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HEAT AND MASS TRANSFER IN FLOWING GAS IN PRESENCE OF LIQUID FILM

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ABSTRACT

In the present work correlation dependence of critical Reynolds number of laminar-turbulent transition is presented for a gas flow in dry or wetting pipes. The new approach to the given problem dealing with quasi-chemical cluster model of a gas developed by authors is offered.

INTRODUCTION

In chemical manufacture, at the process of fuel and oxidizer mixing in aviation engines, at the process of sea water desalination and in variety of other manufactures the irrigated channel with a liquid film flowing down on it at a counter stream of a gas is used. Depending on hydrodynamic and physical parameters of a liquid and gas on a surface of a liquid film waves are formed, and in the gas flow may take place the laminar-turbulent transition [1]. Correlation dependence between value of critical Reynolds number of laminar-turbulent transition and properties of a liquid film (average speed v_l , viscosity coefficient μ_l and surface tension coefficient σ) has been found [2]:

$$Re_{cf} = \left[\frac{86}{0.11 + 0.9 \left(\frac{v_l \mu_l}{\sigma} \right)^{2/3}} \right]^{1.19}$$
 (1)

Usually Reynolds number is considered as the relation of inertial and viscous forces, and critical Reynolds number of laminar-turbulent transition is defined in experiment on sharp increase in drag coefficient in turbulent flow that allows to define critical Reynolds number reliably.

In work [3] other (statistical) treatment of Reynolds number has been offered. Reynolds number was interpreted as the relation of phase volumes of macroscopical and microscopic movements of molecules that has allowed to obtain an estimation of dependence of Reynolds number on the second virial coefficient of investigated gas.

The dependence obtained has been checked up for Hagen-Poiseuille flow in a thin pipe. Correlation of critical Reynolds number of laminar-turbulent transition in Hagen-Poiseuille flow with the second virial coefficient B(T) of considered gas (He, Ne, Ar, Kr, Xe, N_2 , CO_2 , SF_6) at gas temperatures close to T=300K and pressure from 1atm to 2atm has been found. The correlation dependence $Re_c(B(T))$ found in experiments [3] deserves more detailed discussion.

In quasi-chemical cluster model (QCCM) of a real gas developed by authors [4] a real gas is consider in a first approximation as an ideal mixture of monomers(A_1) and clusters (A_n - dimers (n=2), trimers (n=3) and etc.). We suppose that in this gas mixture reactions of cluster formation and destruction are taking place according to the following elementary processes:

$$A_n + A_1 + M \iff A_{n+1} + M \tag{2}$$

Having received on the basis of this QCCM theory the expressions for density and viscosity of real gas, it is possible to obtain the following expression for relation between Reynolds number of ideal gas and Reynolds number of real gas:

$$Re = Re_{real} W_m (\mu_{md} / \mu_m) (f_m + f_d)$$
 (3)

Here W_m - molar mass of a monomer, μ_m - dynamic viscosity coefficient of the gas made from monomers, μ_{md} -dynamic viscosity coefficient of the gas representing an equilibrium mixture of monomers and dimers, f_m , f_d -mol-mass fractions of monomers and dimers accordingly. Equilibrium concentration f_m , f_d of an ideal gas mixture

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of monomers and dimers are defined according to equilibrium constant of reaction of dimerization $K_c(T)$ at given temperature and pressure.

In work [5] expression of the second virial coefficient B(T) is given as the sum of three terms:

$$B = B_f + B_b + B_m \,, \tag{4}$$

where B_f - the contribution of the excluded volume of atoms or gas molecules, $B_b = -K_{cb}(T)$ - the contribution due to bond dimers, $B_m = -K_{cm}(T)$ - the contribution due to metastable dimers (rotary pairs), here K_{cb} and K_{cm} - equilibrium constans of dimerization reaction with formation of bond and metastable dimers, accordingly.

TRENDS AND RESULTS

On **Figure1** dependences of B_f and $B_b + B_m$ coefficients bringing the greatest contribution to the second virial coefficient B(T) on temperature for investigated in work [3] gases are presented.

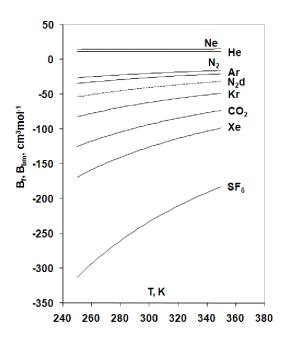


Figure 1. Dependence of components of the second virial coefficient B_f and $B_b + B_m$ on temperature T for various gases.

It is shown (**Figure 1**) that the greatest contribution to the second virial coefficient B(T) in wide range of temperatures B_f (the excluded volume) makes only for atoms Ne and He. For all other investigated in work [3] atoms and molecules in the specified range of temperatures the greatest contribution make bond and metastable dimers. We will notice also that for molecular gases, the more the

molecule contains vibrational degrees of freedom, the more contribution in B(T) make bond and metastable clusters, and the contribution of the excluded volume becomes ever less. Examples of such gases are also steams of a liquid of a film in devices of chemical technology.

In **Figure 2** dependence of Re/Re_{real} on equilibrium constant of dimerization reaction K_c at pressure P=101325Pa and temperature T=300K according to the equation (2) (black small squares, a continuous line – linear correlation) is given. Except for helium for which, at given pressure and temperature, dimerization process is insignificant ($K_c \square 0$), for all other considered gases K_c makes the main contribution to the second virial coefficient. The equation of linear correlation is as follows:

$$Re/Re_{real} = -100.19K_c + 0.9988 \tag{5}$$

The factor of reliability of linear correlation $R^2 = 0.998$ is close to one. This circumstance suggests - to receive dependence of critical Reynolds number of laminar-turbulent transition on equilibrium constant of dimerization $K_c \square - (B_b + B_m)$ for Hagen-Poiseuille flow in a thin pipe (Re_c) and for gas flow in irrigated tubes (see eq.(1)).

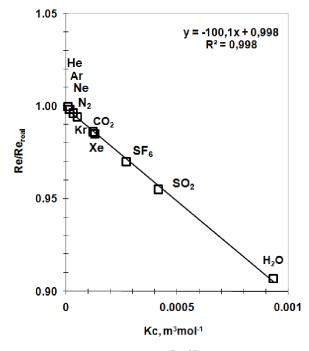


Figure 2. Dependence of Re/Re $_{real}$ on equilibrium constant of dimerization reaction K_c for various noble and molecular gases at pressure P=101325Pa and temperature T=300K.

On **Figure 3** correlation dependence of Re_{cf} on $B_{bm} = B_b + B_m$ size (for the specified substances $B \approx B_{bm}$) in the form of white triangles for variety of substances is given.

As can be seen from Figure 3 the critical Reynolds numbers Re_c , Re_{cf} for two considered types of flow (in thin glass pipes and in irrigated channels) are described approximately by identical parabolic dependences:

$$Re_c = 0.0048B_{bm}^2 + 5.0837B_{bm} + 3447.4$$
 (6)

with factor of statistical reliability $R^2 = 0.9836$ (in thin glass pipes) and

$$Re_{cf} = 10^{-5} B_{bm}^2 + 0.29 B_{bm} + 2243.9,$$
 (7)

with factor of statistical reliability $R^2 = 0.8606$ (in irrigated channels).

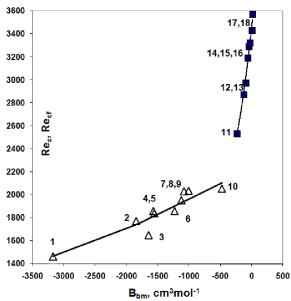


Figure 3. Correlation dependences of Re_c and Re_{cf} on B_{bm} for a number of substances (1- C_2H_5OH , 2- CH_4O , 3- CCl_4 , 4-1,2 C_2H_4Cl , 5- C_2H_6 ,6-1,1 C_2H_4Cl , 7- D_2O ,8- C_3H_6O , 9- H_2O ,10- N_2H_4 ,11- SF_6 ,12-Xe,13- CO_2 ,14-Kr,15- N_2 ,16-Ar,17-He,18-Ne); Δ - processing of results of work [2], ■ - processing of results of work [3]).

These correlation dependences, probably, point out the source of initial disturbances of flow of finite value, because forming and decaying clusters are possessing significant value of energy stored in vibrational degrees of freedom.

In **Table 1** frequencies of intermolecular vibrational modes of complex $Al - H_2O$ and water dimmer $(H_2O)_2$, and also dissociation energy E_{dis} of these molecular association are given. These results are obtained by authors with help of *ab initio* quantum chemical code GAMESS [6]. The complex $Al - H_2O$ serves as model for an estimation of a thermal stream at formation of the adsorbed molecule of water on a surface of a firm body (atom Al is considered motionless).

Table 1

	i	1	2	3	4	5	6	E_{dis} , c
$Al-H_2O$	ω_{i}	108.54	163.45	331.06				2559.9
$(H_2O)_2$	ω_{i}	121.80	153.00	163.10	183.20	354.80	619.60	1003.61

It is shown (**Table 1**) that at the considered temperature all specified vibrational modes are exited.

It is known [1] that one of sources of waves in a film can be chemical reactions on its surface. Evaporation of a film and substance condensation on a film also can lead to formation of waves on a film [1]. At water irrigation of the vertical channel in the presence of ascending stream of air formation and destruction of water dimers can be considered as elementary reaction on surfaces of the liquid film.

In work [1] it is shown that the relative amplitude of waves on a film surface is the key factor influencing critical Reynolds number of laminar-turbulent transition in the gas. Use of the above-stated results of quantum-chemical calculations has allowed us to estimate the contribution of water dimers formation on the film in change of relative amplitude of waves on a liquid surface.

For numerical calculations the input parameters are as follows: $\mathrm{Re}_0=60$, T=293.15K, $Ga_0=44$ $\Gamma_1=0.2$. The account of dimerization leads to change in values of Reynolds number Re on 1.5%, Galileo number Ga, on 1.2%, parameter Γ_1 on 0.4%, relative amplitude of a wave on a surface of a liquid film α on 0.4%. Thus it is shown that for flow in irrigated channels possible influence of clusters on process of laminar-turbulent transition may be not only "energetical" (a thermal source of disturbances in flow), but also "geometrical" ("roughness" growth in this case liquid "wall"). According to experimental criterion of Calo [4] at growth of a relative dimmer fraction above 5 % there is a rapid growth of clusters of greater sizes that will lead to strengthening of the effects considered.

CONCLUSIONS

1. In the present work on the basis of quasi-chemical cluster model of gas developed by authors correlation dependence

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- of Re/Re_{real} on equilibrium constant of reaction of dimerization is obtained.
- 2. Correlation dependences of critical Reynolds number of laminar-turbulent transition on equilibrium constant of dimerization are found for gas flow in dry and irrigated pipes.
- 3. The given work pays attention to a role of clusters of bearing gas in formation and stability of a liquid film on surfaces of the solid body, influencing on turbulization of gas flow that essential impact on processes of inter phase heat and mass transfer.

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