Modelling of a Packed Bed Reactor for Green Ammonia Production

Hossein Asgharian[1], Samuel Simon Araya[1], Mads Pagh Nielsen[1], Vincenzo Liso[1]
[1]AAU Energy, Aalborg University, Aalborg 9220, Denmark

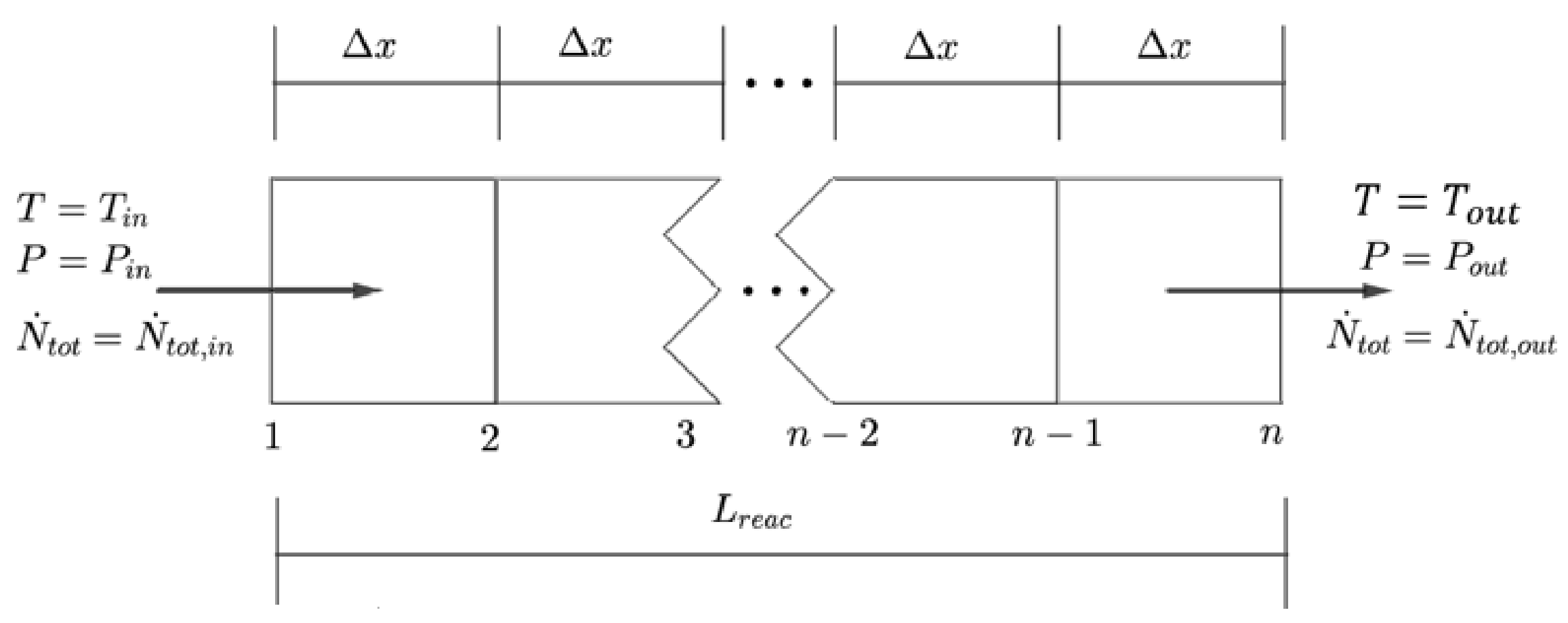
Introduction

Ammonia is one of the most high-demand industrial chemicals. Although more than 75% of the produced ammonia is used in the agriculture sector as a fertilizer, it can also be used for other applications. Haber-Bosch process has been widely used to produce ammonia. However, this process is very energy intensive, with low conversion, while it utilizes fossil fuel, and it leads to greenhouse gas emission. In this study, an ammonia synthesis reactor which utilizes Ruthenium as catalyst is investigated by developing a 1D model in MATLAB. This reactor can be used in the green ammonia synthesis processes since it operates at lower temperatures and pressures because of using a catalyst with very high activity. The performance of adiabatic reactor is investigated at different inlet temperatures and the effect of secondary inlet reactant at the middle of the reactor is also evaluated. RPlug reactor in Aspen Plus is used to validate the results.

Model Description

The reactor is divided into n control volumes as shown by Figure 1. The length of each control volume is Δx, and the reactants which are nitrogen and hydrogen enter the reactor at 20 bar pressure, while the inlet temperature of the reactants varies in the range of 550 to 650 K.

Figure 1: The spatial discretization used for modelling the reactor



n	1000
L_{reac}	0.1 m
Δx	10^{-4}m
$\dot{V}(at\ 377C)$	0.0115 lit/min
m_{cat}	0.005 kg
D	0.0104 m
$\dot{N}_{tot,in}$	7.0559×10^{-4} mol/s
P_{in}	20 bar

The equations for calculating the rate of reaction when ruthenium is used as catalyst , pressure drop along the reactor, and the released heat as a result of exothermic reaction are given as follows:

$$\text{Rate}= 2.9\exp\left(-\frac{62139}{RT}\right)P_{N_2} - 2.31\times10^{9}\exp\left(-\frac{133714}{RT}\right){P_{NH_3}}^{1.3}{P_{H_2}}^{-2.5}\ (\text{mol/g}_{\text{cat}}\text{min})[1] \quad (1)$$

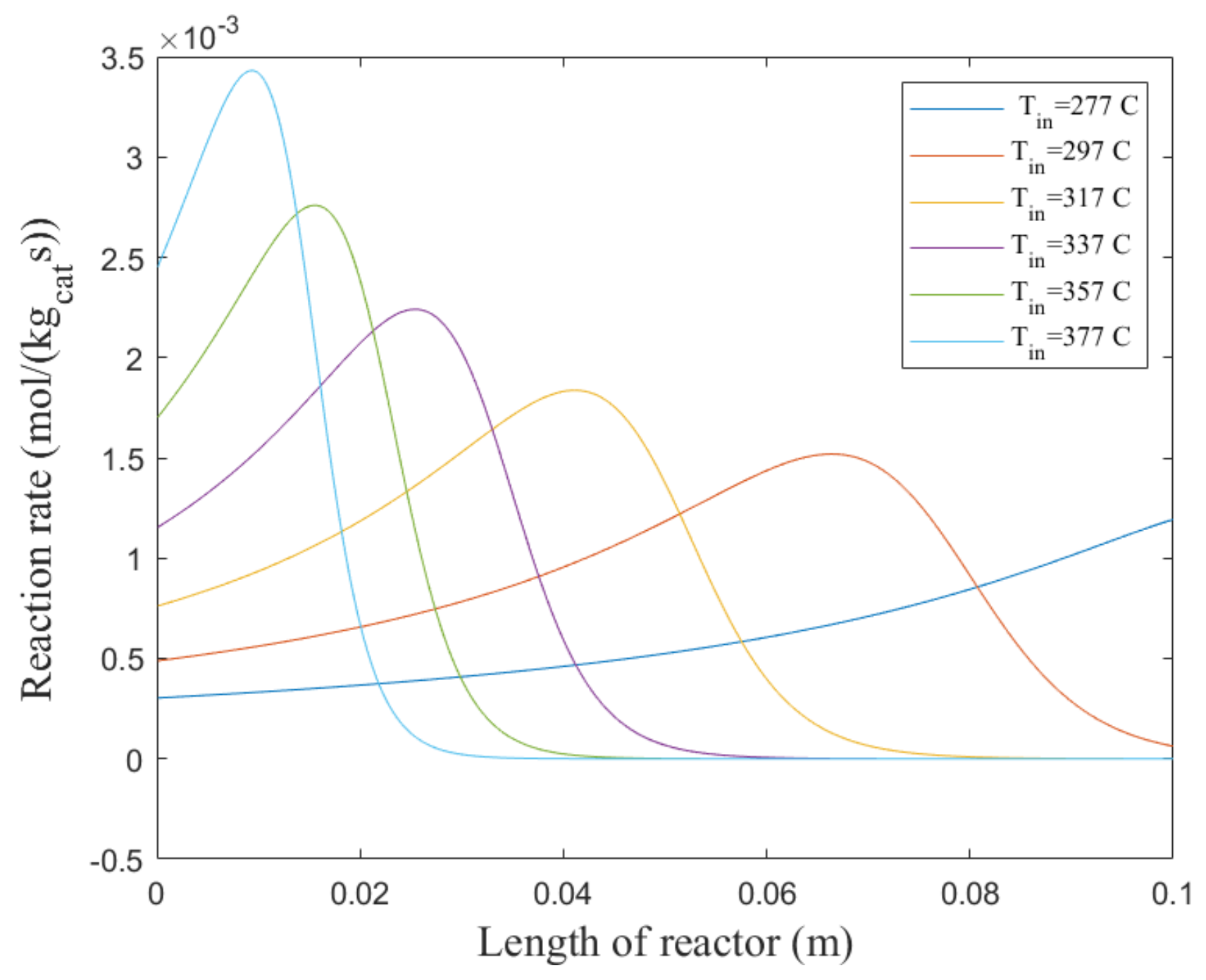
$$\frac{\Delta P}{L} = \frac{150 v_s \mu (1-\varepsilon)^2}{{D_p}^2\varepsilon^3} + 1.75\frac{v_s^2\rho(1-\varepsilon)}{D_p\varepsilon^3}(Pa/m) \quad (2)$$

$$\Delta H_R = 4.184\{-\left[0.54526 + \frac{840.609}{T} + 459.734\frac{10^6}{T^3}\right]p - 5.34685T - 0.2525\times10^{-3}T^2 + 1.69167\times10^{-6}T^3 - 9157.09\}(\text{kJ/kmol})\ [2] \quad (3)$$

Results and discussion

The reaction rate along the reactor for different inlet temperatures is shown by Figure 2. As can be seen, the reaction rate increases to a maximum value and then it decreases and at the end it may reach to equilibrium. Figure 3 also indicates the fraction conversion along the reactor for 3:1 ratio of H_2:N_2 at different inlet temperatures. The fraction conversion is given by equation 4. As can be seen, the fraction conversion increases along the reactor until the reaction reaches to equilibrium. Afterwards, the fraction conversion does not change.

Figure 2: The reaction rates along the reactor



$$F = \frac{\dot{n}_{H_2,in} - \dot{n}_{H_2,out}}{\dot{n}_{H_2,in}} \quad (4)$$

Figure 3: The fraction conversion along the reactor

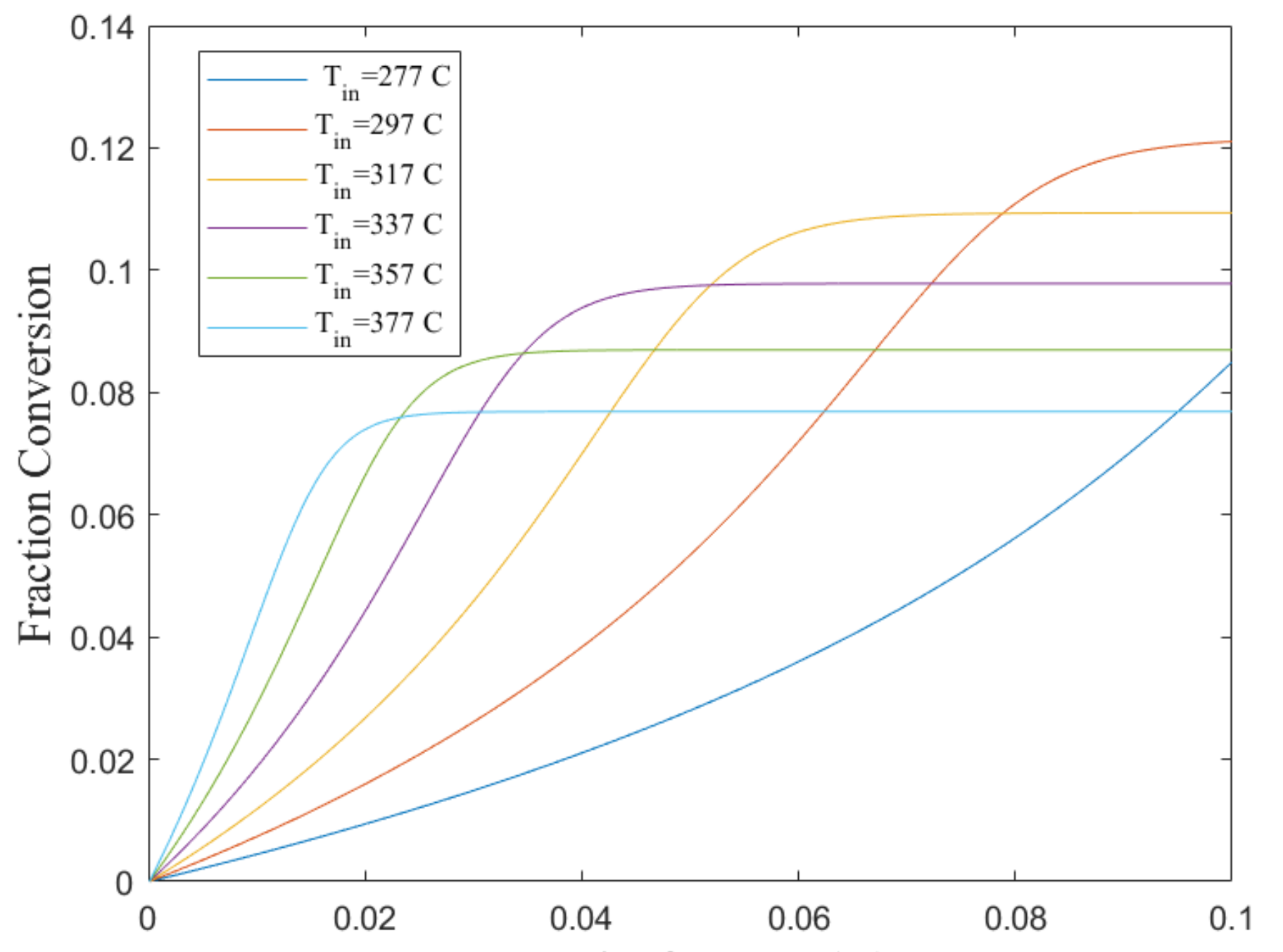


Figure 4 also shows the temperature increase of the gases inside the reactor as a result of the exothermic reaction. As can be seen, the gas mixture temperature increases along the reactor until the reaction reaches to the equilibrium.

Figure 4: The temperature of gas mixture along the reactor

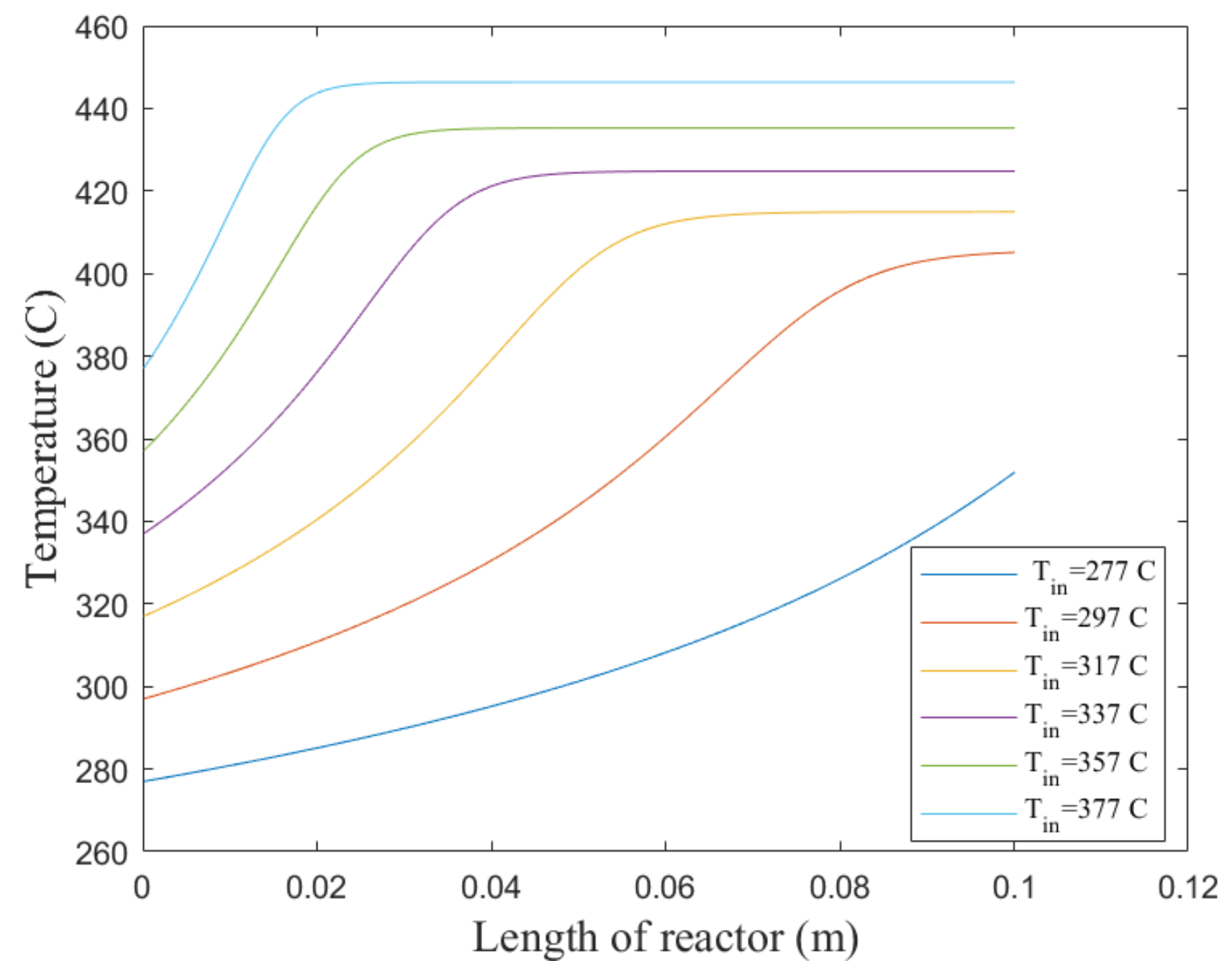


Figure 5 also indicates the temperature of the gas mixture along the reactor when 80% of the reactants enter the reactor from the main inlet and 20% of the reactants enter the reactor from secondary inlet at the middle of the reactor.

Figure 5: The temperature of gas mixture along the reactor when 20% of the reactants enter the reactor from the secondary inlet

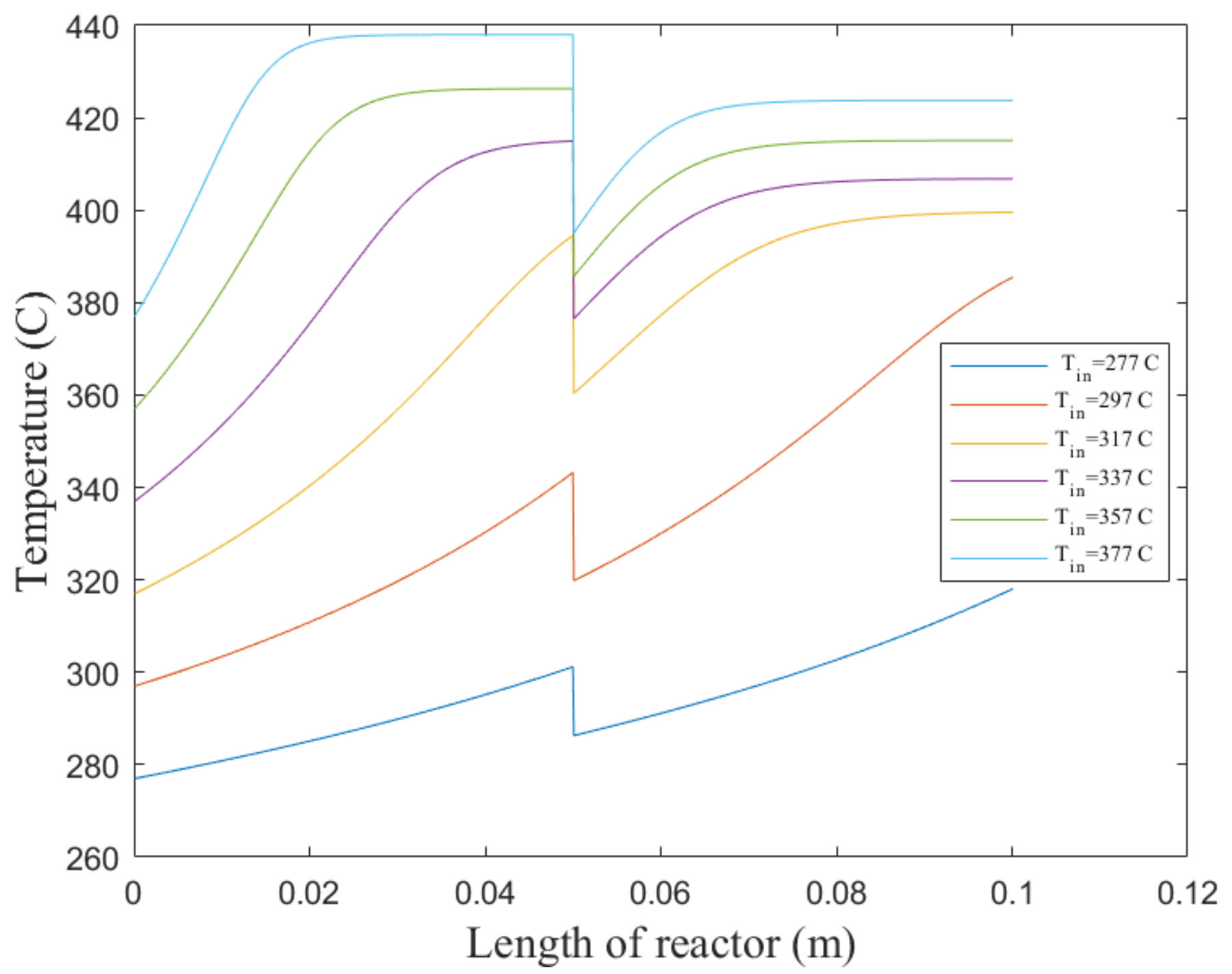


Figure 6 also shows the reaction rate along the reactor when 20% of the reactants enter the reactor from the secondary inlet.

Figure 6: The reaction rate along the reactor when 20% of the reactants enter the reactor from the secondary inlet

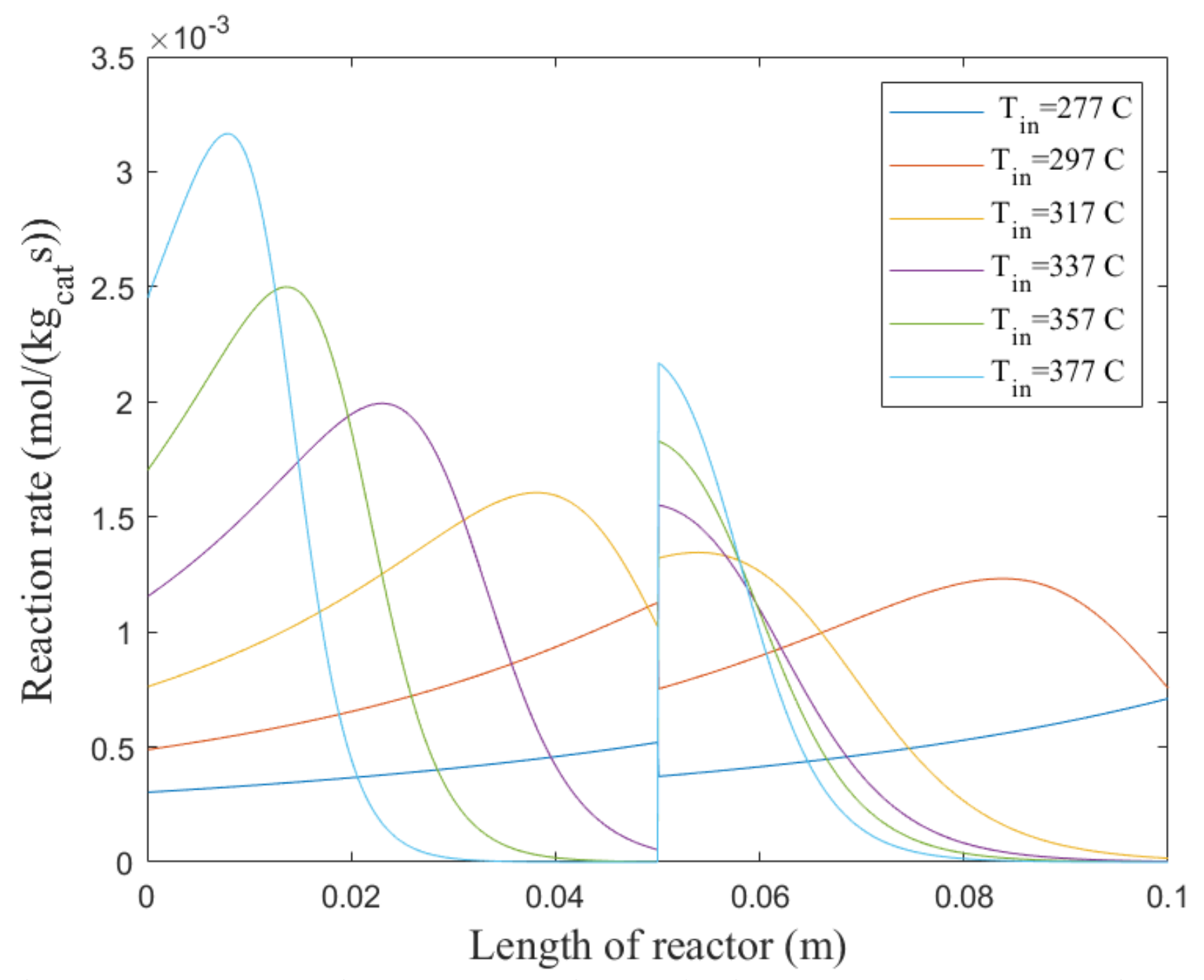
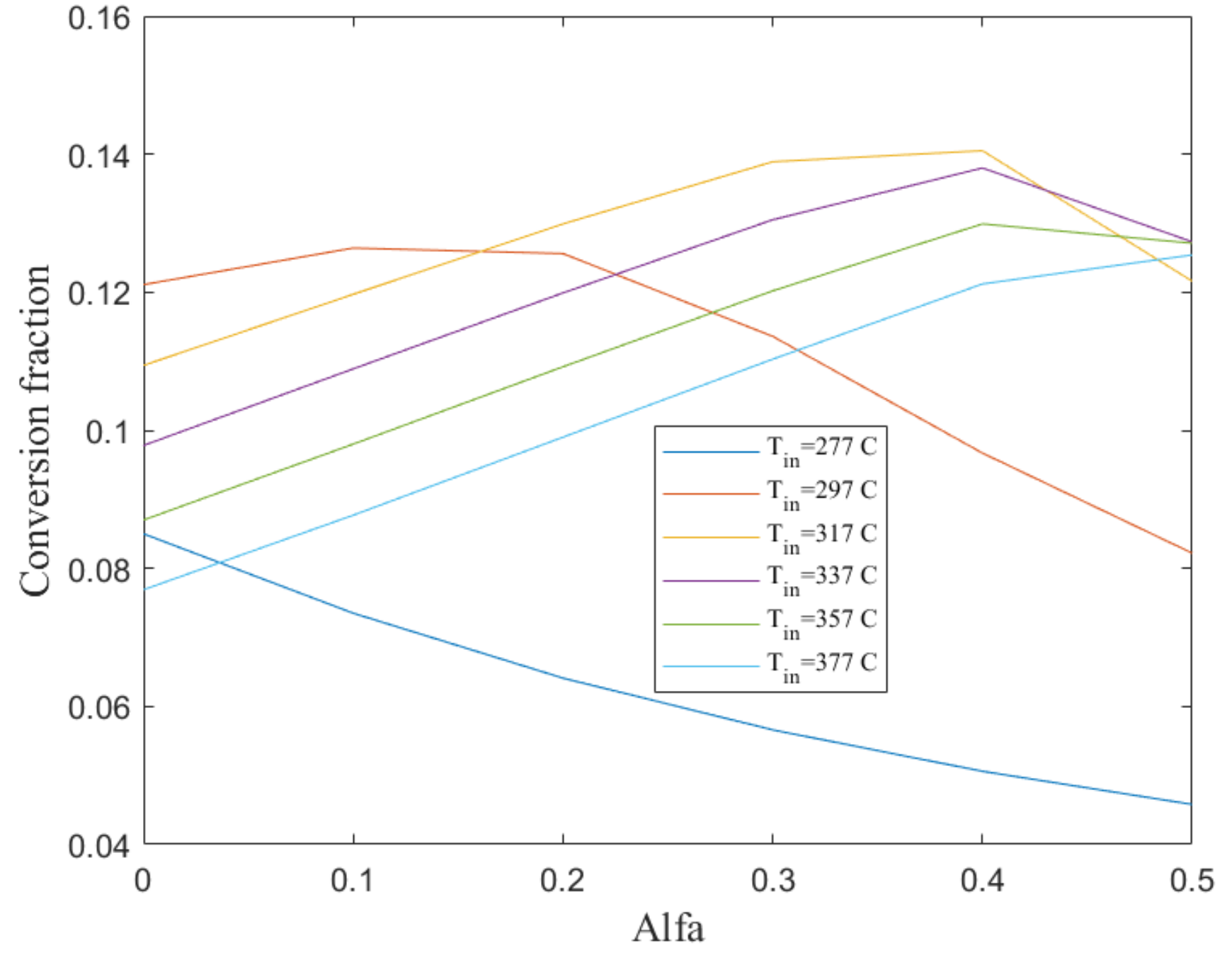


Figure 7 also shows the effect of the secondary inlet reactant on the fraction conversion where the fraction of reactants enter the reactor from the secondary inlet (Alfa) varies from 0 to 0.5.

Figure 7: The effect of secondary inlet reactant on the fraction conversion



Conclusion

- The reactants inlet temperature has a great impact on fraction conversion when an adiabatic reactor is used for ammonia synthesis.
- High inlet temperatures are suitable for short adiabatic reactors.
- Using the secondary inlet reactant can improve the performance of the adiabatic reactor by cooling the reactor and increasing the partial pressure of the reactants.
- Using the secondary inlet reactant is advantageous and can enhance the fraction conversion when the reactants inlet temperature is high.

References:

[1]. Smith, C., & Torrente-Murciano, L. (2021). Exceeding Single-Pass Equilibrium with Integrated Absorption Separation for Ammonia Synthesis Using Renewable Energy—Redefining the Haber-Bosch Loop. *Advanced Energy Materials*, *11*(13), 2003845.

[2]. Suhan, M. B. K., Hemal, M. N. R., Choudhury, M. S., Mazumder, M. A. A., & Islam, M. (2022). Optimal design of ammonia synthesis reactor for a process industry. *Journal of King Saud University-Engineering Sciences*, *34*(1), 23-30.

Contact info: Hossein Asgharian - hoas@energy.aau.dk

Acknowledgment: HySTrAm project funding from the European Union Grant Agreement N° 101058643.

Funded by the European Union

GRANT AGREEMENT N° 101058643

AAU ENERGY
AALBORG UNIVERSITY