

PREDICTION OF THE REACTION CHAMBER EFFICIENCY IN THE PROCESS OF SYNTHESIS OF ACETYLENE FROM METHANE¹⁾

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A model allowing to predict the reaction chamber thermic efficiency value has been elaborated. The quality of heat exchanged across the chamber walls is determined by the average temperature of the reaction mixture in the chamber and the construction parameters. The proposed iteration method of calculations allows to define the mutual influences: the heat chamber efficiency and the methane conversion degree.

ПРОГНОЗ КИД РЕАКЦИОННОЙ КАМЕРЫ В ПРОЦЕССЕ СИНТЕЗА АЦЕТИЛЕНА ИЗ МЕТАНА

В работе описана модель, на основе которой можно определить прогноз кид реакционной камеры. Обмен тепла через стенку камеры зависит как от конструкции камеры, так и от средней температуры реакционной смеси. Предложенный итерационный метод расчета позволяет определить взаимное влияние кид камеры и степени конверсии метана.

1. INTRODUCTION

The acetylene synthesis from methane is one of the processes extensively studied by us. One may attempt to generalize the description of this process on the basis of experimental data. A fundamental difficulty in elaborating such a description is to determine the relationship between the value of heat exchanged across the reaction chamber wall and the conversion degree of methane.

A precise mathematical description of heat exchange across the wall is very complex and is not feasible at present. We have obtained satisfactory results by using an approximate description of heat exchange in the studied system and a simplified model of the chemical process.

¹⁾ Contribution presented at the 3rd Symposium on Elementary Processes and Chemical Reactions in Low Temperature Plasma in Krfáovo, September 22—26, 1980.

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II. METHODS

a) An approximate description of heat exchange in the reaction chamber of a chemical plasma reactor.

From the point of view of heat exchange the reaction chamber may be considered as a tube heat exchanger where the hot gas flowing through the chamber is the heating medium and the cooling medium is water. We have assumed that the heat amount exchanged across the chamber wall of a given thickness is given for a stationary process by the formula:

$$Q = KF(T_q - T_r), \quad (1)$$

where K is the overall heat transfer coefficient, T_q the temperature of gaseous medium (reaction mixture), T_r the temperature of cooling medium (water), F the area of heat exchange.

The reaction chamber of our reactor has been intensively cooled; the water temperature increased in this process so little that it can be assumed to be constant.

The above relationship permits to determine the amount of energy exchanged across the wall at a constant gas temperature. If an endothermal process occurs in the chamber the gas temperature decreases rapidly; it has been found that temperature decreases linearly along the chamber [1]. It seems justified to use the mean gas temperature in the calculation of the exchanged heat amount instead of the local one. It also applies for the case where no chemical process takes place in the chamber and the temperature decrease is then due to the energy transfer across the wall.

Taking into account the above considerations one obtains the relationship (2):

$$Q = KF(T_{in} + T_{out})0.5 - const = aT + b, \quad (2)$$

where T_{in} is the gas temperature at the reaction chamber inlet, T_{out} the gas temperature at the reaction chamber outlet, $a = KF$, $b = -KT$ const.

The chamber efficiency η [2] is defined by the formula (3):

$$\eta = \frac{E_{pl} - Q}{E_{pl}}, \quad (3)$$

where E_{pl} is the plasma jet energy at the inlet of the reaction chamber.

The above definition implies that at a constant T the chamber efficiency increases with the energy fed to the reactor.

The temperature T_{in} is related with the amount of fed energy and with the plasma gas (argon) flow rate, G , as well as with the methane flow rate, M . It can be calculated by solving the equation (4):

$$E_{pl} = G \int_{T_0}^{T_{in}} c_{p,Ar} dT + M \int_{T_0}^{T_{in}} c_{p,CH_4} dT \quad (4)$$

where T_0 is the reference temperature, c_p the specific heat capacity at constant pressure.

The final temperature T_{out} can be calculated from the energy balance and from the reaction stoichiometry (5):

$$E_{pl} - Q = 0.5MU \int_{T_0}^{T_{out}} c_{p,CH_4} dT + 1.5MU \int_{T_0}^{T_{out}} c_{p,H_2} dT + (1-U)M \int_{T_0}^{T_{out}} c_{p,Ar} dT + G \int_{T_0}^{T_{out}} c_{p,N} dT + 0.5MU\Delta H_0, \quad (5)$$

where U is the methane-to-acetylene conversion degree, ΔH_0 the heat effect of the reaction $CH_4 - 1/2 C_2H_2 + 3/2 H_2$ at the temperature T_0 . The relationship (5) is correct only in the case where no side reactions take place.

b) A simplified model of the chemical process is as follows.

We have assumed that the only chemical reaction occurring in the studied process is acetylene formation and that equilibrium concentrations are attained and that the equilibrium temperature is that of the outlet gas. Under such conditions the methane-to-acetylene conversion degree is given by

$$U = \frac{\sqrt{x^2 + 4(1 + 0.75\sqrt{3/K_p})(1+x)} - x}{2(1 + 0.75\sqrt{3/K_p})}, \quad (6)$$

where $x = G/M$, $\ln K_p = -\Delta G/RT$.

c) Calculation algorithm

The system is characterized by the magnitudes G , M , E_{pl} and the coefficients a and b . The equation system (2), (4), (5), and (6) has been solved by the iterative method:

- calculation of the temperature T_{in} ,
- calculation of the conversion degree of methane assuming $Q = 0$ and $T_{in} = T_{out}$,
- calculation of temperature T_{out} for the calculated conversion degree,
- calculation of heat loss of the reaction chamber,
- calculation of the conversion degree of methane for the calculated Q and T_{in} values, and so on.

Iteration has been continued until the difference between consecutive Q values has been lower than the assumed accuracy.

The coefficients a and b were determined earlier in an experiment where the argon and nitrogen plasma passed through the reaction chamber.

III. RESULTS

We have compared 163 experimental and calculated results. The linear correlation coefficient of the dependence $U_{exp} = f(U_{calc})$ has been 0.877 and the value for $Q_{exp} = f(Q_{calc})$ 0.911.

IV. DISCUSSION

The calculation results indicate that the above presented simplifications are acceptable. Completion of the calculations with an algorithm taking into account acetylene decomposition during the process of freezing can serve as a base of process optimization.

REFERENCES

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Received October 20th, 1980