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OPTIMIZATION OF A METHANOL SYNTHESIS REACTOR

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The gas-phase methanol synthesis is usually carried out in a reactor consisting in a series of adiabatic fixed beds with intermediate cooling using the synthesis gas raw material. Due to the equilibrium limitations, the optimization reaction system in order to maximize the carbon oxides conversion and methanol productivity is necessary. In this paper, an optimization problem for a methanol synthesis reactor, operated both using direct and indirect cooling technologies, have been formulated and solved using the genetic algorithms combined with pattern search numerical techniques. A comparison of the two reactor configurations behavior in terms of methanol productivity was performed and the results showed a superior efficiency of the indirect cooling approach.

Keywords: Methanol synthesis, fixed-bed reactor, reactor optimization, genetic algorithms

1. Introduction

The methanol is one of the most important products in chemical industry used mainly as an intermediary in the manufacture of formaldehyde, amines, acetic acid or as a solvent. Due to the development of fuel industry, the methanol importance on the market increased considerably, because the manufacture of fuel additives (methyl-tert butyl ether) or the synthesis of dimethyl-ether are using methanol as a raw material [1].

The methanol is commercially manufactured from synthesis gas by using the low pressure technology (50- 100 bar) over copper-zinc based catalysts [2, 3]. There are two providers for methanol synthesis technology on the market, ICI and Lurgi, the first one offering a reactor concept based on the adiabatic quench converter, where the feed flow rate is split into fractions and injected between catalyst beds to control the reaction, whereas the second is proposing a quasi-

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isothermal design [3]. The chemical system consists in a series of three reactions, two of which being highly exothermal, severely limited by the equilibrium [4].

Different kinetic models, developed over the commercial $Cu/ZnO/Al_2O_3$ catalysts, have been proposed in the literature, the main ones being those published by Graaf et al [4] and Vanden Bussche and Froment [5]. Lim et al [6] proposed a kinetic model developed on a $Cu/ZnO/Al_2O_3/ZrO_2$.

Different studies regarding the methanol process optimization have been published in literature, most of them considering the Lurgi-type as an optimization candidate. Lovik [7] reported a study of modeling, estimation and optimization of a Lurgi shell and tube methanol synthesis reactor, using pseudo-homogeneous and heterogeneous mathematical models. The goal of the optimization study was to maximize the reactor productivity in respect with the recycle rate and the coolant temperature. Fuad et al [3] reported an optimization study taking into account the catalyst deactivation, considering inlet temperature and composition, feed flow rate and coolant temperature as decision variables, in order to maximize the methanol production rate. Shahrokhi and Baghmisheh [8] study concerning the modeling, optimization and control of a Lurgi-type reactor, had as a goal maximization of the reactor yield by changing the shell temperature, feed composition and recycle ratio. There are only few studies in the literature regarding the optimization of an ICI adiabatic reactor. In their study, Agachi et al [9] reported an optimization study of an adiabatic methanol synthesis reactor using the Pontryagin's Maximum Principle. The authors determined the optimal temperature profile in order to maximize the reactor productivity.

There are few studies in the literature regarding the optimization of a cold-shot reactor (injection of cold reactant between the catalyst beds). The optimal control problem considering several beds with uniform temperature have been reported by Crowe and Lee [10]. The optimal adiabatic cold-shot reactor policy, considering the conversion of sulfur dioxide to sulfur trioxide, have been reported by Lee and Aris [11]. Bozga [12] developed and solved an optimal control problem for a multi-bed catalytic reactor hosting an exotermic, reversible reaction.

From our knowledge there is not study in the literature presenting a comprehensive comparison of the optimal operation for the low pressure methanol synthesis reactor. The present papers focuses on the optimization of a methanol synthesis over a commercial $Cu/ZnO/Al_2O_3$catalyst, consisting in a series of adiabatic fixed beds, operated at low pressure, both with direct and indirect cooling.

2. Reactor mathematical model

The syngas conversion to methanol in the low pressure process takes place by the chemical reactions (1)-(3) [13]:

$$CO + 2H_2 \rightleftarrows CH_3OH,\ \Delta H_{298} = -21.7\,kcal \cdot mol^{-1} \qquad (1)$$

$$CO_2 + H_2 \rightleftarrows CO + H_2O,\ \Delta H_{298} = 11.9\,kcal \cdot mol^{-1} \qquad (2)$$

$$CO_2 + 3H_2 \rightleftarrows CH_3OH,\ \Delta H_{298} = -9.8\,kcal \cdot mol^{-1} \qquad (3)$$

In this study it was considered a methanol synthesis process carried out over a commercial Cu/ZnO/Al_2O_3 catalyst. The kinetic model developed by Graaf et al (1990) [13] was taken into account. In order to evaluate the chemical equilibrium, the expression proposed by Graaf et al (1986) [14] are implemented. The kinetic model is described by relations (4) to (6) and the rate and equilibrium constants are given in Table 1.

The reaction rates expressions are:

$$v_{p1} = \frac{k_1 K_{CO}\left[f_{CO} f_{H_2}^{3/2} - f_{CH_3OH} / \left(f_{H_2}^{1/2} K_{p1} \right) \right]}{\left(1 + K_{CO} f_{CO} + K_{CO_2} f_{CO_2}\right)\left[f_{H_2}^{1/2} + \left(K_{H_2O} / K_{H_2}^{1/2} \right) f_{H_2O} \right]} \qquad (4)$$

$$v_{p2} = \frac{k_2 K_{CO_2}\left[f_{CO} f_{H_2} - f_{H_2O} f_{CO} / K_{p2} \right]}{\left(1 + K_{CO} f_{CO} + K_{CO_2} f_{CO_2}\right)\left[f_{H_2}^{1/2} + \left(K_{H_2O} / K_{H_2}^{1/2} \right) f_{H_2O} \right]} \qquad (5)$$

$$v_{p3} = \frac{k_3 K_{CO_2}\left[f_{CO_2} f_{H_2}^{3/2} - f_{CH_3OH} f_{H_2O} / \left(f_{H_2}^{3/2} K_{p3} \right) \right]}{\left(1 + K_{CO} f_{CO} + K_{CO_2} f_{CO_2}\right)\left[f_{H_2}^{1/2} + \left(K_{H_2O} / K_{H_2}^{1/2} \right) f_{H_2O} \right]} \qquad (6)$$

The results reported by Bartholomew and Farrauto [15] and our preliminary numerical simulation studies, shown that, at the operating temperature and pressure at which the methanol synthesis process is carried out, the behavior of the gas mixture is ideal. Consequently, the fugacities f_j in the rate expressions (4)-(6) can be replaced by partial pressures of the components, p_j.

The physical properties of the mixture and the reactions enthalpies were evaluated from literature data and correlations [16].

Table 1.

Kinetic and equilibrium constants for methanol synthesis

Reaction	Kinetic and equilibrium constants
(1)	$k_1 = 4.89 \cdot 10^7 \cdot \exp\left(\frac{-113000}{R_G T}\right), mol\ bar^{-1.5}\ kg_{cat}^{-1}\ s^{-1}$ $K_{CO} = 2.16 \cdot 10^{-5} \cdot \exp\left(\frac{46800}{R_G T}\right), bar^{-1};\ K_{CO_2} = 7.05 \cdot 10^{-7} \cdot \exp\left(\frac{61700}{R_G T}\right), bar^{-1}$ $\frac{K_{H_2O}}{K_{H_2}^{1/2}} = 6.37 \cdot 10^{-9} \cdot \exp\left(\frac{84000}{R_G T}\right), bar^{-1}; \lg K_{p1} = \frac{5139}{T} - 12.621, \left[K_{p1}\right] = bar^{-2}$
(2)	$k_2 = 9.64 \cdot 10^{11} \cdot \exp\left(\frac{-152900}{R_G T}\right), mol\ bar^{-1.5}\ kg_{cat}^{-1}\ s^{-1}$ $\lg K_{p1} = -\frac{2073}{T} + 2.029$
(3)	$k_2 = 1.09 \cdot 10^5 \cdot \exp\left(\frac{-87500}{R_G T}\right), mol\ bar^{-1.5}\ kg_{cat}^{-1}\ s^{-1}$ $K_{p3} = K_{p1} K_{p2}$

Other data taken into account into reactor simulation are given in Table 2.

Table 2.

Reactor simulation data *[17]*

Parameter	Value
Catalyst bed void fraction, ε	0.45
Catalyst bed density, ρ_{SC}, kg m^{-3}	1000
Catalyst particle diameter, m	$4.2 \cdot 10^{-3}$
Total length of catalyst beds, m	10
Reactor diameter, m	5
Feed composition	15 % CO, 74 % H_2, 0.04 % CH_3OH, 8 % CO_2, 0.1 % H_2O, 2.86 % CH_4
Feed pressure, bar	54

In order to evaluate the composition and temperature variation and to describe the process behavior inside the reactor, a pseudo-homogeneous one-dimensional ideal mathematical model including mass and thermal balance equations as well as pressure drop equation was taken into account. The mathematical model equations and the corresponding boundary conditions for the first catalyst bed are:

$$\frac{d\xi_{m,n}}{dz}=\frac{1}{\dot{D}_m}v_{R,n};n=1,2,3;\ z=0,\xi_{m,n}=0 \tag{7}$$

$$\frac{dT}{dz}=\frac{1}{\dot{D}_m c_p}\sum_{i=1}^{3}\left(-\Delta H_{R,n}\right)v_{R,n};\ v_{R,n}=\eta_{i,n}\cdot v_{p,n}\cdot\rho_{sc};\ n=1,2,3;\ z=0,T=T_0 \tag{8}$$

$$\frac{dp}{dz}=-ff\,\frac{\dot{D}_m^2}{\rho\cdot d_p};\ z=0,\ p=p_0 \tag{9}$$

$$ff=\frac{(1-\varepsilon)}{\varepsilon^2}\left[1.75+150\cdot\left(\frac{1-\varepsilon}{\mathrm{Re}_p}\right)\right] \tag{10}$$

where $\xi_{m,n}$ - the extent of reaction n over the total mass flowrate, kmol kg^{-1}; $\dot{D}_m$ - the specific mass flow rate, kg m^{-2} s^{-1}; T-reaction temperature, K; c_p – reaction mixture specific heat, cal mol^{-1} K^{-1}; $v_{R,n}$ - reaction rate, kmol m^{-3} s^{-1}; $\eta_{i,n}$-efectiveness factor for reaction n; p-pressure inside the reactor, bar; ρ-reaction mixture density, kg m^{-3}; ff-friction factor; Re_p – Reynolds number.

Two reactor configurations have been taken into account, both consisting in maximum 4 catalyst beds, each of them operated adiabatically. The first one (denoted further as direct cooling, DC) uses cold reactant to cool down the reaction mixture between catalyst beds (cold shot cooling). In order to achieve the cooling, the feed flow rate is split into fractions, injected between the catalyst beds. In order to evaluate the composition and temperature change due to the feed of cold reagent between the catalyst beds, the balance equations in the mixing point given by relations (11) will be used:

$$T_{0,k}^{(+)}=\frac{D_{m,k-1}T_{k-1}+D_m^{(k)}T_0}{D_{m,k-1}+D_m^{(k)}};\ \xi_{m,n,k}^{(+)}=\frac{D_{m,k-1}\xi_{m,n,k-1}^{(-)}}{D_{m,k-1}+D_m^{(k)}} \tag{11}$$

where $T_{0,k}^{(+)}$ - temperature of the mixture after the mixing point, K; $D_{m,k-1}$ - mass flowrate coming from the previous catalyst bed, kg s^{-1}; $D_m^{(k)}$ - fraction of the mass flowrate fed on the current (k) catalyst bed, kg s^{-1}; T_0- feed temperature, K; $\xi_{m,i,k}^{(+)}$ - reaction extent on the kth catalyst bed, for the reaction n after the mixing point; kmol kg^{-1}; $\xi_{m,i,k-1}^{(-)}$ -reaction extent before the mixing point.

The boundary conditions of the mathematical model for the direct cooling approach will become:

$$z = Z_{k-1}, \xi_{m,n} = \xi_{m,n,k}^{(+)}, T = T_{0,k}^{(+)}; p = p_{k}^{(+)} \tag{12}$$

The second configuration, takes into account the cooling between the catalyst beds performed by external heat exchangers (indirect cooling, IC). In this case, the boundary conditions for the reactor mathematical model between the catalyst beds, expressed by equations (7)-(9), become:

$$z = Z_{k-1}, \xi_{m,n} = \xi_{m,n,k-1}^{(+)}, T = T_{0,k}^{(+)}; p = p_{k-1}^{(+)} \tag{13}$$

The superscript (-) is denoting the variables values before the mixing point, whereas the superscript (+) is denoting the same variable values after the mixing with the cold reactant feed (DC) or the outlet cooling in an external heat exchanger (IC).

The scheme of the two approaches is presented in Fig. 1.

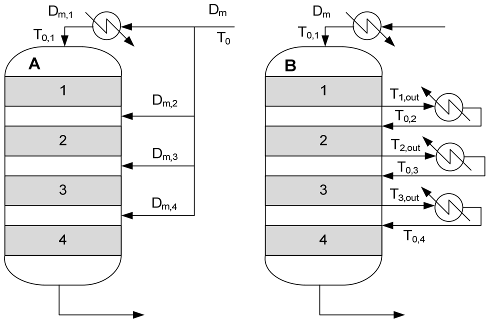

Fig. 1. Direct (A) and indirect (B) cooling methanol synthesis reactor scheme

3. Optimization study

In this paragraph will be formulated and solved an optimization problem for a methanol synthesis reactor, in order to determine the most appropriate reactor structure to maximize the methanol production.

Problem formulation

The objective of this study was to determine the operating parameters that maximize the carbon oxides conversion along with the simultaneous maximization of methanol production flowrate, by optimally distributing a given catalyst amount over the reactor catalyst beds. The objective function is expressed by:

$$J = \frac{w(1)}{D_{M,MeOH}} - w(2)\, X_{CO+CO_2} \tag{14}$$

with $D_{M,MeOH}$ - methanol flowrate at the reactor outlet, kg s^{-1}; X_{CO+CO_2} - global carbon oxides conversion.
The weighting coefficients, *w*, were equal to 1.

For the direct cooling technology, the decision variables are: feed temperature on the first bed $\left(T_{0,1}\right)$, the fractions from the feed flowrate fed between the catalyst beds$\left(fb_k, k=1..4\right)$, the total mass flowrate $\left(D_m\right)$and the catalyst distribution among the beds. The indirect cooling reactor optimization considered as decision variables the feed temperature on each catalyst bed,$\left(T_{0,k}, k=1..4\right)$, the total mass flowrate $\left(D_m\right)$ and the height of the catalyst beds $\left(Z_k, k=1..4\right)$.

In order to solve these problems involving several decision variables, different numerical algorithms can be implemented. One of the most efficient numerical techniques is the genetic algorithm (GA). This type of algorithms are efficient search and optimization techniques inspired by natural evolution [18] and due to their working principle are more robust in the localization of global optima [19]. As reported by Costa et al., the genetic algorithms are efficient in identifying promising regions of the search space (exploration step) but not very efficient when it comes down to fine tuning of the optimum (exploitation step) [20]. In this work, the Genetic Algorithm Toolbox included in Matlab® programming environment has been used. The algorithm is initialized by a set of S population elements, each element consisting in decision variables values uniformly distributed between 0 and 1. The quality of each element is evaluated by the performance index (fitness) function and the calculated values are ordered in increasing order. Then an iterative procedure is applied, according to the classical structure of a genetic algorithm. A selection of individuals by the roulette wheel approach is performed, and on the selected elements the crossover and mutation operators are applied. The selection by roulette wheel consist in the creation of a wheel where each individual has a section proportional with its fitness value [21]. The weighted wheel is spun several times to select individuals undergoing further crossover and mutation operations. The individuals with the lowest value of the performance index value have the highest chance to survive. In this work a single-point crossover operator is used along with a mutation scheme named “adaptive feasible” that, according to Matlab® documentation, randomly generates directions that are adaptive with respect to the last successful or unsuccessful generation. By performing preliminary runs and in order to ensure a good diversity, a population size of 100 was chosen. In order to achieve a fine tuning of the solution, a pattern search (Hooke-Jeeves) algorithm implemented in the Optimization Toolbox of the Matlab programming environment was used. The optimal solution of the Genetic Algorithm technique was used as the initialization step for the pattern search algorithm. The final solution reported in this study is, for all the cases, the combination of the two numerical algorithms.

Optimization problem 1 (no restriction on the feed temperature on the catalyst beds)

The optimization problem was solved for the two technological approaches, in order to evaluate their efficiency in terms of carbon oxides conversion and methanol production. The weighting factors, *w*, were equal to 1.

The decision variables ranges considered in our study are:

- Feed mass flow rate: $40 < D_m < 200,\ kg \cdot s^{-1}$
- Temperature: $300 < T < 700, K$
- Feed flow rate fractions (only for DC) $0 < fb_k < 1$
- Catalyst beds lengths: $0.5 < Z_i < 10,\ m$

A comparison of the optimization results for the two technological approaches in terms of decision variables values and reactor performances are given in Table 3.

Table 3

Comparison of the optimization results for problem 1

Direct cooling		Indirect cooling	
Feed temperature on the first catalyst bed, K	522	Feed temperature on the first catalyst bed, K	524
Total feed flowrate, kg s^{-1}	200	Total feed flowrate, kg s^{-1}	200
Catalyst bed lengths, m	Z_1=0.81 Z_2=2.4 Z_3=3 Z_4=3.79	Catalyst bed lengths, m	Z_1=1.86 Z_2=2.29 Z_3=2.67 Z_4=3.18
Feed flowrate fractions	fb_1=0.358 fb_2=0.189 fb_3=0.214 fb_4=0.239	Temperatures between catalyst beds, K	$T_{0,1}$=524 $T_{0,2}$=518 $T_{0,3}$=514 $T_{0,4}$= 510
Methanol flowrate, D_{MeOH}, kg s^{-1}	34.26	Methanol flowrate, D_{MeOH}, kg s^{-1}	40.63
Carbon oxides conversion, X_{CO+CO2}, %	22.41	Carbon oxides conversion, X_{CO+CO2}, %	26.61

The reactor behavior, both for direct and indirect cooling corresponding to the optimal parameters given in Table 3, is described in *Fig. 2-4*. It can be observed from the optimization results that the optimal catalyst bed lengths increases from first to last, in order to ensure a conversion value close to the equilibrium one at the bed outlet (*Fig. 2*).

In *Fig. 3* there are shown the evolutions of the reactor temperature (T_{eff}) and methanol formation rates (v_{MeOH}eff) in respect with the reactor length. The temperature that maximizes the methanol formation rate (T_{max}), at the composition existing for each reactor length was also determined. It can be observed that both for DC and IC technologies, the effective methanol formation rate approaches the maximum one for reactor axial positions close to the bed outlet.

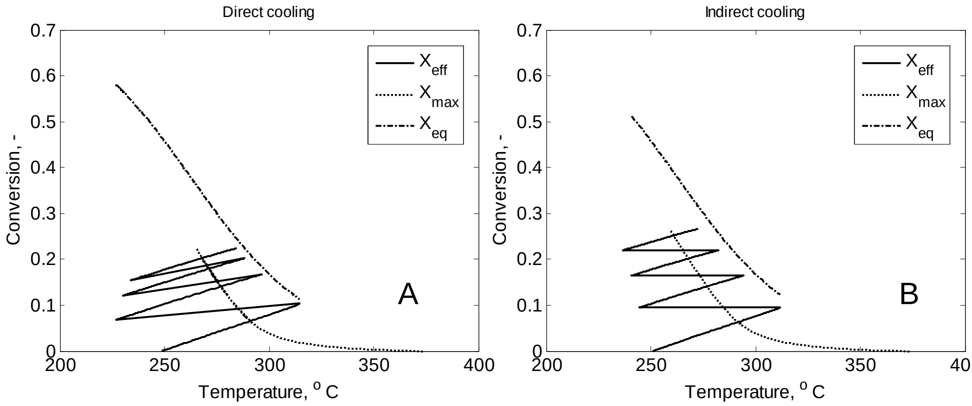

Fig. 2. Conversion-temperature diagrams for direct (A) and indirect (B) cooling technologies (Problem 1)

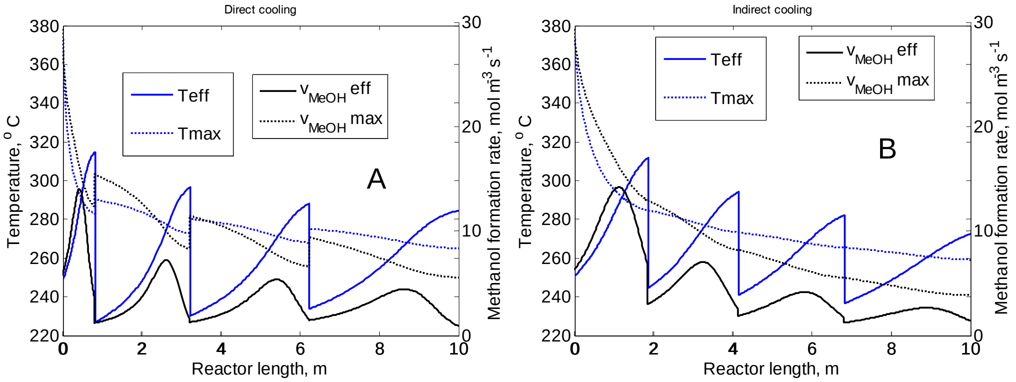

Fig. 3. Temperature and methanol formation rate profiles in the methanol synthesis reactor (Problem 1)

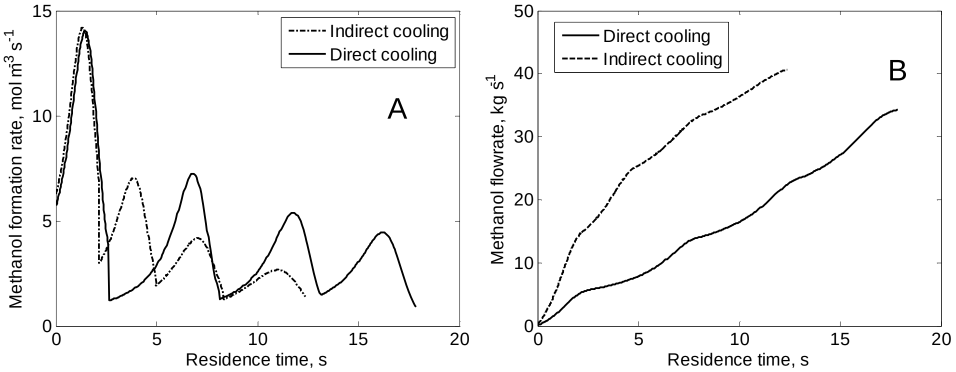

Fig. 4. Methanol formation rate and methanol flowrate evolutions in respect with the residence time in the bed for DC and IC technologies (problem 1)

On the first catalyst bed, even if the methanol formation rates have close values, the difference in the feed flowrates leads to a higher methanol flowrate for IC (*Fig. 3*). It can be observed from Table 3 that for the same total mass feed flowrate, the indirect cooling is more efficient both in terms of global carbon oxides conversion (26.61 % for IC by comparison with 22.41 % for DC) and methanol outlet flowrate (40.63 kg/s in comparison with 34.26 kg/s).

Influence of the weighing factors

The minimization of the objective function (14) is acquired by maximizing the methanol flowrate along with the carbon oxides conversions. The results depend on the weighting factors that ensure the relative influence of the carbon oxides conversion and methanol flowrate at the reaction system outlet. Different values of the weighting factors have been tested. If the ratio *w(1)/w(2)* is higher than 1, the optimization results in terms of carbon oxides conversion and methanol flowrate are the ones given in Table 3. If the weight factors combination favor the carbon oxides conversion (ratio *w(1)/w(2)* lower than 0.01), the optimization results given in Table 4 are determined. It is worth to mention that this optimal solution provides relatively high carbon oxides conversions (25.9 % for DC and 38.9 % for IC), but relatively low methanol productivity, due to the diminishing of the feed flow rate. The temperatures at the inlet of each catalyst bed are lowered by the optimization algorithm in order to increase the equilibrium conversion.

Given the results, it can be emphasized that in respect with the *w(1)/w(2)* ratio, optimal solutions providing high mass feed flowrates and low conversions, or low flowrates with high conversions, can be determined. Depending of the methanol synthesis process priorities, different weighting factors combinations can be used in order to favor the global conversion of carbon oxides irrespective the feed flow rate, or the reactor productivity, expressed as mass feed flowrate (irrespective the global conversion).

Table 4

Optimization results for low w(1)/w(2) ratio

Direct cooling		Indirect cooling	
Feed temperature on the first catalyst bed, K	522	Feed temperature on the first catalyst bed, K	480
Total feed flowrate, kg s^{-1}	74.1	Total feed flowrate, kg s^{-1}	40
Catalyst bed lengths, m	Z_1=1.34 Z_2=2.45 Z_3=2.91 Z_4=3.3	Catalyst bed lengths, m	Z_1=1.99 Z_2=2.11 Z_3=2.87 Z_4=3.03
Feed flowrate fractions	fb_1=0.261 fb_2=0.184 fb_3=0.248 fb_4=0.307	Temperatures between catalyst beds, K	T_1=480 T_2=484.4 T_3 =480.8 T_4 = 481.2
Methanol flowrate, D_{MeOH}, kg s^{-1}	14.66	Methanol flowrate, D_{MeOH}, kg s^{-1}	11.84
Carbon oxides conversion, X_{CO+CO2}, %	25.9	Carbon oxides conversion, X_{CO+CO2}, %	38.9

Optimization problem 2 (restrictions on the feed temperature on the catalyst beds)

In order to limit the deactivation of the catalyst, Bartholomew and Farrauto recommends that the temperature inside the catalyst bed to be kept below 250 ºC [15]. The decrease of temperature inside the catalyst bed can be achieved by lowering the inlet temperature of the reaction mixture. An optimization study was performed imposing a feed temperature range between $300 < T < 500\ K$. The weighting factors were equal to 1. The optimization results are presented in

Table 5.

Table 5.

Optimization results for problem 2

Direct cooling		Indirect cooling	
Feed temperature on the first catalyst bed, K	500	Feed temperature on the first catalyst bed, K	500
Total feed flowrate, kg s^{-1}	197	Total feed flowrate, kg s^{-1}	168
Catalyst bed lengths, m	Z_1=2.40 Z_2=3.65 Z_3=3.95 Z_4=0	Catalyst bed lengths, m	Z_1=3.1 Z_2=3.44 Z_3=3.46 Z_4=0

Feed flowrate fractions	fb_1=0.646 fb_2=0.291 fb_3=0.063 fb_4=0	Temperatures between catalyst beds, K	T_1=500 T_2=500 T_3=500 T_4=500
Methanol flowrate, D_{MeOH}, kg s^{-1}	33.4	Methanol flowrate, D_{MeOH}, kg s^{-1}	31.8
Carbon oxides conversion, X_{CO+CO2}, %	22.2	Carbon oxides conversion, X_{CO+CO2}, %	24.8

The results presented in *Table 5* show that, by restricting the inlet temperature on each catalyst bed, the most efficient technological solution is the direct cooling. The carbon oxides conversion is 22.2 % for DC in comparison with 24.8 % for IC, but the methanol flowrate is slightly higher (33.4 vs 31.8 kg/s). It is worth to be mentioned that both technologies require the distribution of the catalyst only in 3 beds, with the amount of catalyst increasing from first to last bed (*Table 5*). The conversion-temperature diagrams, the profiles of temperature and methanol formation rates in respect with reactor length, as well as the evolutions of methanol flowrate in respect with the residence time in the reactor are given in *Fig. 5*-7.

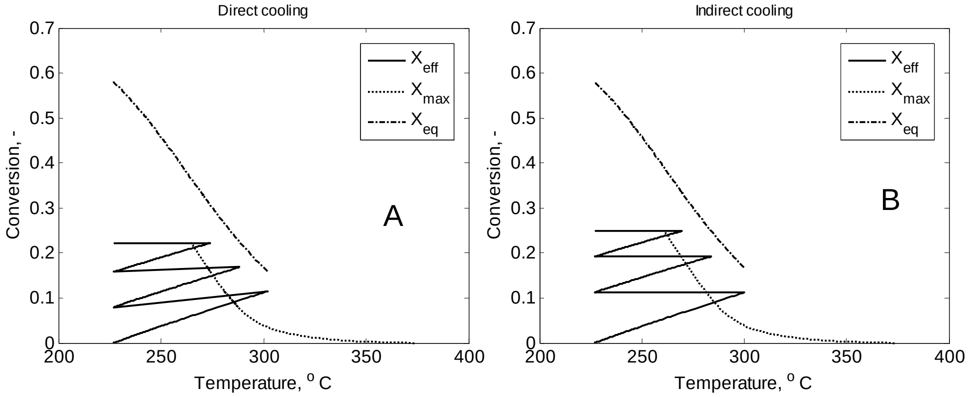

Fig. 5. Conversion-temperature diagrams for direct (A) and indirect (B) cooling technologies (Problem 2)

In Fig. 7A there are evidenced evolutions with respect to the residence time in the catalyst beds for the methanol formation rates for DC and IC reactors. It is worth to be mentioned that, on the first catalyst bed, the methanol formation rates are relatively similar. Even if the optimal lengths are different, it is acquired a similar residence time of the reaction mixture. This is also emphasized in Fig. 7*A*, where the higher methanol formation rates in DC reactor observed for beds 2 and 3 can be explained by the modification in the composition at the bed inlet for DC reactor, that will lead to a departure from the equilibrium, and consequently, higher methanol formation rates.

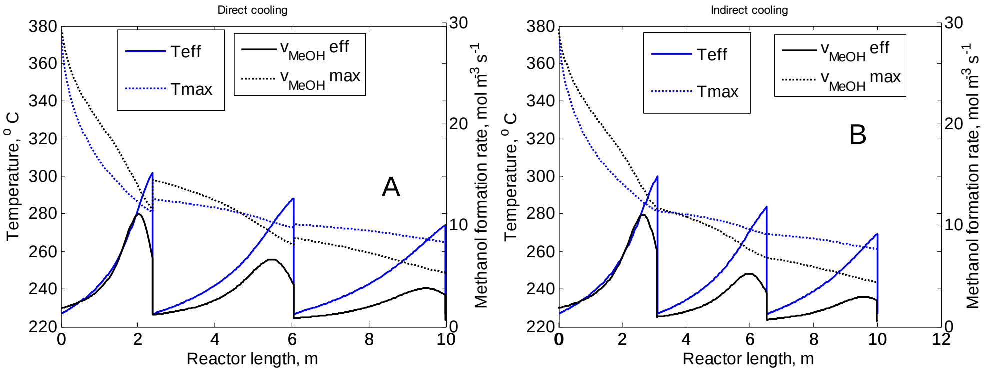

Fig. 6. Temperature and methanol formation rate profiles in the methanol synthesis reactor (Problem 2)

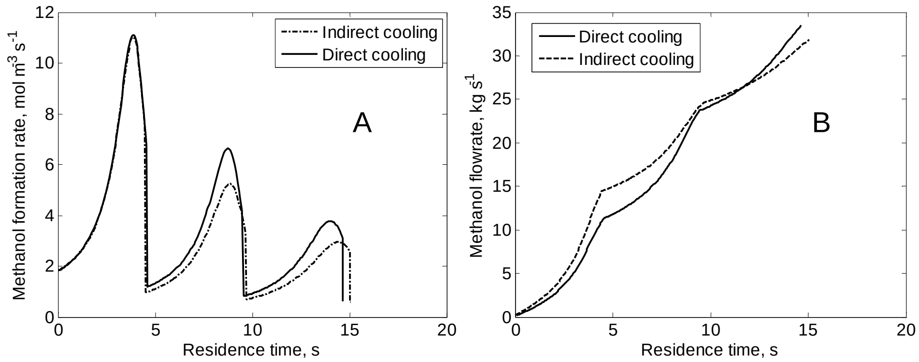

Fig. 7. Comparison of methanol formation rate and methanol flowrate for DC and IC approaches (Problem 2)

6. Conclusions

In the present study a multi-bed methanol synthesis reactor consisting in a series of adiabatic catalyst beds was optimized using a combination of genetic algorithms – pattern search numerical techniques in order to maximize both the methanol production and the carbon oxides global conversion. The direct cooling and indirect cooling technologies were considered and compared. Two optimization problems were formulated and solved for each operating technique, one considering no temperature restrictions and the second taking into account the temperature limitation at the inlet of each catalyst bed. The results of the first optimization problem shown the IC as the most efficient technology, due to the highest temperatures at the bed inlet correlated with the shorter residence time that will favor the methanol formation reaction. The results obtained for second optimization problem shows the DC reactor as the most efficient, due to the composition effect that will boost the methanol formation rate on the last catalyst bed.

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