

# Modeling and Simulation of a Water Gas Shift Reactor operating at a low pressure

Wail El Bazi<sup>1,\*</sup>, Abderrahim El-Abidi<sup>2,3</sup>, Moulay Saddik Kadiri<sup>1</sup>, Said Yadir<sup>2,3</sup>

<sup>1</sup>Laboratory of Process Engineering and Industrial Systems Optimization (LIPOSI)  
ENSAKhouribga, Sultan Moulay Slimane University,  
BéniMellal, Morocco

<sup>2</sup>Laboratory of Materials, Processes, Environment and Quality (LMPEQ),  
ENSA Safi, Cadi Ayyad University,  
Marrakech, Morocco

<sup>3</sup>Laboratory of Electronics, Instrumentation and Energy (LEIE),  
Faculty of Science, Chouaib Doukkali University,  
El Jadida, Morocco

## ABSTRACT

In order to study the WGS on an industrial scale at a low pressure, the modeling and simulation of a WGS reactor operating at a pressure close to  $P_{atm}$  and processing an industrial charge in the presence of a high temperature shift catalyst ( $Fe_2O_3/Cr_2O_3$ ) were performed. The Profiles of the carbon monoxide conversion, temperature and pressure along the reactor were obtained. The effect of several operating parameters (inlet temperature,  $H_2O/CO$  ratio) on the conversion of carbon monoxide along the reactor has been determined. The estimated catalytic mass to convert 60.5% of the carbon monoxide contained in the inlet is 170.76 t. The pressure drops in the reactor are not negligible and the maximum temperature reached is without any harmful effect on the catalyst. The choice of an optimal inlet temperature and a high  $H_2O/CO$  ratio improves the conversion of carbon monoxide.

**Keywords**—Packed bed reactor, catalyst, water gas shift reaction

## I. INTRODUCTION

Hydrogen is an important source of energy and is involved in various industrial processes such as: ammonia synthesis, methanol synthesis, etc. [1]. The production of this molecule can be carried out through several ways: Production from methane [2], biological production [3], water electrolysis [4], chemical production of aluminum and sodium hydroxide [5], or WGS (water gas shift reaction) which is a chemical reaction converting a mixture of carbon monoxide (CO) and water vapor ( $H_2O$ ) into a mixture of carbon dioxide ( $CO_2$ ) and hydrogen ( $H_2$ ):



This slightly exothermic reaction discovered by the Italian physicist Felice Fontana in 1780 [1] can occur in the presence of catalysts based on several metals such as Cu, Fe, Ni, Pd, Pt, Rh, Ru [6] or even metal oxide [7]. At high temperatures (350-450°C) catalysts based on iron oxides and chromium oxide III ( $Cr_2O_3$ ) can be used [7]. At low temperatures (120-240°C) copper or copper oxide catalysts can be used with promoters of alumina oxide ( $Al_2O_3$ ) [7] and zinc oxide (ZnO) [8]. WGS can occur at pressures ranging from 1 to 83.75 bars [7-10]. But often industrial reactors operate at high pressures [8, 11-12]. Numerous models of the water gas shift reactors have been published to date. Elnashaie et al developed a steady-state one-dimensional heterogeneous model to study the behavior of industrial reactors operating at high temperatures [11]. Their work also focused on the effect of temperature on the conversion of carbon monoxide. Adams et al used a dynamic two-dimensional heterogeneous model to study the behavior of reactors operating at both high and low temperatures [13]. Adams was also interested in the effect of important parameters on  $X_{CO}$  ( $H_2O/CO$ - temperature ratio). Falleiros

Barbosa Lima et al investigated an industrial reactor operating at high temperatures, using different one-dimensional pseudo homogeneous models [14]. The effect of catalyst deactivation on reactor performance was also investigated. A steady-state one-dimensional pseudo-homogeneous model was also used by Shokry et al to predict the evolution of molar flow rate along and at the outlet of an industrial WGS reactor operating at low temperatures [12]. These authors also studied the effect of pressure, inlet temperature,  $H_2O/CO$  ratio on  $X_{CO}$ . The major disadvantage of operating at high pressures is the enormous energy costs that it would be interesting to reduce them by carrying out the WGS at low pressures. In addition, the operating life of the catalyst can reach 15 years if the reactor operates at a low pressure [15]. Indeed, several papers have been carried out to study this reaction and to determine its kinetic expressions in the presence of catalysts allowing its activation at pressures close to the atmospheric pressure [8,16-23]. It would therefore be interesting to use these expressions in the simulation and study of the behaviour of reactors operating at pressures on the order of 1 atm. In fact, the work of Maklavany et al has been interested in this topic. These authors used the kinetic expression of WGS in the presence of a low temperature shift catalyst ( $CuO/ZnO/Al_2O_3$ ) to simulate a laboratory reactor operating at 1.2 bar. Two models were used: a steady state 2D homogeneous isothermal model [24] and a 1D homogeneous isothermal model with axial dispersion [25]. The effect of temperature on the variation of several parameters along the reactor (CO concentration, pressure, reaction rate, superficial velocity) was also studied. In our study, we also carried out the simulation of a reactor operating at a low pressure. But in our case, it is in the presence of a high temperature shift catalyst ( $Fe_2O_3/Cr_2O_3$ ) and for a large reactor. This will allow the industrial-scale study of the reaction at a low pressure and clarified the strengths and weaknesses of the realization of WGS under this condition. The model we used to simulate the fixed catalytic bed is the steady state one-dimensional pseudo homogeneous model that is widely used in the study of the behaviour of industrial catalytic convertors, sites of the WGS [12,14,26] or other gas phase reactions [27,28,29]. In the first part of this study, we used the kinetic rate expression corresponding to this catalyst in the modeling and simulation of an industrial WGS reactor. This allowed the prediction of profiles of the carbon monoxide conversion, temperature and pressure along the reactor. Then, the work was continued by studying the effects of the operating parameters (inlet temperatures,  $H_2O/CO$  ratios) on the conversion of carbon monoxide in order to define the optimal conditions of the reaction realization.

## II. DESCRIPTION

### A. Description of the studied catalyst and the operating conditions for establishing the kinetic rate expression

The kinetic rate expression corresponding to the chosen catalyst was carried out by Keiski et al [18]. The characteristics of the catalyst, as well as the operating conditions under which the kinetic rate expression was established, are presented in Table I [7,13,18].

TABLE I. CATALYST CHARACTERISTICS AND OPERATING CONDITIONS FOR THE ESTABLISHMENT OF THE WGS KINETICS [7,13,18]

Catalyst	Composition	Operating conditions for the establishment of WGS kinetics	Equivalent spherical diameter, $d_p$ ( $\mu m$ )	Shape	Catalyst density, $\rho_c$ ( $kg/m^3$ )
CCE C12 Ref: [7,13,18]	$Fe_2O_3/Cr_2O_3$ (89/9%)	T : [575-675 K], P : 1 atm $H_2O/CO$ (molar) : [2.4-12.1] Gas mixture of different fractions of: $CO, CO_2, H_2O, H_2, N_2$	2800	Cylinder	3730

### B. Description of the reactor and the operating conditions considered in the simulation

The characteristics of the simulated reactor are presented in Table II.

TABLE II. REACTOR CHARACTERISTICS

Packed bed diameter D (m)	Packed bed length, L (m)	Number of packed beds (tubes)	Thermal property of the packed bed	void fraction in the packedbed $\epsilon$
0.09	2.2	6000	Adiabatic	0.4

The first simulations were run to predict the profiles of carbon monoxide conversion, temperature and pressure along the reactor operating at a low pressure and for a feed flow of an industrial nature. We ran these Simulations under the operating conditions presented in Table III.

TABLE III. OPERATING CONDITIONS USED FOR THE PREDICTION OF  $X(Z)$ ,  $T(Z)$  AND  $P(Z)$ 

Molar flow rate of the feed gas mixture, $F_{i,0}(\text{mol. s}^{-1})$	Inlet pressure, $P_0$ (atm)	Inlet temperature, $T_0$ (K)
CO : 23.28 CO <sub>2</sub> : 94.19 H <sub>2</sub> : 364.149 H <sub>2</sub> O : 228.93 N <sub>2</sub> : 134.354	1.12	590

The compositions and the inlet pressure of the gas mixture of table 3 are close to those studied when establishing the kinetic rate expression of the WGS [18]. The temperatures remain within the temperature range of the kinetic study [18]. At the same time, in order to evaluate the WGS at low pressures in a situation close to an industrial case, each partial molar flow rate of WGS reagent (CO, CO<sub>2</sub>, H<sub>2</sub>O, H<sub>2</sub>) presented in Table 3 is equal to 30% of the actual partial molar flow rate of the same reagent feeding the high pressure WGS reactor of the Alexandria Fertilizers Company (AlexFert) [12]. The molar flow rate of nitrogen shown in this table is equal to 30% of the real molar flow rate of the inerts feeding the company's reactor.

To study the effect of temperature on the carbon monoxide conversion along the reactor, other simulations were performed for other inlet temperatures (575 K, 605 K, 620 K) while keeping the other operating conditions (Table 3) and the same reactor characteristics (Table 2).

Finally, the study of the effect of the H<sub>2</sub>O/CO ratio on the  $X_{\text{CO}}$  profile along the reactor required further simulations for  $[H_2O]/[CO]=3$  which corresponds to  $F_0(H_2O) = 69.84 \text{ mol.s}^{-1}$  and  $F_0(CO) = 23.28 \text{ mol.s}^{-1}$  and for  $[H_2O]/[CO]=5$  which corresponds to  $F_0(H_2O) = 116.4 \text{ mol.s}^{-1}$  and  $F_0(CO) = 23.28 \text{ mol.s}^{-1}$ . These last simulations were established by varying only the molar flow rate of the water vapor. While the other operating conditions (Table III) and reactor characteristics (Table II) have not been changed.

### III. EQUATIONS

#### A. kinetic expression

The kinetic expression used is a simple power-law model [7,18]:

$$-r_{\text{co}} (\text{mol. kg cata}^{-1} . \text{h}^{-1}) = 2623447 \exp\left(\frac{-79759}{RT}\right) C_{\text{co}}^{0.74} C_{\text{H}_2\text{O}}^{0.47} C_{\text{CO}_2}^{-0.18} [1 - \beta] \quad (1)$$

Where  $-r_{\text{CO}}$  is the CO conversion rate,  $C_i$  is the molar concentration of species  $i$  ( $\text{mol.dm}^{-3}$ ) and  $\beta$  is the reversibility factor:

$$\beta = \frac{C_{\text{CO}_2} C_{\text{H}_2}}{C_{\text{CO}} C_{\text{H}_2\text{O}} K_e}$$

The equilibrium constant,  $K_{\text{eq}}$ , is given by the equation 2 [7,18]:

$$K_{\text{eq}} = \exp\left(\frac{4577.8}{T} - 4.33\right) \quad (2)$$

### B. Process modeling and numerical solution

The following assumptions were made to develop the used mathematical model for the packed bed reactor simulation:

- Adiabatic reactor.
- Steady state condition.
- Axial dispersion is neglected, because the flow rate is sufficiently high to create a turbulent flow ( $Re = \frac{G \cdot d_p}{\mu} > 40$ ) and ( $L/d_p > 150$ ) [30]. Where  $Re$  is the Reynolds number,  $G$  is the superficial mass velocity ( $\text{kg} \cdot \text{m}^{-2} \cdot \text{s}^{-1}$ ) and  $\mu$  is the dynamic viscosity of the mixture ( $\text{Pa} \cdot \text{s}$ ).
- Radial dispersion is neglected, because the tube diameter is narrow, the reactor is adiabatic and the WGS is a moderately exothermic. Under these conditions, radial gradients of concentrations and temperatures are not important [30,31,32].
- The heat and mass transfer as well as the diffusion in the catalyst were lumped in the rate constant.

The system of differential equations used is as follows [14]:

$$\frac{dX_{CO}}{dz} = \frac{-r_{CO} F_{Pres} \rho_B S}{F_{CO,0}} \quad (3)$$

$$\sum F_i C_{pi} \frac{dT}{dz} = \Delta H_R r_{CO} F_{Pres} \rho_B S \quad (4)$$

$$\frac{dp}{dz} = -f \frac{\rho_g u_s^2}{d_p} \quad (5)$$

$C_i$  is expressed using the perfect gas equation:

$$C_i = \frac{P_i}{RT} \quad (6)$$

Where  $P_i$  is the partial pressure (Pa), expressed as follows:  $P_i = \frac{F_i}{\sum_{i=0}^n F_i} \cdot P = y_i \cdot P$

With  $y_i$  is the molar fraction of the species  $i$

The expression of the molar flow rate,  $F_i$  ( $\text{mol} \cdot \text{s}^{-1}$ ), of each component depends on its nature, be it a reagent, a product or an inert:

- For the reagent:

$$F_i = F_{i,0} - F_{CO,0} \cdot X_{CO} \quad (7)$$

- For the product:

$$F_i = F_{i,0} + F_{CO,0} \cdot X_{CO} \quad (8)$$

- For the inert:

$$F_i = F_{i,0} \quad (9)$$

The kinetic expression rate presented in equation 1 is applicable at  $P=1$  atm, while the pressures in the reactor are slightly above the atmospheric pressure. To consider this difference between the reactor pressures and the atmospheric pressure, a pressure scale-up factor ( $F_{pres}$ ) can be used to apply the kinetic equation derived at  $P=1$  atm to higher pressures [13]:

$$F_{pres} = P(atm)^{(0,5 - \frac{P(atm)}{250})} \quad (10)$$

The catalyst bulk density,  $\rho_B$  ( $\text{kg.m}^{-3}$ ), is expressed by equation 11:

$$\rho_B = (1 - \varepsilon) \cdot \rho_c \quad (11)$$

The molar specific heat capacity of each component,  $C_{pi}$  ( $\text{J.mol}^{-1} \text{K}^{-1}$ ), as a function of temperature is given by the empirical equation:

$$C_{pi} = \alpha + \beta \cdot T + \gamma \cdot T^2 \quad (12)$$

The values of  $\alpha$ ,  $\beta$  and  $\gamma$  are provided in Table IV:

TABLE IV. CONSTANTS EXPRESSING  $C_{pi}$  ACCORDING TO TEMPERATURE

Speciesi	$\alpha$	$\beta \times 10^3$	$\gamma \times 10^6$
H <sub>2</sub>	29.3	-0.84	2.09
CO <sub>2</sub>	32.22	22.18	-3.35
CO	27.62	5.02	0
H <sub>2</sub> O	30.13	10.46	0
N <sub>2</sub>	27.62	4.19	0

The heat of the reaction,  $\Delta H_R$  ( $\text{J.mol}^{-1}$ ), is expressed by equation 13:

$$\Delta H_R = -4,12 \times 10^4 + \int_{298}^T (C_{pCO_2} + C_{pH_2} - C_{pCO} - C_{pH_2O}) \cdot dT \quad (13)$$

The friction factor  $f$ , presented in equation 5 can be calculated using Ergun's equation [33]:

$$f = \frac{1 - \varepsilon}{\varepsilon^3} \left( a + b \frac{1 - \varepsilon}{Re} \right) \quad (14)$$

with  $a=1.75$  and  $b=150$ .

$G$  is calculated by equation 15:

$$G = \sum_{i=1}^{i=n} \frac{F_i M_i}{S} \quad (15)$$

Where  $S$  ( $\text{m}^2$ ) is the cross section of the reactor ( $S = \frac{\pi D^2}{4}$ ) and  $M_i$  is the molecular weight of the species  $i$  ( $\text{kg.mol}^{-1}$ )

$\mu$  is expressed by equation 16 [34]:

$$\mu = \sum_{i=1}^n \frac{\mu_i}{1 + \frac{1}{y_i} \sum_{j=1, j \neq i}^n \frac{y_j [1 + (\frac{\mu_j}{\mu_i})^{1/2} (\frac{M_j}{M_i})^{1/4}]^2}{2\sqrt{2} [1 + (\frac{M_i}{M_j})^{1/2}]}} \quad (16)$$

When the pressure level is moderate, its impact on the viscosity of the gas is low. In this case, the parameter that most impacts viscosity is mainly temperature [35].

The dynamic viscosity of species  $i$ ,  $\mu_i$  (Pa.s), is expressed as a function of temperature by the empirical equation 17:

$$\mu_i = \frac{AT^B}{1 + \frac{C}{T} + \frac{D}{T^2}} \quad (17)$$

Table V below gives the values of A, B, C and D for each species  $i$ :

TABLE V. CONSTANTS EXPRESSING  $\mu_i$  ACCORDING TO TEMPERATURE

species $i$	A x $10^7$	B	C	D
H <sub>2</sub>	1.797	0.685	-0.59	140
CO <sub>2</sub>	2.148	0.46	290	0
CO	1.113	0.534	94.7	0
H <sub>2</sub> O	6.1839	0.678	847.23	-73930
N <sub>2</sub>	6.56	0.608	54.71	0

The density of the gas mixture,  $\rho_g$  (kg.m<sup>-3</sup>), is expressed by equation 18:

$$\rho_g = \frac{P}{RT} \sum_{i=1}^{i=n} y_i M_i \quad (18)$$

The superficial velocity,  $u_s$  (m.s<sup>-1</sup>), is defined as:

$$u_s = \frac{G}{\rho_g} \quad (19)$$

The catalyst mass corresponding to a longitudinal position  $z$  in the reactor,  $w(z)$  (kg), is expressed by equation 20:

$$w(z) = S. z. \rho_B \quad (20)$$

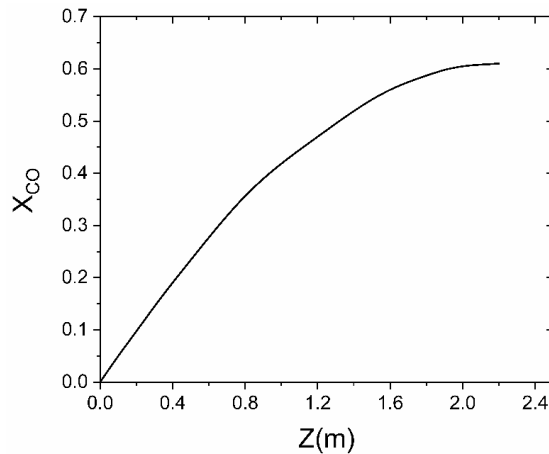
Differential equations (3-5) were numerically solved by MATLAB by using the fourth-order Runge-Kutta method. The boundary conditions are:  $X_{CO}(Z=0) = 0$ ,  $P_0(Z=0) = 1,134 \times 10^5$  Pa,  $T_0(Z=0) =$  The inlet temperature.

#### IV. RESULTS AND DISCUSSIONS

##### A. Profile of the carbon monoxide conversion along the reactor

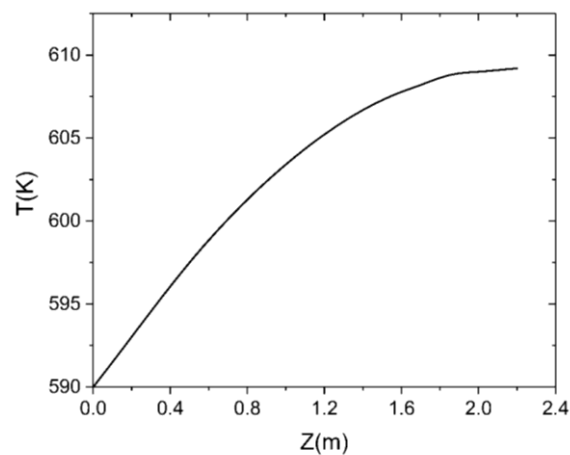
Figure 1 has an asymptotic shape. From  $Z=0$  m to  $Z=1.8$  m, the conversion of carbon monoxide increases along the reactor until a value of  $X_{CO} = 0.6$ . From 1.8 m to 2 m, the increase of  $X_{CO}$  according to the longitudinal position is very weak and  $X_{CO}$  obtained at  $Z=2$  m is 0.605. Beyond 2 m,  $X_{CO}$  remains constant. Under the conditions studied, the equilibrium conversion would be 0.605. The catalytic mass required to reach this conversion is 170.76 t. In order to increase the conversion of carbon monoxide or/and lower the necessary catalytic mass, several possibilities remain to be explored:

- Determination of optimal operating conditions (inlet temperature, H<sub>2</sub>O/CO ratio, etc.).
- Optimization of the catalyst composition (choice of the promoter or/ and promoter fraction increasing catalytic activity [7]),
- ...etc.

Fig. 1.  $X_{CO}=f(Z)$ .

### B. Variation of temperature, along the reactor height

The curve showing the temperature variation along the reactor also has an asymptotic shape. From  $Z=0$  m to  $Z=1.8$  m, the temperature increases along the reactor until it reaches 608.95 K. From  $Z=1.8$  m to  $Z=2$  m, the temperature increase along the reactor is very slight.  $T$  obtained at  $Z=2$  m is 609 K. Beyond 2m, the temperature remains constant. In fact, at this longitudinal position the equilibrium is reached and since the reactor is an adiabatic one, the temperature rise stops.

Fig. 2.  $T=f(Z)$ .

The maximum temperature reached in the case studied has no damaging effect on the catalyst. In fact, when the temperature exceeds 823 K, the catalyst will quickly be deactivated by sintering and the thermodynamic limitation becomes very important [8].

### C. Pressure profile across the catalyst bed

The pressure drops from 1.12 atm to 1.021 atm ( $\Delta P = 8.8\%$  of inlet pressure). This loss of pressure is not negligible [24] and can affect the good functioning of the reactor. In fact, the decrease in pressure between the inlet and outlet of the reactor causes an increase in the superficial velocity, which leads to a decrease in contact time and therefore in catalytic activity. In addition, it is necessary to compress the inlet flow when its pressure is low in order to overcome the pressure drop along the reactor and ensure a downstream flow at a pressure higher than the atmospheric pressure. If the pressure in the reactor is lower than the atmospheric pressure, it is necessary to use a vacuum pump in order to evacuate the reactor.

Several solutions can be studied to reduce pressure drops, including:

- The selection of the catalyst shape offering the lowest possible pressure loss. In fact, several studies have demonstrated that the shape of the catalyst has an important effect on the pressure loss [36, 37].
- The use of a foamsince it limits the pressure drops compared to a conventional fixed bed [38].
- ...etc

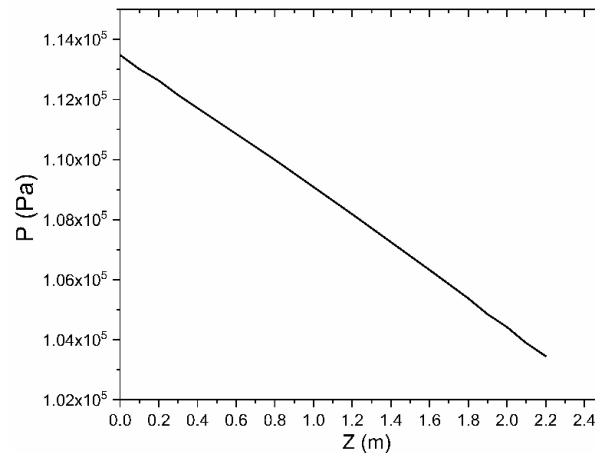


Fig. 3.  $P = f(Z)$ .

#### D. The effect of inlet temperature on carbon monoxide conversion

Figure 4 shows that the increase in the inlet temperature from 575 K to 590 K causes an increase in the CO conversion along the reactor. It should also be noted that the equilibrium is not reached in the reactor when the inlet temperature is 575 K. For the inlet temperature range between 590 K and 620 K, the conversion of CO is thermodynamically limited. The higher the inlet temperature, the faster the equilibrium is reached (located in the most remote longitudinal positions) and the lower the equilibrium conversion. In fact, according to Le Chatelier's principle, to counter the constraint of a temperature increase, the equilibrium is shifted following the reverse reaction, which leads to this decrease in the carbon monoxide conversion. According to Figure 4, the inlet temperature giving the highest conversion at the reactor outlet ( $X_{CO} = 0.605$ ) is 590 K.

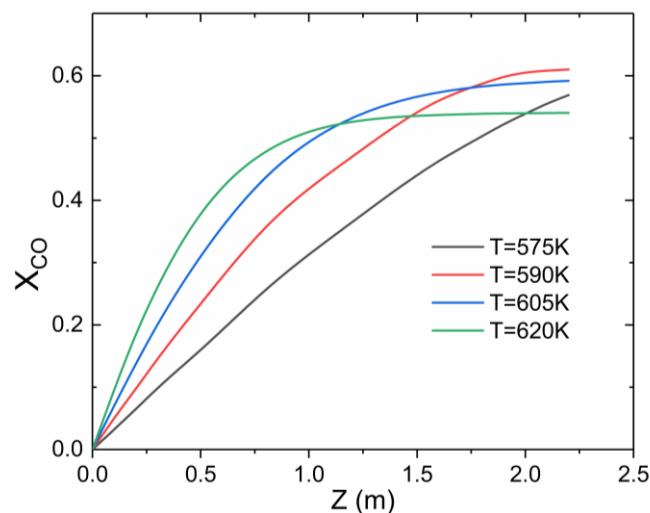


Fig. 4. The effect of inlet temperatures on  $X_{CO}$  along the reactor



### E. The effect of $H_2O/CO$ ratio on $X_{CO}$

It is clear from figure 5 that the higher the  $H_2O/CO$  ratio, the more carbon monoxide conversion is important. The highest conversion is obtained for a ratio of  $H_2O/CO=10$ . In fact, in the studied case, the reaction rate is accelerated with the increase in water concentration (see Equation 1) and therefore the  $H_2O/CO$  ratio. The same effect of this ratio on  $X_{CO}$  has been observed in experimental studies conducted at the atmospheric pressure, at high temperatures (573 K-773 K) and in the presence of catalyst also composed of  $Fe_2O_3$  and  $Cr_2O_3$  [39]. In fact, the role of the water vapour is extremely important, because its use with sufficiently high flow rates prevents over-reducing of the catalyst [7]. If the WGS is conducted with low  $H_2O/CO$  ratios, this results in methanation, Fischer Tropsch reaction and carbon deposition on the catalyst [7]. However, it should be noted that the carrying out of WGS with high  $H_2O/CO$  ratios requires significant energy costs related to the water vapor production.

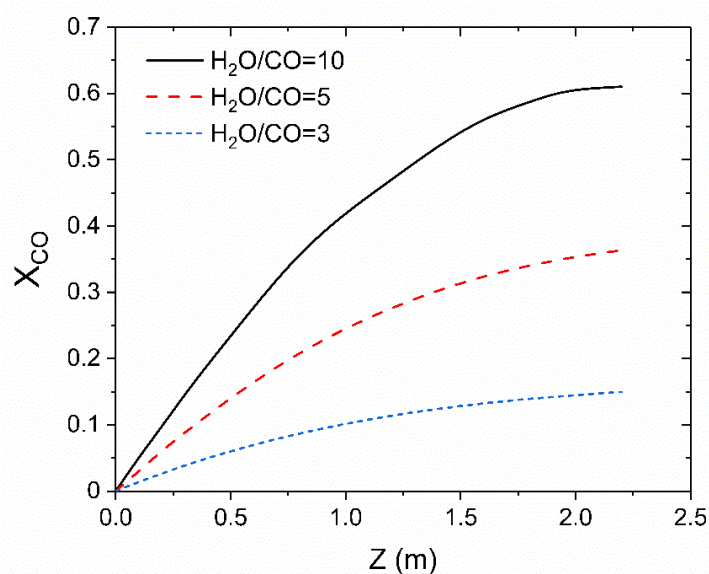


Fig. 5. The Effect of  $H_2O/CO$  ratios on  $X_{CO}$  along the reactor.

## V. CONCLUSION

This study investigated the modeling and simulation of a WGS reactor processing an industrial load operating at a low pressure. The model used to predict the profiles of carbon monoxide conversion, temperature and pressure along reactor is the steady state one-dimensional pseudo homogeneous model and the kinetic rate expression of the WGS corresponding to the catalyst used is taken from the literature. The estimated catalytic mass to convert 60.5% of carbon monoxide contained in inlet flow is 170.76 t. To lower the catalytic mass needed and/or increase the conversion of carbon monoxide there are several paths to explore such as the choice of promoter or a fraction of promoter allowing to improve catalytic activity. The pressure drop is not negligible ( $\Delta P = 8.8\% P_{inlet}$ ) which can have many harmful effects on the proper functioning of the installation. The use of foam, for example, should limit pressure drops. The maximum temperature reached (609 K) has no damaging effect on the catalyst. This work confirmed the important role of choosing an optimal inlet temperature and a high  $H_2O/CO$  ratio in increasing the conversion of carbon monoxide at the reactor outlet. The best conversion ( $X=0.605$ ) is obtained for a ratio  $H_2O/CO=10$  and for an inlet temperature of 590 K.

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