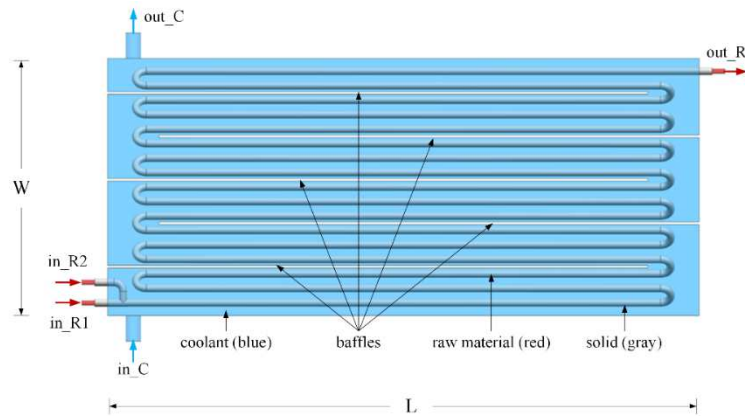


Figure 2 Domains of raw material, coolant and solid in PFR-3 reactor

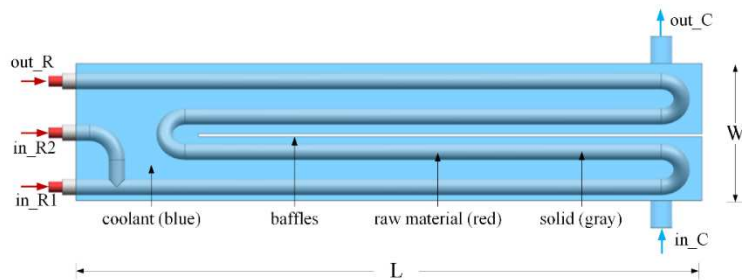


Figure 3 Domains of raw material, coolant and solid in PFR-6 reactor

Meanwhile, two kinds of traditional tubular reactors are selected and manufactured to compare

the performances with TPMS reactor. Figure 2 and Figure 3 depict the domains of raw material, coolant and solid in PFR-3 and PFR-6 reactors, respectively. These tubular reactors are designed with smaller geometric dimensions, with inner diameters of 2mm and 4mm, respectively. Additionally, the tube bundle adopts a typical staggered arrangement and several flow baffles are used to reduce flow short circuit and dead zones, enhancing cooling efficiency. As illustrated in Table 1, these three reactors are provided with similar residence volumes for chemical reaction. Although the characteristic length of TPMS reactor is greater than the other two reactors, its specific surface area is obviously larger, causing more remarkable heat transfer. Constrained by manufacturing process, the two tubular reactors possess dramatically larger residence volumes than TPMS reactor, greatly decreasing volumetric utilization.

Table 1 The detailed geometric parameters of the present reactors

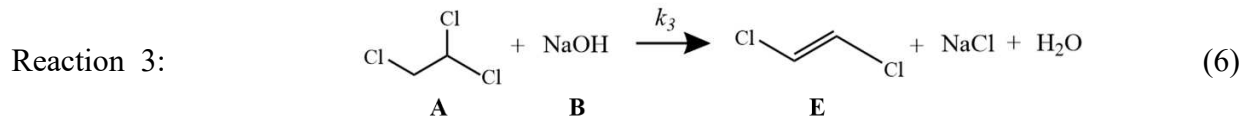
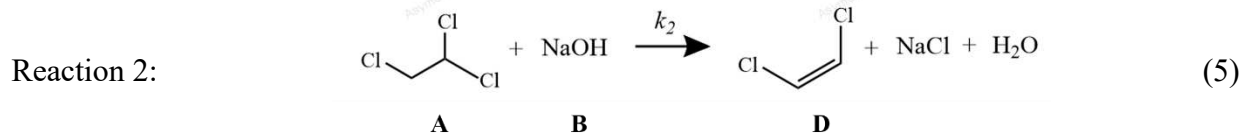
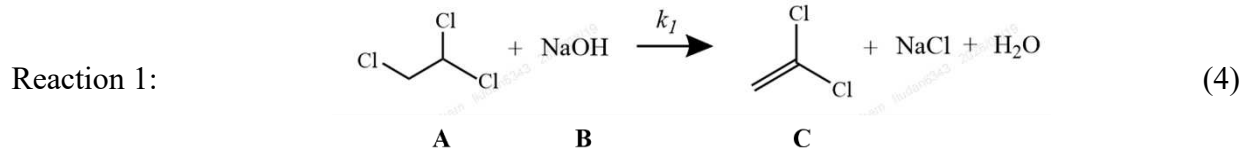
|                                                                           | TPMS reactor | PFR-3 reactor | PFR-6 reactor |
|---------------------------------------------------------------------------|--------------|---------------|---------------|
| Length (L) / mm                                                           | 108          | 235           | 235           |
| Width (W) / mm                                                            | 52           | 105           | 55            |
| Thickness (T) / mm                                                        | 12           | 12            | 23            |
| Wall thickness / mm                                                       | 0.6          | 0.5           | 1.0           |
| Unit cell size / inner diameter of reactor / mm                           | 6            | 2             | 4             |
| 1 <sup>st</sup> inlet diameter of raw material (in_R1) / mm               | 2            | 2             | 4             |
| 2 <sup>nd</sup> inlet diameter of raw material (in_R2) / mm               | 2            | 2             | 4             |
| Outlet diameter of raw material (out_R) / mm                              | 2            | 2             | 4             |
| Inlet diameter of coolant (in_C) / mm                                     | 8            | 8             | 8             |
| Outlet diameter of coolant (out_C) / mm                                   | 8            | 8             | 8             |
| Residence volume of raw material / ml                                     | 9.98         | 11.2          | 13.06         |
| Residence volume of coolant / ml                                          | 24.6         | 245.65        | 223.74        |
| Surface area of raw material / m <sup>2</sup>                             | 0.0328       | 0.0228        | 0.0112        |
| Specific surface area of raw material / (m <sup>2</sup> /m <sup>3</sup> ) | 2269         | 2036          | 854           |

### 3、Methodology

The combination of several research methods can neutralize their inherent respective limitations. As the multi-physics coupling technology has been advanced recently, the combination of CFD simulation and reaction kinetics seems to be the most effective approach at present, for analyzing the performances of chemical reactors and evaluating the scale-up consistency of chemical process.

#### 3.1 Reaction system

As a raw material and organic polymer, Vinylidene chloride (VDC) has been widely used for various manufacturing products. The dehydrochlorination of 1,1,2-trichloroethane (112TCE) under the alkaline condition of NaOH is the most economically approach to produce VDC. The reaction system of 112TCE and NaOH involves three parallel reactions, as shown below.



where  $k_1$ ,  $k_2$  and  $k_3$  refer to the reaction rate constants, respectively. Using A, B and C to represent raw materials, the reaction kinetics are expressed and the related parameters are obtained according to the reported literature [46].

Reaction 1:

$$-r_1 = \frac{dC_C}{dt} = k_1 \cdot C_A \cdot C_B = 1.668 \times 10^{11} \cdot e^{-\frac{75662}{RT}} \cdot C_A \cdot C_B \quad (7)$$

Reaction 2:

$$-r_2 = \frac{dC_D}{dt} = k_2 \cdot C_A \cdot C_B = 8.996 \times 10^9 \cdot e^{-\frac{85722}{RT}} \cdot C_A \cdot C_B \quad (8)$$

Reaction 3:

$$-r_3 = \frac{dC_E}{dt} = k_3 \cdot C_A \cdot C_B = 2.310 \times 10^{10} \cdot e^{-\frac{90213}{RT}} \cdot C_A \cdot C_B \quad (9)$$

Additionally, the reaction kinetics and chemical exothermic heat are strongly bidirectionally coupled. Owing to the distinct activation energy, the reaction 1, reaction 2 and reaction 3 are affected with different sensitivity. Without adequate heat transfer for exothermic reaction, local thermal hotspot could be possibly induced and the produce yield is decreased to different extents. The heat source induced by chemical reaction can be described as followed.

$$q_v = -\frac{dC_A}{dt} \cdot h_r \quad (10)$$

### 3.2 Numerical method

For this reaction system, there exist several numerical frameworks to implement reaction kinetics into CFD simulations. The multi-component model and Euler-Euler model are mainly adopted to resolve the concentration distribution of components. But these two mainstream methods require massive computational resources and possibly lead to low efficiency for large-scale industrial

reactors. Accordingly, a high-efficiency numerical method is proposed on the basic of a split-type solution mode. Considering the little effect of solvent concentration change on the solution properties, the momentum equation is firstly solved without the source terms of mass and momentum. The conservation equations for mass, momentum and energy are:

Conservation of mass:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{U}) = 0 \quad (11)$$

Conservation of momentum:

$$\frac{\partial(\rho \mathbf{U})}{\partial t} + \nabla \cdot (\rho \mathbf{U} \cdot \mathbf{U}) = -\nabla \mathbf{P} + \rho \mathbf{f} \quad (12)$$

Conservation of energy:

$$\frac{\partial(\rho T)}{\partial t} + \nabla \cdot (\rho \mathbf{U} T) = \nabla \cdot \left( \frac{k}{C_p} \nabla T \right) + S_T \quad (13)$$

where  $\mathbf{U}$ ,  $\mathbf{P}$  and  $\mathbf{f}$  are velocity vector, pressure vector and force vector, respectively.  $\rho$ ,  $k$  and  $C_p$  denote density, thermal conductivity and specific heat capacity of methanol aqueous solution, respectively.  $T$  represents temperature.  $S_T$  refers to the source term of energy, which is calculated according to Equation 10. Given the Reynolds number obviously lower than 2000, laminar flow model is adopted in this work.

Subsequently, the flow field is frozen as a fixed field. The concentration distribution, heat and mass transfer are calculated with the pre-calculated velocity field. The concentration conservation for the component  $\phi_i$  is:

$$\frac{\partial(\rho \phi_i)}{\partial t} + \nabla \cdot (\rho \mathbf{U} \phi_i) = \nabla \cdot J_i + S_{\phi_i} \quad (14)$$

where  $J_i$  is diffusion flux due to concentration gradient.  $S_{\phi_i}$  denotes the source term, which is derived from Equation 7~Equation 9.

### 3.3 Method validation

Two kinds of methanol-water solutions are separately prepared using solute A and solute B, with these two solutes maintained at the same molar concentration. TPMS reactor is selected to compare the conversions obtained by experiment and simulations. As summarized in Table 2, the simulated results agree well with the experimental results within a 5% error range, verifying the reliability and accuracy of the developed numerical method. Furthermore, the mesh sensitivity is carried out to exclude the size effect on numerical results. As the domain grid is further refined from simulation 2 to simulation 1, the numerically calculated conversions exhibit only negligible

variation. With a comprehensive consideration of computational efficiency and numerical accuracy, the grid scheme in simulation 2 is chosen for the subsequent simulations. Without continuous iterative solution of the momentum equation throughout the simulation, this numerical approach possesses significant computational efficiency, which is capable to precisely resolve the heat, mass and momentum transfer and reaction performance within the studied domains of chemical reactor and potentially applied to scale-up optimization and validation.

Table 2 The raw material conversion obtained by experiment and simulations

|            | Experiment | Simulation 1<br>(857W cells) | Simulation 2<br>(663W cells) | Simulation 3<br>(384W cells) | Simulation 4<br>(326W cells) |
|------------|------------|------------------------------|------------------------------|------------------------------|------------------------------|
| Conversion | 72.5%      | 75.65%                       | 75.64%                       | 75.45%                       | 75.37%                       |
| Error      | /          | 4.34%                        | 4.33%                        | 4.01%                        | 3.96%                        |

#### 4、Results and discussions

In this work, a 70 wt% methanol-water mixed solvent is employed to separately prepare 112TCE solution and NaOH solution. For this homogeneous reaction system, the effect of solute on the thermophysical properties of the solution can be reasonably neglected under low-concentration condition. The flow and heat transfer characteristics are researched with water fluid and the reaction performances are analyzed with 70 wt% methanol-water fluid. The corresponding fluid properties are listed in Table 3.

Table 3 Thermophysical properties of water and 70 wt% methanol-water solution <sup>[47-48]</sup>

|                                         | Density<br>/(kg/m <sup>3</sup> ) | Dynamic viscosity<br>/(Pa·s) | Specific heat capacity<br>/(J/kg·K) | Thermal conductivity<br>/(W/m·K) |
|-----------------------------------------|----------------------------------|------------------------------|-------------------------------------|----------------------------------|
| Water (at 298.15K)                      | 997                              | 0.890                        | 4186                                | 0.606                            |
| Methanol-water solution<br>(at 323.15K) | 847                              | 0.722                        | 3133                                | 0.284                            |

##### 4.1 Flow characteristics

Perfectly mixed flow and plug flow are two fundamental ideal flow models widely adopted in chemical reaction engineering. The flow pattern in a real flow reactor is intermediate between these two ideal flows. Residence Time Distribution (RTD) is always used to quantitatively characterize the non-ideal flow and back-mixing behavior in a flow reactor. The RTD tests are performed on these three flow reactors with step-input method. A steady-state flow is firstly

achieve in the reaction domains using deionized water. The inlet stream is rapidly switched to the NaCl solution with pre-calibrated constant concentration, and the solution conductivity at the reactor outlet is simultaneously measured by a Hamilton conductivity meter. After eliminating the baseline offset, the recorded real-time conductivity data is converted to the solution concentration using the pre-calibrated correlation. The concentration is normalized by the feeding solution, yielding a residence time distribution function  $F(t)$ . By differentiating  $F(t)$  with respect to time, the RTD density function  $E(t)$  is derived, satisfying the strict normalization.

$$E(t) = F'(t) \quad (15)$$

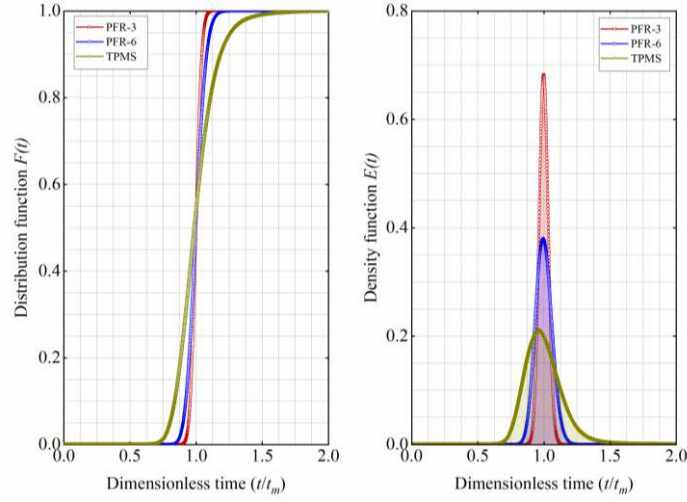
$$\int_0^{\infty} E(t) dt = 1 \quad (16)$$

$$t_m = \int_0^{\infty} t \cdot E(t) dt \quad (17)$$

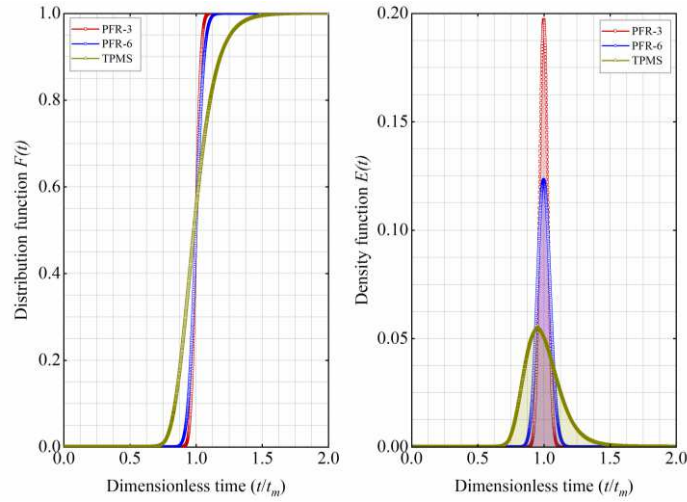
The mean residence time  $t_m$  is defined as the statistically averaged duration of raw material residing in the studied flow reactor, calculated by Equation 17. Through comparing  $t_m$  and theoretical space time  $\tau$ , direct diagnostics can be conducted to identify unaccounted dead volume, unexpected fluid bypassing, or system leakage within the flow reactors. Due to different residence volumes of PFR-3, PFR-6 and TPMS, the physical time is also normalized by the mean residence time  $t_m$ . As shown in Figure 4 the residence time distribution functions  $F(t)$  in these three reactors sharply increase from 0 to 1 within a narrow time window. The  $F(t)$  curve of PFR-3 reactor displays the steepest ascent, whereas the TPMS reactor shows the most gradual one. Consequently, the derivative  $E(t)$  curve of PFR-3 reactor exhibits a sharp, narrow peak, while the  $E(t)$  curve of TPMS reactor presents a relatively broad, low peak. As the flow rate decreases from 40.56 ml/min to 10.14 ml/min, the  $F(t)$  curves of these three reactors increase relatively more gently and the  $E(t)$  curves are provided with a broader and lower peak, which can be attributed to higher degree of axial dispersion and back-mixing compared with the near-ideal plug flow reference system. Generally, the absence of a long tailing in the  $E(t)$  curves suggests the absence of significant dead volume that would otherwise cause some fluid to reside in reactor far longer than the theoretical space time  $\tau$ . Additionally, it can be known from Figure 5 that  $t_m$  is approximately equal to  $\tau$  in PFR-3 reactor and TPMS reactor, with no significant flow bypassing or channeling. But  $t_m$  greatly less than  $\tau$  indicates the presence of flow bypassing or channeling inside the PFR-6 reactor. Therefore, the flow pattern in PFR-3 and TPMS reactors can be approximately treated as plug flow under the present conditions.

$$\delta_{\theta}^2 = \int_0^{\infty} (t - t_m)^2 \cdot E(t) dt \quad (18)$$

$$N = \frac{t_m^2}{\delta_{\theta}^2} \quad (19)$$



(a) Flow rate of 40.56ml/min



(b) Flow rate of 10.14ml/min

Figure 4  $F(t)$  and  $E(t)$  in reaction domain

The dimensionless variance  $\delta_{\theta}^2$  and  $N$  value in the tanks-in-series model are always used to quantitatively characterize the non-ideality of flow in flow reactor. These two parameters lay the quantitative foundation for subsequent flow model fitting. A  $\delta_{\theta}^2$  of 0 suggests ideal plug flow, while a value of 1 represents ideal mixed flow. As illustrated in Figure 6, the TPMS reactor is provided with the maximum value of  $\delta_{\theta}^2$ ; however, all  $\delta_{\theta}^2$  values of these three reactors are less than 0.025. The reciprocal of  $\delta_{\theta}^2$  is  $N$  value in the tanks-in-series model, approximating the real flow pattern through  $N$  equal-volume, ideal-mixed tanks. Under the present conditions, the  $N$  values of these three flow reactors are greater than 45, far higher than the reported criterion ( $N \geq 45$ ).

10<sup>[49-50]</sup> and  $N \geq 30$ <sup>[51]</sup>) for near-ideal plug flow.

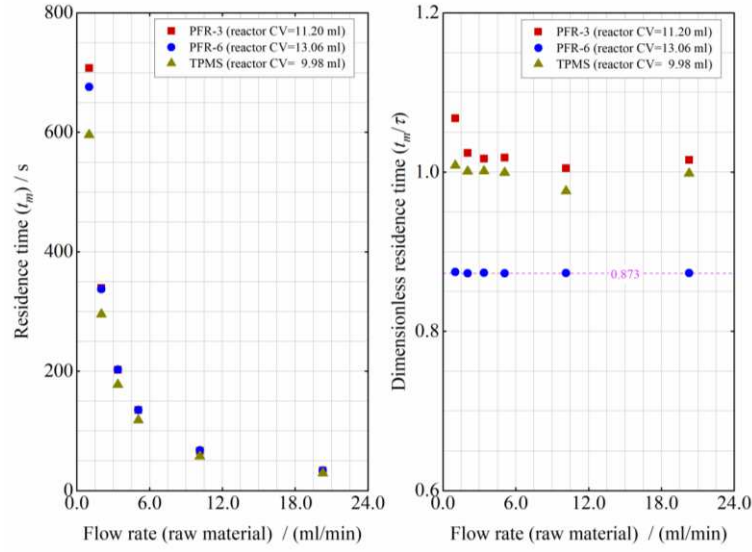


Figure 5 Mean residence time  $t_m$  in reaction domain under various flow rates

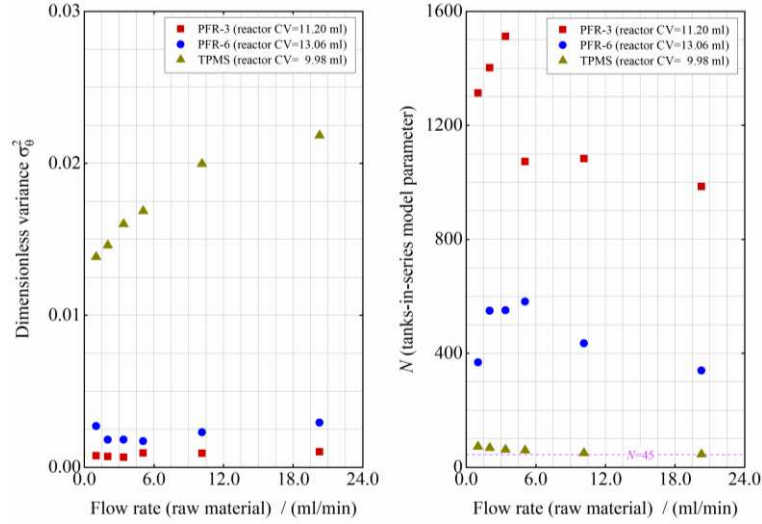
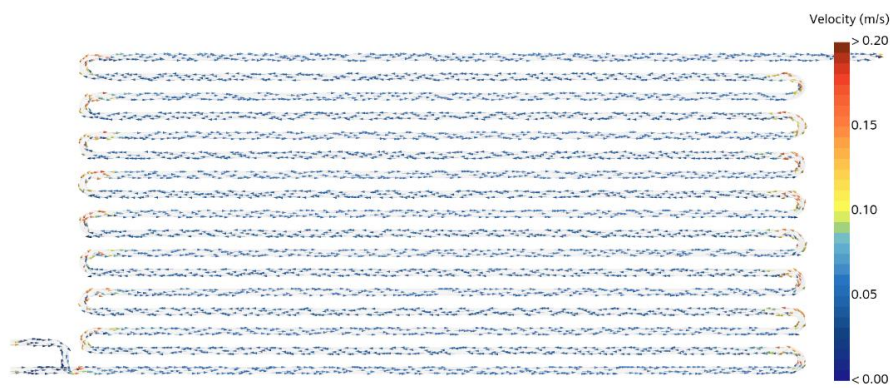


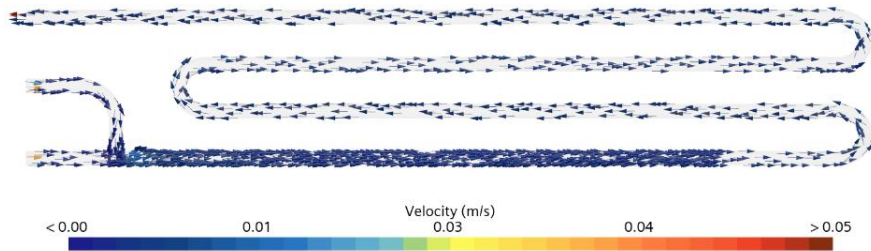
Figure 6 Dimensionless variance  $\delta_\theta^2$  and N values in reaction domain under various flow rates

Furthermore, the pressure drop is especially concerned, as it directly determines the selection of the feed delivery pump and the pressure rating of the reactor. In this work, the flow field and pressure drop are numerically analyzed with water fluid for these three reactors. As seen in Figure 7, the flow distribution in the reaction domain of PFR-3 reactor exhibits more uniform than that of PFR-6 reactor. The partial flow bypassing could be concluded from non-uniform flow distribution in PFR-6 reactor, leading to  $t_m$  less than  $\tau$ . A relatively uniform velocity field and repetitive interpenetrating flow are observed in Figure 7 (c), contributing to transverse mixing and suppressing axial dispersion. Localized dead zones are identified in the corners of TPMS reactor, requiring further geometric optimization. Figure 8 and Figure 9 display the relationships of volume-averaged velocity and pressure drop with respect to flow rate in reaction domain and

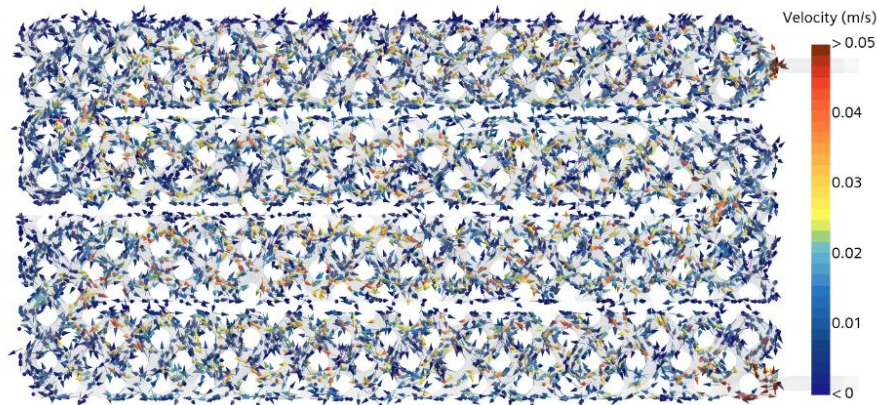
coolant jacket. As shown in Figure 8, the volume-averaged velocity and pressure drop linearly increase with flow rate, indicating the predominance of viscosity effect in reaction domain. The smallest diameter and longest flow path in the reaction domain of PFR-3 produce largest velocity and pressure drop, greatly higher than the other two reactors. And it can be as seen from Figure 9 that the large cavity of cooling jacket in PFR-3 and PFR-6 reactors results in less pressure drop than that of TPMS reactor. The non-linear relationship of volume-averaged velocity and pressure drop with respect to flow rate can be attributed to the comparable effect of inertia and viscosity. Overall, the magnitude of pressure drop under the present conditions is well within the acceptable range for industrial applications.



(a) In reaction domain of PFR-3 reactor



(b) In reaction domain of PFR-6 reactor



(c) In reaction domain of TPMS reactor

Figure 7 Velocity vector in reaction domain (flow rate of 40.56ml/min)

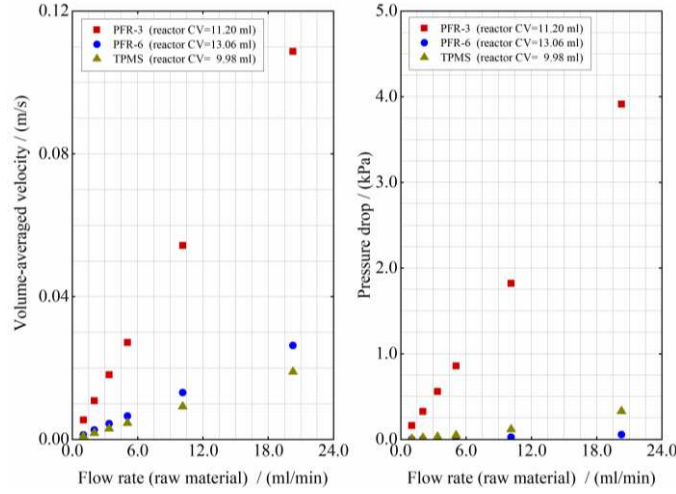


Figure 8 Volume-averaged velocity and pressure drop in reaction domain

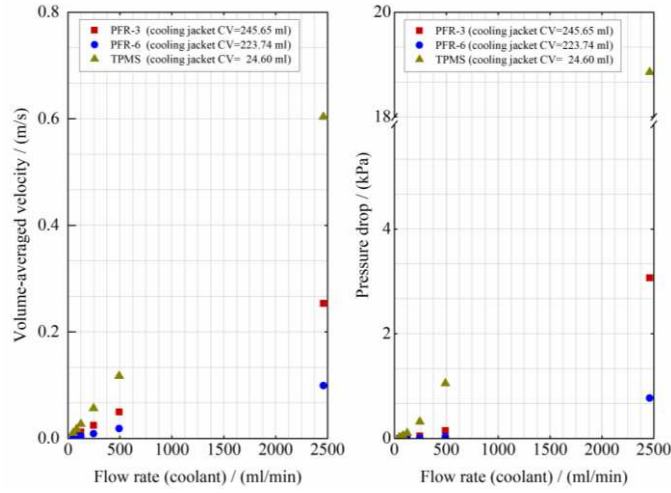


Figure 9 Volume-averaged velocity and pressure drop in cooling jacket

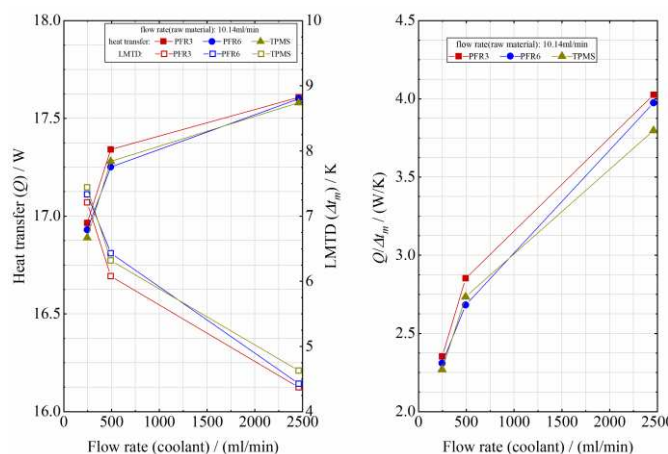
## 4.2 Heat transfer characteristics

Flow reactors are always designed with sufficient heat transfer capacity to remove the exothermic heat generated by chemical reactions. According to the fundamental theory of heat transfer, the heat transfer can be quantitatively characterized by the product of the total heat transfer area, the overall heat transfer coefficient and the logarithmic mean temperature difference (LMTD). Although the outlet temperature of reaction system can be maintained within expected operating range, the residence time that the reaction system experiences at elevated temperatures varies significantly across different reactor configurations. To deeply distinguish the heat transfer capacity of flow reactors, an exponential heat source is hypothetically introduced to simulate the exothermic reactions, as formulated below.

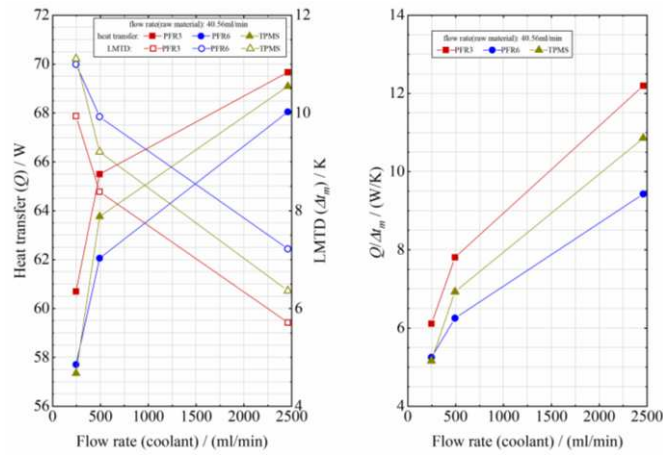
$$\frac{d\phi_i}{dt} = -0.2 \cdot \phi_i \quad (\phi_{i0} = 500) \quad (20)$$

$$q_v = \left| \frac{d\phi_i}{dt} \right| \cdot h_i = 100 \cdot \phi_i \quad (\text{W/m}^3) \quad (21)$$

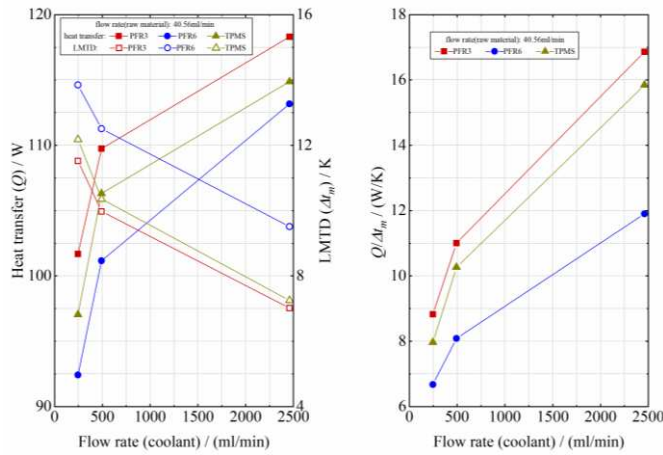
The heat transfer characteristics of these flow reactors are numerically investigated, with water selected as both raw material in reaction domain and coolant in cooling jacket. The inlet temperatures of raw material and coolant are 323.15K and 298.15K, respectively. As observed in Figure 10, the overall heat transfer ( $Q$ ) increases consistently with the flow rate of coolant and the LMTD ( $\Delta t_m$ ) decreases reversely with the flow rate of coolant, indicating that the raw material is further cooled. The increased  $Q/\Delta t_m$  can be attributed to the enhanced convective heat transfer induced by elevated velocity and thinned thermal boundary layer. When the flow rate of raw material is 10.14ml/min, the sensible heat of raw material is sufficiently small to be cooled for high-flow-rate coolant. Therefore, few differences in heat transfer ( $Q$ ) and LMTD ( $\Delta t_m$ ) are observed for PFR-3, PFR-6 and TPMS reactors in Figure 10 (a). As the heat from the reaction domain is raised through increasing flow rate of raw material and introducing heat source, remarkable differences in  $Q$ ,  $\Delta t_m$  and  $Q/\Delta t_m$  are clearly presented in Figure 10 (b) and (c). The PFR-3 reactor exhibits the best comprehensive heat transfer performance, followed by the TPMS reactor, while the PFR-6 reactor delivers the poorest performance. And the difference in heat transfer performances of these flow reactors is greatly enlarged with an increased heat from raw material, such as raised temperature, increased flow rate and reaction heat source. However, the heat transfer performance between TPMS reactor and PFR-3 reactor becomes gradually converges under strong exothermic heat. Because the heat of raw material is mainly removed by the temperature rise of the coolant, the smallest residence volume in cooling jacket of the TPMS reactor results in minimized heat transfer especially under the condition of a relatively low coolant flow rate. Therefore, the TPMS reactor is highly applicable to the reaction system with high heat removal demand under sufficient coolant flow rate conditions.



(a) Flow rate of 10.14ml/min in reaction domain without heat source



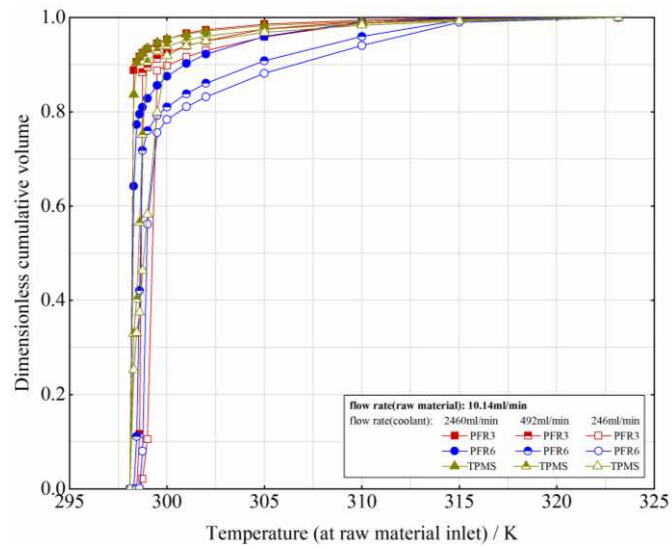
(b) Flow rate of 40.56ml/min in reaction domain without heat source



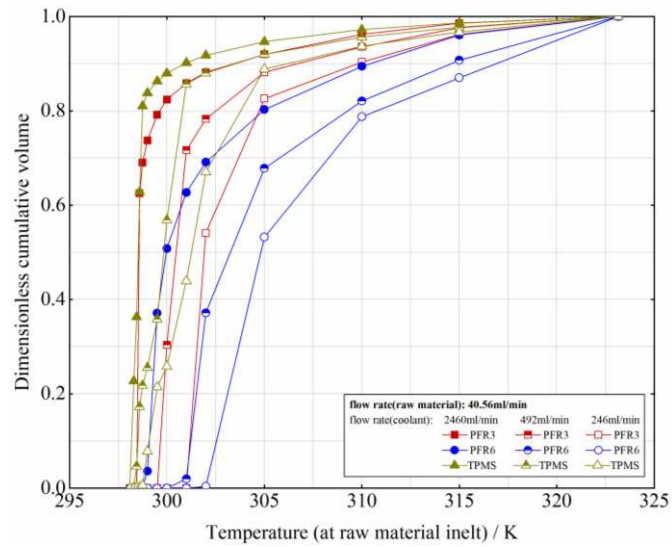
(c) Flow rate of 40.56ml/min in reaction domain with exponential heat source

Figure 10 Overall heat transfer under different flow rates of coolant

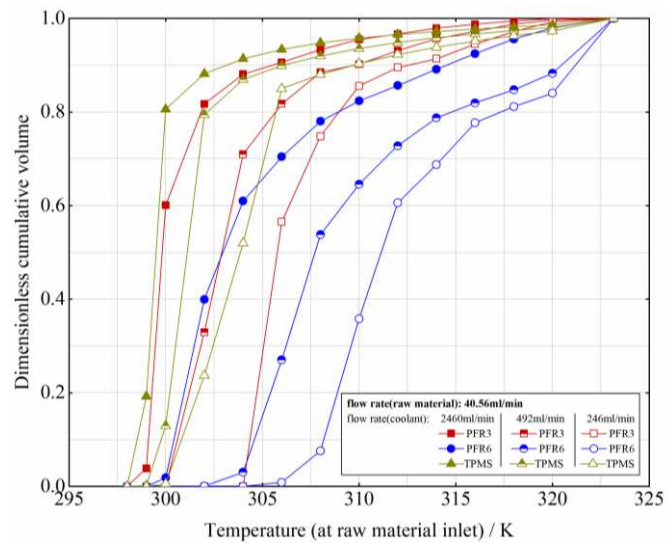
The comprehensive heat transfer does not represent the thermal characteristics of each individual domain cell. As shown in Figure 11 (a), the raw material with low flow rate can be rapidly cooled within a short flow path, leading to few differences among these three flow reactors. As the flow rate of raw material is increased in Figure 11 (b) and volumetric heat source is introduced in Figure 11 (c), the TPMS reactor demonstrates superior heat transfer to achieve a rapid cooling on the reaction domain cells. It can be noted from Figure 11 that the inherent advantages of TPMS reactor becomes more prominent with the increasing of heat removal demand. A larger proportion of residence volume under low-temperature condition refers to that the time for the reaction system to deviate from the expected temperature is shorter.



(a) Flow rate of 10.14ml/min in reaction domain without heat source



(b) Flow rate of 40.56ml/min in reaction domain without heat source



(c) Flow rate of 40.56ml/min in reaction domain with exponential heat source

Figure 11 Dimensionless cumulative volume under different temperatures

### 4.3 Reaction performances

The residence time of reaction system at different temperature intervals dramatically differs with reactor configurations, affecting the side reactions to varying degrees. A homogenous reaction system between 112TCE and NaOH is selected for numerical investigation on the effect of reactor configurations on the raw material conversion and selectivity. Ignoring the effect of 112TCE and NaOH, the bulk flow fields are firstly resolved for both the reaction domain and cooling domain, where 70 wt% methanol-water solution and deionized water are separately adopted as raw material and coolant. The numerical simulations on flow reaction behavior are carried out under the raw material flow rate of 40.56ml/min and the coolant flow rate of 10.14ml/min respectively, with identical inlet temperatures for both streams. Generally, the activation energy of the side reaction is much greater than that of the main reaction, making it more sensitive to temperature variation. Insufficient heat transfer capacity leads to a non-uniform temperature distribution, producing more impurity and lower selectivity.

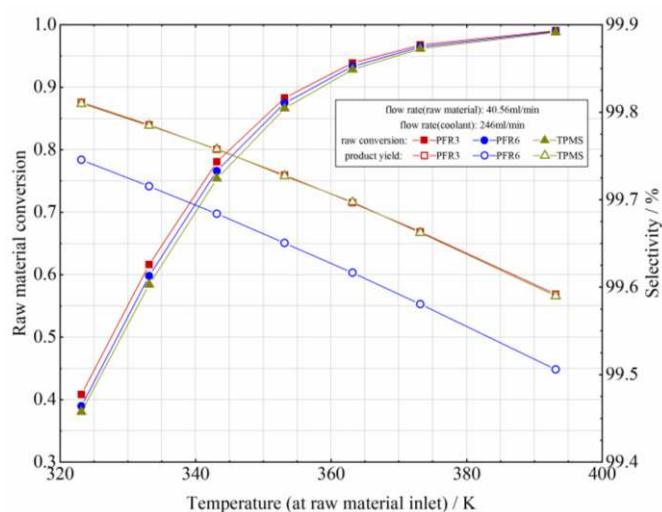


Figure 12 Raw conversion and selectivity under negligible exothermic conditions

Meanwhile, the exothermic power of continuous flow reaction is scaled up by 500 times to simulate more extreme exothermic scenarios. More significant differences in temperature control, raw material conversion and selectivity among these three reactors can be seen from Figure 13 and Figure 14. Although the comprehensive heat transfer of these three reactors can meet the requirement of several tens of watts, distinguished temperature distribution in domain cells results in different results. The raw material in the TPMS reactor and PFR-3 reactor can be maintained at relatively lower temperature than PFR-6 reactor, producing higher selectivity. Under low-

temperature condition, the lower conversion in TPMS reactor is also caused by the shorter residence time and lower temperature control, yielding a smaller exothermic heat. As the reaction temperature is increased, the reaction domain becomes enough for complete conversion. The conversion and exothermic power among the three reactor are approximately equal. However, the increasingly prominent heat transfer performance of the TPMS reactor results in a slightly higher selectivity than that of the PFR-3 reactor.

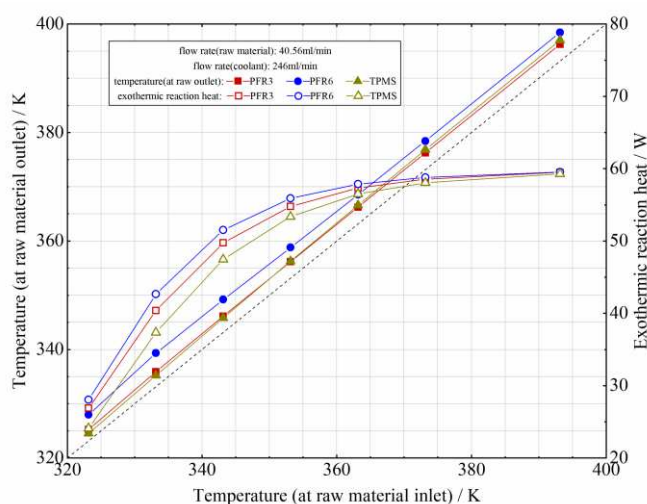


Figure 13 Temperature change of raw material and heat source of exothermic reactions

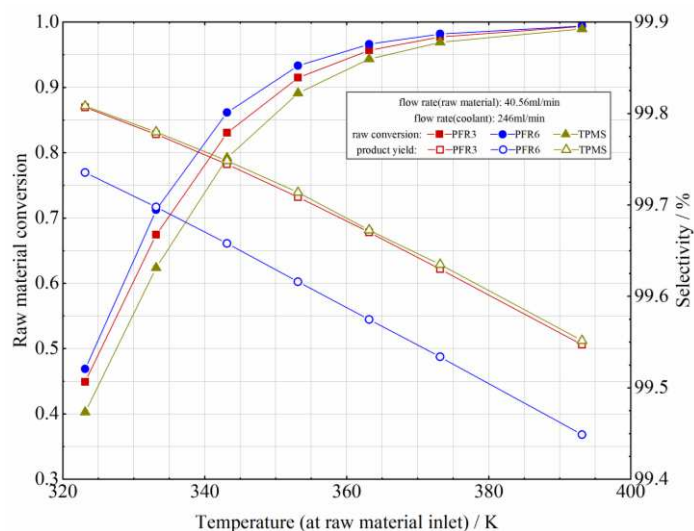


Figure 14 Raw conversion and selectivity under strongly exothermic conditions

Based on the above analysis, the dimensional scale-up of tubular reactor exerts a remarkable influence on the heat and mass transfer, deserving special attention. The positive feedback effect between heat and reaction is the fundamental cause of thermal runaway. Although the characteristic length of the TPMS reactor is comparable to that of PFR-6 reactor, the heat and mass transfer, reaction performance in TPMS reactor are superior to that of the PFR-3 reactor,

especially under extreme exothermic conditions. The present achievements are only conducted under the condition that the main reaction rate is 2~3 orders of magnitude larger than that of the side reactions. When the dominance of the side reactions increases, the superiority of the TPMS reactor will be further highlighted.

## 5、Conclusions

In this study, a TPMS-based flow reactor is developed with interconnected flow passages to enhance flow mixing and heat transfer. The flow and heat transfer characteristics, and reaction performances of the novel flow reactor are comprehensively researched through combining CFD simulation and chemical reaction kinetics, comparing with traditional tubular flow reactors. Some conclusions are drawn as followed.

(1) Experiments on RTD are conducted to characterize the non-ideal flow and back-mixing behavior in the flow reactors. As the flow rate of working fluid increases, the  $F(t)$  curves present a steep ascent, producing a sharper and narrower peak in  $E(t)$  curves. According to the quantitative evaluation by the tanks-in-series model, the  $N$  value exceeds 45, which can be considered as near-ideal plug flow in TPMS reactor. And the pressure drops in reaction domain and cooling jacket can be guaranteed within a reasonable range for industrial applications.

(2) The heat transfer characteristics are numerically studied under various conditions. The heat transfer can be convectively enhanced by increased coolant flow rate. As more heat is released from the reaction domain, the diameter scale-up of tubular flow reactors greatly decreases the heat transfer capacity. With a hypothetical heat source applied, the TPMS reactor demonstrates superior heat transfer, maintaining the reaction domain cells at the expected temperature.

(3) Due to the enhanced heat transfer, the reaction progression in the TPMS reactor is slower than the other two. When the reaction domain becomes enough for complete conversion, higher selectivity can be achieved in the TPMS reactor especially under extreme exothermic conditions, which could be further highlighted under the increasing dominance of the side reactions.

(4) Despite the greater characteristic length, the TPMS reactor is potentially scaled up with the consistency of heat and mass transfer. The implementation of reaction kinetics into CFD simulations could be an efficient method to resolve the heat and mass transfer, and reaction performance, with reasonable computational resources and efficiency for industrial scale-up.

## **CRedit and authorship contribution statement**

**Liang Hu:** Conceptualization, Methodology, Investigation, Data curation, Writing – original draft, Formal analysis, Writing - review & editing; **Botao Liu:** Resources, Data curation, Methodology, Validation, Visualization, Writing – original draft; **Dan Liu:** Investigation, Data curation, Software, Writing – original draft; **L. Wang:** Resources, Software, Validation, Project management, Formal analysis, Methodology, Supervision, Writing - review & editing.

## **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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