Table 1. Simulation parameters for the convection-diffusion system with the surface adsorption process

L	C_0	u_{max}	D_F	k	Pe_M
100	1.0	0.001	0.0005	1.0	200
100	1.0	0.005	0.0005	1.0	1000
100	1.0	0.01	0.0005	1.0	2000

Table 2. Physical properties of each component

Property	Value
Specific heat capacity ($kJ \cdot kg^{-1} \cdot K^{-1}$)	
H_2	$C_{p,H_2} = 15.04 - 2.50 \times 10^{-3} T + 3.16 \times 10^{-6} T^2 - 7.11 \times 10^{-10} T^3 + T^{-2}$
CO_2	$C_{p,CO_2} = 0.54 + 1.30 \times 10^{-3} T - 7.30 \times 10^{-7} T^2 + 1.55 \times 10^{-10} T^3 + T^{-2}$
H_2O	$C_{p,H_2O} = 1.73 + 2.59 \times 10^{-4} T + 4.65 \times 10^{-7} T^2 - 1.62 \times 10^{-10} T^3 + T^{-2}$
CH_4	$C_{p,CH_4} = 0.65 + 5.20 \times 10^{-3} T - 1.26 \times 10^{-6} T^2 + 3.14 \times 10^{-10} T^3 + T^{-2}$
Thermal conductivity ($W \cdot m^{-1} \cdot K^{-1}$)	
H_2	$\lambda_{H_2} = 6 \times 10^{-8} T^2 + 3 \times 10^{-4} T - 1.33 \times 10^{-2}$
CO_2	$\lambda_{CO_2} = -1 \times 10^{-8} T^2 + 1 \times 10^{-4} T - 3.47 \times 10^{-2}$
H_2O	$\lambda_{H_2O} = 3 \times 10^{-8} T^2 + 8 \times 10^{-5} T - 9.90 \times 10^{-3}$
CH_4	$\lambda_{CH_4} = 9 \times 10^{-8} T^2 + 5 \times 10^{-5} T - 2.34 \times 10^{-2}$
Molecular diffusivity ($m^2 \cdot s^{-1}$)	
H_2	$D_{H_2} = 4.11 \times 10^{-5} \left(\frac{T}{T_0}\right)^{\frac{3}{2}} \left(\frac{P_0}{P}\right)$ ($T_0 = 298\ K$ and $P_0 = 0.1\ MPa$)

CO_2	$D_{CO_2}=1.64\times10^{-5}\left(\frac{T}{T_0}\right)^{\frac{3}{2}}\left(\frac{P_0}{P}\right)$ (T_0=298 K and P_0= 0.1 MPa)
H_2O	$D_{H_2O}=2.55\times10^{-5}\left(\frac{T}{T_0}\right)^{\frac{3}{2}}\left(\frac{P_0}{P}\right)$ (T_0=298 K and P_0= 0.1 MPa)
CH_4	$D_{CH_4}=2.64\times10^{-5}\left(\frac{T}{T_0}\right)^{\frac{3}{2}}\left(\frac{P_0}{P}\right)$ (T_0=298 K and P_0= 0.1 MPa)

Table 3. The kinetic parameters of Sabatier reaction with three different pressures

Pressure (MPa)	$k_{f,0}$	$k_{r,0}$	$K_{CO_2,0}$ (MPa^{-1})	$K_{H_2O,0}$ (MPa^{-1})	$E_{a,f}$ (kJ/mol)	$E_{a,r}$ (kJ/mol)	ΔH_{CO_2} (kJ/mol)	ΔH_{H_2O} (kJ/mol)
0.35	1.23×10^3	3.89×10^8						
0.60	6.36×10^2	1.95×10^8	2.50×10^{-5}	5.51×10^7	22.77	114.40	-32.33	77.61
1.09	3.05×10^2	9.11×10^7						

($k_{f,0}$ unit is $mol\cdot s^{-1}\cdot g\text{-}cat^{-1}\cdot MPa^{-0.5}$; $k_{r,0}$ unit is $mol\cdot s^{-1}\cdot g\text{-}cat^{-1}\cdot MPa^{-2}$)

Table 4. The carbon conversion rate of different Dilution packing methods with the same number of catalysts

Dilution packing methods	Carbon conversion rate
Without bed dilution	47.41%
Layered dilution methods:	
Inert particle and catalyst in 9 layers	57.63%
Inert particle and catalyst in 5 layers	57.59%
Mixing dilution methods:	
Catalyst uniformly mixed with inert particle	59.87%

Gradient distribution based on original heat profile	65.22%
Gradient distribution based on original temperature profile	59.83%

Table 5. Thermal conductivities of two types of inert particles

	Thermal conductivities
Inert particle made of Al_2O_3	35 $W \cdot m^{-1} \cdot K^{-1}$
Inert particle made of SiC	120 $W \cdot m^{-1} \cdot K^{-1}$