Rarefied reactive gas flow in T-shape microreactors

Mubashir Hussain∗, Patric Müller†

†Institute of Multiscale Simulation, University of Erlangen-Nürnberg, Germany
∗Magnetic Resonance Institute for Safety, Technology and Research GmbH, Germany
email: hussain@mri-star.com

Abstract – The present study investigates the reactive gas flows in T-shape microreactors by means of a 3D direct simulation Monte-Carlo method (DSMC). The reactive process is modeled by incorporating a single step irreversible exothermic reaction of gas species A and B. The energy released in each reaction is added to the system by increasing the kinetic energy of the product gas specie C. The reactive collisions are modeled by means of a momentum preserving hard sphere collision model in 3D DSMC.

We analyzed several process and gas parameters to observe their extent of influence on the characteristics of the reactive flow. The T-microreactor with thermal walls showed much higher mass carrying capacity as compare to the specular walls. The reaction front, which initially for maximum reaction rate was close to the inlet of gas specie of higher mass density, moved towards the center of the inlet part of T-channel and eventually dissolved with decreasing reaction rates. This transition was smooth in T-channel with thermal walls, whereas, quite abrupt in case of specular walls. Moreover, in T-microreactors with thermal walls, the amount of A and B converted to C follows an exponential decrease especially in moderate to low reaction rates. Further, with a clear separation between high and low reactive flows, a piece-wise exponential decay in concentration of C with respect to decreasing reaction rates was also observed in T-channel with specular walls.

Keywords – Reactive flow, T-shape, microreactor, DSMC, gas flow

1 Introduction

Reactive fluid flow occurs in many micro-fluidic devices such as microreactors, microturbines, microengines etc. These flows are characterized by their high Knudsen number meaning that the length of the mean free path of the fluid molecules is comparable to the characteristic length of the microchannel. On such small length scales, the assumption of continuum flow no longer remains valid (5) and a particle-based approach such as direct simulation Monte-Carlo (DSMC) is required to simulate the fluid flow (1).

DSMC is a particle-based method to solve the Lattice Boltzmann equation and is well suited for simulating rarefied gas flows such as in microchannels. The present study extends our work on mixing of rarefied gases in T-mixers (4) with an aim to investigate the effect of reactions on the gas flow in T-shape microchannels by means of an in-house built object oriented 3D DSMC C++ code. The code is written in state-of the-art C++ features and can be run both on shared and distributed memory. Moreover, the code is based on quite novel particle tracking algorithms in complex geometries and has been thoroughly tested on several benchmark problems. For details on the code, the readers are refereed to these articles (12–14).

Several studies have been done so far on the behavior of the fluid flow through T-shape reactors. These studies, however, mostly comprise of simulating non-reactive gases through different type of microreactors (see e.g. (5, 9, 15–18)). Thorough studies on characteristics of reactive flow in different kind of microreactors especially T-shape microreactors are rather limited in literature. Zhang and Xie (19) recently did a detailed study of 2D reactive flow in Y-shaped microreactors. They simulated a combustion network of H₂ and O₂ with a non premixed gas flow and analyzed Knudsen number and wall temperature effects on the flow characteristics. Their study provides a
micro-level insight into the combustion dynamics. However, neglecting the concentration, pressure
and temperature gradients in the third dimension on such a small scale may result in reduced wall
effects and inconsistent results with respect to the 3D flow (3, 4). Palharini et al. (6) also quite
recently studied the characteristics of hypersonic rarefied gas flow with chemical reactions over
3D cavities using DSMC. Their focus was on the structure of flow field formed in the microscale
cavities. DSMC has also been used to simulate the surface reactions in the microchannels. For
instance, Pesch et al. (7) modeled the gas-solid catalytic reactions in the nanoscale cavities of
highly porous particles using DSMC. Their study revealed a transition between low and high
temperatures. They further showed that at high temperature three regions with different reaction
rates exist in the cavities.

This study investigates the rarefied reactive gas flow in the T-shape microreactor with an aim
to develop better understanding of reactive fluid flow on such small scales. Moreover, our focus
is to study the influence of reaction rates and wall conditions on the flow characteristics of gas
species with different mass densities. We start first by explaining the momentum preserving hard
sphere reactive collision model used in the 3D DSMC, which is followed by the discussion on the
simulations results.

2 Reactive Collisions in DSMC

DSMC is a particle-based fluid flow simulation method that is based on the principle of kinetic
theory of gases. This means that flow of an ensemble of point-like particles with mass and
momentum representing the large number of real gas molecules are simulated in order to model
the real fluid dynamics. A particle enters into or leaves the system with respect to certain boundary
conditions e.g. dirichlet boundary condition and moves through the system due to the pressure
gradient. The equation of state is usually taken to be the ideal gas law and to fill the vessel with a
gas before the pressure driven gas flow, the quasi-particles are evenly distributed over the domain
with the Maxwell-Boltzmann velocity distribution.

To simulate the movement of particles and their collisions with other particles and walls, DSMC
method executes two events in each time step, namely the streaming and the collision events. In
streaming event, particles are moved to new locations according to their velocities and size of the
time step. Whereas in the collision event, particles pairs, chosen randomly within each geometrical
cell, experience collision with respect to the collision model accounted for e.g. hard sphere collision
model. The macroscopic quantities such as mass density, pressure, velocity, temperature etc. are
computed from the moments of the velocity distribution of these particles and the ideal gas law.
These quantities are usually averaged over several thousand time steps to minimize the statistical
fluctuations. The complete description of the method along with its implementation in C++,
boundary conditions, wall properties etc. can be found in (11).

2.1 Particle-based reaction process

The reaction considered in this study is a one-step irreversible exothermic binary reaction given
as

\[ \text{A + B} \rightarrow 2\text{C} + \Delta E. \]  

(1)

In reaction (1), species A and B are reactants, and specie C is a product. Whereas, \( \Delta E \) represents
heat added in the system due to the exothermic reaction.

In particle-based framework this means that species A and B are converted to specie C upon every
reactive collision which is based on a certain reaction probability. Moreover, the pre-collision
masses of molecules A and B are not equal to their post-collision masses. Their sum, however,
remain the same i.e.,
\[ m_1 \neq m'_1 \quad ; \quad m_2 \neq m'_2, \]
\[ m_1 + m_2 = m'_1 + m'_2. \]

Here, without loss of generality, \( m_1 \) and \( m_2 \) denote pre-collision masses of particles A and B, respectively, and \( m'_1 \) and \( m'_2 \) denote post-collision masses of A and B, respectively. It is to be noted that in the given scenario \( m'_1 = m'_2 \) which are represented by specie C after reactive collision as shown in reaction (1).

To model the exothermic nature of the reaction, a certain amount of heat is also added in the system with every reactive collision. In Monte-Carlo direct simulation, we added all such heat in the system by increasing accordingly the kinetic energy of the product molecules (specie C). This means that not only the post-collision velocities of the individual particles are different from the pre-collision velocities but also the sum of the pre- and post-collision kinetic energies are not equal. In fact, sum of the post-collision kinetic energies is greater than the sum of the pre-collision kinetic energies due to the added heat in the system.

The necessary condition for the reaction (1) to take place is that the kinetic energy, \( E \), associated with the relative motion of the colliding particles must exceed the activation energy \( E_a \), i.e.
\[ E = \frac{1}{2} \mu_{1,2} |\vec{v}_1 - \vec{v}_2|^2 > E_a, \]
where, \( \mu_{1,2} = \frac{m_1 m_2}{m_1 + m_2} \), and, \( \vec{v}_1 \) and \( \vec{v}_2 \) are velocities of A and B, respectively. However, not every collision with kinetic energy greater then the activation energy results in a reaction. This is accounted by considering a reaction probability model which is chosen to be rather simple in the current study and is given by
\[ P = \begin{cases} 
0 & \text{if } E \leq E_a, \\
1 - \frac{E_a}{E} & \text{if } E > E_a. 
\end{cases} \]

Since, our aim here is to investigate the flow characteristics under the influence of reaction rates, rather then incorporation of reactions be means of some sophisticated reaction model e.g. total collision energy, the above reaction model adequately serves this purpose. Further, the microscopic reaction probability (5) leads to the macroscopic Arrhenius reaction rate, \( A \exp^{-E_a/RT} \), by taking into account the Maxwell-Boltzmann distribution of the relative velocities (10). Here, \( R \) is the ideal gas constant, \( T \) is the temperature and \( A = \pi \sigma (8k_b T/\pi M)^{1/2} \), where \( \sigma \), \( k_b \) and \( M \) are the collision radius, the Boltzmann’s constant and the reduced mass, respectively.

To simulate the reaction mechanism in DSMC, particle pairs are randomly chosen in each geometrical cell in a collision step. We then check if the pair of particles are the species A and B, and if its not, then we move on to the next time step by performing simple elastic hard-sphere collision. If, however, the colliding particles are found to be of species A and B, we compute the probability of reaction by using equation (5) and generate a random number from uniform distribution in the unit interval [0 1]. If the generated random number is greater then the reaction probability then once again both particles experience simple elastic hard-sphere collision without any reaction. However, if the random number is less then the reaction probability then we perform a reactive collision by changing the masses and velocities of the particles as explained above. To perform the reactive collisions we make sure that the pre- and the post collision momenta of the particles remain same which is explained in the following section.
2.2 Momentum conservation in reactive collisions

The current study of gas flow in microchannel is done by assuming Dirichlet boundary conditions for pressure, temperature and flow velocity in the 3D DSMC (2). Moreover, the binary collision of particles are simulated as hard sphere collisions. In a conventional elastic hard sphere collision, colliding particles neither change mass nor release heat energy upon collision. Thus the post-collision velocities of the colliding particles can be computed from the conservation of momentum and energy. However, in exothermic reactive collisions particles can change their masses and release heat. This means that momentum of the colliding particles is conserved, however, the total kinetic energy of particles is not. It is assumed in the current study that all heat released in a reaction is utilized to raise the kinetic energy of the products. By keeping this fact into account, the corresponding post-collision velocities, \( \vec{v}_1' \) and \( \vec{v}_2' \), are then given by (Polewczak (8))

\[
\vec{v}_1' = \frac{1}{M} \left[ m_1 \vec{v}_1 + m_2 \vec{v}_2 + m_2' \sqrt{\frac{\mu_{1,2}}{\mu_{1,2}'} \left( (\vec{v}_1 - \vec{v}_2) - \hat{\epsilon} (\hat{\epsilon}, \vec{v}_1 - \vec{v}_2) + \hat{\epsilon} \alpha \right)} \right],
\]

(6)

\[
\vec{v}_2' = \frac{1}{M} \left[ m_1 \vec{v}_1 + m_2 \vec{v}_2 - m_1' \sqrt{\frac{\mu_{1,2}}{\mu_{1,2}'} \left( (\vec{v}_1 - \vec{v}_2) - \hat{\epsilon} (\hat{\epsilon}, \vec{v}_1 - \vec{v}_2) + \hat{\epsilon} \alpha \right)} \right].
\]

(7)

Here, \( M = m_1 + m_2 = m_1' + m_2', \mu_{1,2}' = m_1' m_2' / m_1 + m_2', \hat{\epsilon} \) is a unit vector, \( \langle ., . \rangle \) is the inner product, and \( \alpha = \sqrt{((\hat{\epsilon}, \vec{v}_1 - \vec{v}_2))^2 + 2 \Delta E / \mu_{1,2}} \). The unit vector \( \hat{\epsilon} \) is chosen arbitrarily since collision between particles in DSMC does not depend on the spatial location or motion of particles within the geometric cell. The post-collision velocities, eqs. (6) and (7), satisfy the following equalities,

\[
m_1 \vec{v}_1 + m_2 \vec{v}_2 = m_1' \vec{v}_1' + m_2' \vec{v}_2'
\]

(8)

\[
m_1 \vec{v}_1 \cdot \vec{v}_1 + m_2 \vec{v}_2 \cdot \vec{v}_2 + 2 \Delta E = m_1' \vec{v}_1' \cdot \vec{v}_1' + m_2' \vec{v}_2' \cdot \vec{v}_2'.
\]

(9)

This is depicted in Fig. 1 which shows the conservation of the total momentum of the reactive gas flow (specie A, B and C) in a T-shape microchannel with thermal walls. The small fluctuation are expected due to the interaction of particles with the boundary walls.

![Figure 1: Total momentum of reactive gases over time in a T-shape microchannel with thermal walls.](image)

3 Simulation Results

The simulation results for reactive gas flow in T-shape microchannel are presented here. In all simulations carried out in this study, the outlet boundary condition is assumed to be vacuum and
the inlet pressure is taken to be $1 \times 10^5$ Pa. Moreover, the temperature of the walls and the inlet gas species is always taken to be 300K. Further, the properties of the gas specie A correspond to the hydrogen gas, $\text{H}_2$, with mass $3.347 \times 10^{-27} \text{kg}$, whereas, the characteristics of the gas specie B correspond to Oxygen, $\text{O}_2$, with mass $5.313 \times 10^{-26} \text{kg}$. In every reaction, gas species A and B are converted to the specie C which corresponds to OH with mass $2.82 \times 10^{-26} \text{kg}$. Additionally, a total $7.64 \times 10^{-19}$ joules of heat is added into the system by increasing the kinetic energy of the gas specie C.

The gas flow is simulated with variations in the reaction rate by changing the activation energies of the reactions as given in Table 1. In case i we artificially decreased the activation energy, $E_a$, to 0 such that every collision between A and B results in a reactive collision. The purpose is to simulate the scenario with very high reaction rate, for instance, due to the presence of a catalyst. In such a case, a reaction takes place and heat is added to the system as soon as the gas species A and B collide. Similarly, the activation energies for all other cases are decreased systematically to analyze the effect of reaction rates on the characteristics of the reactive flow.

<table>
<thead>
<tr>
<th>case#</th>
<th>$E_a$ [joule]</th>
</tr>
</thead>
<tbody>
<tr>
<td>case i</td>
<td>0</td>
</tr>
<tr>
<td>case ii</td>
<td>$3 \times 10^{-20}$</td>
</tr>
<tr>
<td>case iii</td>
<td>$4 \times 10^{-20}$</td>
</tr>
<tr>
<td>case iv</td>
<td>$4.75 \times 10^{-20}$</td>
</tr>
<tr>
<td>case v</td>
<td>$4.85 \times 10^{-20}$</td>
</tr>
<tr>
<td>case vi</td>
<td>$5 \times 10^{-20}$</td>
</tr>
<tr>
<td>case vii</td>
<td>$6 \times 10^{-20}$</td>
</tr>
<tr>
<td>case viii</td>
<td>$E$</td>
</tr>
</tbody>
</table>

3.1 T-shape microchannel

The dimensions of the T-shape microchannel considered in this study are shown in Fig. 2. The inlet part of the channel has the dimensions $1 \times 4.8 \times 1 \mu\text{m}^3$, whereas, the dimensions of the main part of the channel are $10 \times 1.2 \times 1 \mu\text{m}^3$. The gas species A and B enter separately into the microchannel from the two inlets, as shown in Fig. 2 and, whilst interacting with each other and walls, flow towards the outlet due to the pressure gradient between the inlets and outlet of the microchannel.

To simulate the gas flow, the T-shape geometry is discretized into $2.625 \times 10^5$ cubic cells with an edge length of 0.04$\mu\text{m}$. The time step, $2 \times 10^{-11} \text{s}$, is small enough to accommodate all collisions taking place with in the mean free time. Further, to capture only the steady state data, the first $10^5$ time steps are ignored. Similarly, to reduce fluctuation due to the statistical nature of the simulation, the data are averaged over $10^4$ time steps.

3.2 Influence of wall conditions

We first simulate gas species flow with specular wall conditions. Fig. 3 shows the flow behavior and mass density of the gas specie C under maximum reaction rate (case i) through the T-shape microchannel. The reactive region i.e. the part of the channel where most reactive collisions take place, is found to be much closer to the inlet of the gas specie B, though the inlet conditions for both gas species were the same. The is due to the thermal velocity of the gas specie A, which represents the characteristics of $\text{H}_2$ in our simulation, that is almost 4 times higher than the gas specie B or $\text{O}_2$. Since both gas species enter into the system at identical operating conditions, $\text{H}_2$
travels faster than $O_2$, hence making their point of collision closer to the inlet of $O_2$. The mass density of specie C is represented by the colors and the arrows show the direction of its velocity in Fig. 3.

Effect of the variation in reaction rate on the flow fields with specular walls is depicted in Fig. 4. Figs. 4a to 4c show the flow fields and mass densities of the gas specie C in the reactive flow carried out with activation energies $4 \times 10^{-20}$J, $5 \times 10^{-20}$J, and $6 \times 10^{-20}$J, respectively. Since the probability of reaction decreases as activation energy increases, the mass density as well as the heat added to the system decreases. Moreover, with higher reaction probability i.e. with lower activation energy, the reactions are more probable to take place as soon as gas species A and B collide with each other. This can be clearly observed from the mass densities of C shown in Figs. 3 and 4. The mass densities of C are much more concentrated near the inlet of specie B in simulations (cases) i and iii. However, as the reaction probability decreases the reaction front moves towards the center of the inlet channel and almost appears to be in the middle of the inlet channel in case vi due to a relatively low reaction rate. Further, for a much lower reaction probability as in case vii, the mass density of C significantly decreases and no longer concentrated to a certain region. In fact, it approaches to almost a uniform distribution in space as shown in Fig. 4c.
Figure 4: Mass density and flow field of the gas specie C in simulations iii, vi and vii with specular walls.

Figure 5: Mass density and flow field of the gas specie C in simulations i, iii, vi and vii with thermal walls.
The reactive gas flow in T-channel with thermal walls also showed a similar character (Fig. 5). For high reaction rates (cases i,ii) the reaction front is located close to the inlet of specie B. However, with decrease in reaction rates, the reaction front moves towards the center of the inlet part of T-channel (Fig. 5b). However, contrary to the specular walls, the concentration of specie C is higher in the main part of the T-channel with thermal walls as can be seen in Figs. 5b to 5d. This is due to the thermally diffusive character of the walls which reflect the gas molecules in random directions, hence, making the probability of collision between A and B higher which leads to a higher probability of reaction during the outward flow of gases in main part of the T-channel.

3.3 Pressure distribution in T-channel

Due to the extreme reaction rate, immense amount of heat is expected to be released during the reactive flow with $E_a = 0$. This results in severe pressure increase especially in the inlet part of the T-channel as shown in Figs. 6 and 7. The average static pressure shown in these figures is computed along the inlet and main parts of the T-channel separately. In figures describing flow characteristics in inlet part of the T-channel, (e.g. Figs. 6a and 7a), 0 represents the location of the inlet of the specie B and 1 denotes the location of the inlet of the specie A on the abscissa, which shows normalized length of inlet part of T-channel. Similarly, in figures describing flow characteristics in main part of the T-channel, (e.g. Figs. 6b and 7b), abscissa represents the normalized length of the main part of T-channel with 0 being the start of the main channel and 1 being the outlet of the T-channel.

Figure 6: Average pressure distribution along the inlet and main parts of the T-microreactor with specular walls.

The sudden increase in the pressure around the inlets of the T-channel (Figs. 6a and 7a) for high reaction rates are due to the immense resistance created by the outward flow of the specie C. Further, this sudden increase in pressure is much higher in the vicinity of the inlet of the gas specie B as compare to the vicinity of the inlet of the gas specie A due to the high number of reactions tacking place very close to it. This effect is, however, rather moderate in case of thermal walls. This is due to the chaotic moment of gas molecules that is created due to their interactions with walls of the channel. The diffusive character of the walls create resistance in the flow of the gas which in turn leads to the higher pressure in T-channel before any reactive collision has taken place as compare to the specular walls. This can be observed by comparing pressure for the non reactive flow in Figs. 6a and 7a. Further, this much more chaotic flow of the gas molecules in case of thermal walls allow the gas species A and B to diffuse into each other by making a direct jet-like collision less probable as compare to the specular walls where gases flow more like jets. Hence, we have not only moderate peak pressure with $E_a = 0$J but also this peak pressure is closer to the center of the inlet channel in case of thermal walls as compare to the specular walls.

In the main part of the T-channel, the pressure decreases monotonically and shows no significant
difference from one another in case of thermal walls (Fig. 7b), i.e., change in reaction rate does not have a significant effect in terms of pressure drop in simulations with thermal walls. However, in case of specular walls, we see a clear shift from high pressure to low pressure reactive flow (see Fig. 6). The reason could be that in specular walls molecules interact with each other less as compare to the thermal walls. Especially at the critical reaction rate where flow changes its behavior from highly reactive to almost non reactive, if molecules of species A and B do not react during their first few interactions then the probability of reaction decreases whilst flowing towards outlet. However, in case of thermal walls, molecules move in a much more chaotic manner and in case they don’t react in the first few collisions they still have good chance of getting collided and get reacted during their flow. Therefore, in thermal walls the transition from highly reactive flow to low reactive flow due to change in the reaction rates is rather smooth, whereas, in specular walls this transition takes place abruptly.

3.4 Temperature profile in T-channel

To highlight this further, we have shown the temperature profile of the gas along the main part of the T-channel in Fig. 8. Since every reactive collision adds energy to the system, a very high temperature is observed at the start of the main channel for simulations with high reaction rates ($E_a = 0J$, $E_a = 3 \times 10^{-20}J$, and $E_a = 0J$) in case of specular walls (see Fig. 8a). There does exist small differences in the temperature profile for $E_a = 5 \times 10^{-20}J$, $E_a = 6 \times 10^{-20}J$ and $E_a = 0J$ but are not visible in Fig. 8a due to the scale difference with high reaction rate scenarios. Once again a clear and very big difference in the temperature profile appears to form two distinct groups of reaction rates: high reaction rate group and low reaction rate group. This shows that most of the
reactions between specie A and B take place until the start of the main channel for high reaction rates in case of specular walls, otherwise, the flow observe little to no reactions for low reaction rates. In case of thermal walls, the change in temperature profile is rather smooth for different reaction rates. In fact it can be observed that the temperature for simulation with $E_a = 3 \times 10^{-20}$J is higher as compare to the simulation with 0 activation energy. This is due to the fact that more reactive collisions take place in case of $E_a = 3 \times 10^{-20}$J as compare to $E_a = 0$J since the sudden pressure barrier created by instant reactions in case of $E_a = 0$J close to the inlet of specie B is not present here (see Fig. 7a). This results in better and more flow of specie B and hence higher total number of reactive collisions as compare to the simulation with $E_a = 0$J.

![Diagram](image)

**Figure 9:** Ratio of specie C in the main part of T-microreactor.

### 3.5 Degree of conversion

To compute the number of species A and B converted to specie C or amount of C with respect of other species, we define the quantity of degree of conversion, $D$ as

$$D = 1 - \frac{m_a + m_b}{m_a + m_b + m_c}, \quad (10)$$

where, $m$ denotes mass and subscripts $a$, $b$ and $c$ represent the specie. The scale of $D$ ranges from 0 to 1 with 0 meaning no concentration of C and 1 represents all A and B entered in T-channel are converted to specie C. Fig. 9 shows the computed values of $D$ in the main part of T-channel for various reaction rates. The degree of conversion is plotted on a logarithmic scale to capture the smaller values at low reaction rates. In addition to the reaction rates mentioned in previous figures, a couple of additional simulations are done with $E_a = 4.75 \times 10^{-20}$J and $E_a = 4.85 \times 10^{-20}$J to observe the sensitivity of flow characteristics with respect to the reaction rates. As can be seen in Fig. 9 the conversion rate of species A and B to C decreases with increasing activation energies. A steep change in the degree of conversion is observed right from the beginning for the thermal walls which follows an exponential decrease quite accurately. The change in $D$ for specular walls is, however, quite moderate until $E_a = 4.75 \times 10^{-20}$J. Only around 2% increment in the activation energy after this point brought more than 90% change in the whole flow dynamics such as conversion degree, pressure, etc. The dynamics of flow in specular walls are observed to be extremely sensitive in the range of $E_a = 4.75 \times 10^{-20}$J to $E_a = 4.85 \times 10^{-20}$J. It can, however, be observed from Fig. 9 that the degree of conversion also follows an exponential decay with different rates in both high and low reactive zones leading to a piece-wise exponential behavior with respect to reaction rates.
3.6 Mass flow ratio

Fig. 10 shows the mass carrying capacity of T-microreactors under various reaction rates with thermal and specular walls. It shows that mass flow rate of T-channel with thermal walls is always higher than the mass flow rate of T-channel with specular walls, both in reactive and non reactive flow. It further shows that the mass flow rate or mass carrying capacity of T-channel is reduced by increasing the reaction rate. Once again here, we observe a sudden change in the mass flow rate of T-channel with specular walls as soon as the reaction rate crosses a certain critical value. In Fig. 10, we have plotted the ratio of reactive mass flow ($m_r$) to the ratio of non-reactive mass flow ($m_{nr}$) on a normalized activation energy scale. This gives us an aspect of looking the flow characteristics from an approximated reaction probability scale. For instance, the critical reaction rate which triggers the sudden transition from high reactions to low reactions in specular walls appears to take place when a collision between species A and B have around 70% chance of reaction. This is an interesting and important factor that must be taken into account during designing of the T-microreactors.

4 Conclusions

A comprehensive mesoscopic study of 3D DSMC of rarefied reactive gas flow in T-shape microreactors was presented. The 3D DSMC simulations were carried out by incorporating a momentum preserving hard sphere collision model. The method characterized a powerful tool to investigate quite complex dynamics of rarefied reactive flows in microscale geometries. We investigated a one step irreversible exothermic reaction with respect to the reaction rates and T-channel wall characteristics. It was found that nature of the walls of the T-microreactors has a huge effect on the flow characteristics of the gas species. Under identical inlet conditions and reaction rates, much more reactions take place in T-microreactors with thermal walls as compare to the specular walls. Moreover, diffusive character of the thermal walls increases the probability of collisions and hence reactions during the outward flow in the main part of T-channel as compare to the specular walls. This leads to relatively higher concentrations of specie C in main part of the T-microreactors especially for low reaction rates. It was further found that T-microreactors with thermal walls not only carry more mass but also the pressure drop is much less in moderate to high reaction rates as compare to the T-microreactors with specular walls. Moreover, the concentration of specie C followed a continuous and piece-wise exponential decrease in main part of T-channel with specular and thermal walls, respectively. It is expected that the results of this mesoscopic study of reactive flow of gases in microscale geometries would help in better understanding of the flow characteristics. Moreover, this study would also be very useful for designing of microscale reactors, and identifying and optimizing the influencing parameters in mesoscopic reactive flows.
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