# NUMERICAL INVESTIGATION OF HEAT-AND-MASS TRANSFER IN THERMOCHEMICAL REACTOR

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# MOTIVATION

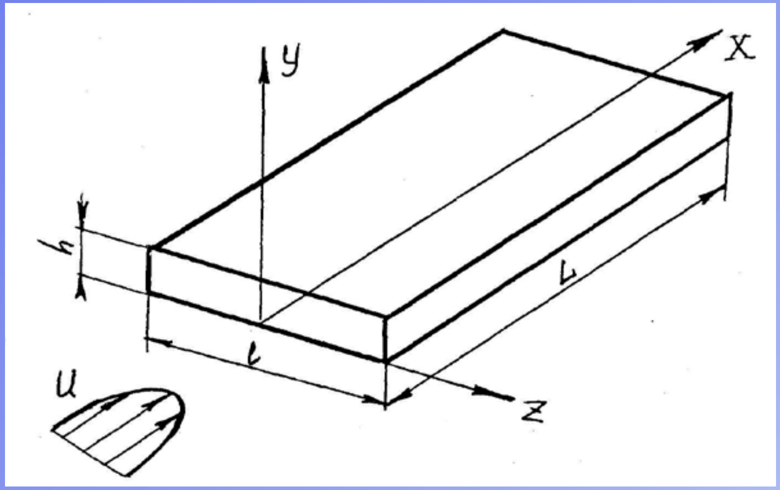
Usage of chemically reacting gas as a coolant is promising for two reasons:

- the effective heat capacity of the gas increases considerably on account of the heat effect of the endothermic reaction.
- the heat transfer process in the chemically reacting gas incorporates common convective heat transfer with diffusive transmission of the latent heat of the reaction.

Therefore, when both types of heat transfer act in parallel at the boundary layer, the overall heat transfer at the cooled wall increases considerably.

The computer simulation of heat-and-mass transfer in the thermochemical reactor (TCR) is considered in this work.

# METHOD OF TCR COMPUTATION



***h = 3 мм, L = 1000 мм, l = 1000 мм***

Planar TCR represents a parallelepiped with its catalytic upper wall being heated ( $T\big|_{y=h} = const$ ) while lower wall is heat-insulated ( $\left.\frac{\partial T}{\partial y}\right|_{y=0} = 0$ ). Uniformly heated steam-methane mixture with the known parameters of pressure, temperature and mixture consumption is supplied to TCR inlet.

In the performance of a task the following conditions are used:

1. Approximation of “slender” channel (h << l<L)
2. “quasi-laminar” approximation ( $\mu_{eff} = \mu + \mu_T$ )
3. Chemical reaction is of equilibrium character $\tau_{chem} << \tau_{gas}$

$CH_4 + H_2O \leftrightarrow 3H_2 + CO$

$CO + H_2O \leftrightarrow H_2 + CO_2$

# MATHEMATICAL MODEL

Differential equation system in partial derivatives describing viscous gas mixture flow when chemical reactions in TCR occur is of parabolic type and it was solved by highly economic march method.

$$\frac{\partial}{\partial x}(y^{\alpha}\rho u)+\frac{\partial}{\partial y}(y^{\alpha}\rho v)=0,$$

$$\rho u\frac{\partial u}{\partial x}+\rho v\frac{\partial u}{\partial y}=-\frac{1}{\gamma M_0^2}\frac{dp}{dx}+\frac{1}{\mathrm{Re}_y\,\varepsilon\cdot y^{\alpha}}\frac{\partial}{\partial y}(y^{\alpha}\tau_{\Sigma}),$$

$$\rho u\frac{\partial c_i}{\partial x}+\rho v\frac{\partial c_i}{\partial y}=\sum_{S=1}^{N_k}Da_S w_{i,S}-\frac{1}{\mathrm{Re}_y\,Sc\varepsilon\, y^{\alpha}}\frac{\partial}{\partial y}(y^{\alpha}J_{i\Sigma}),$$

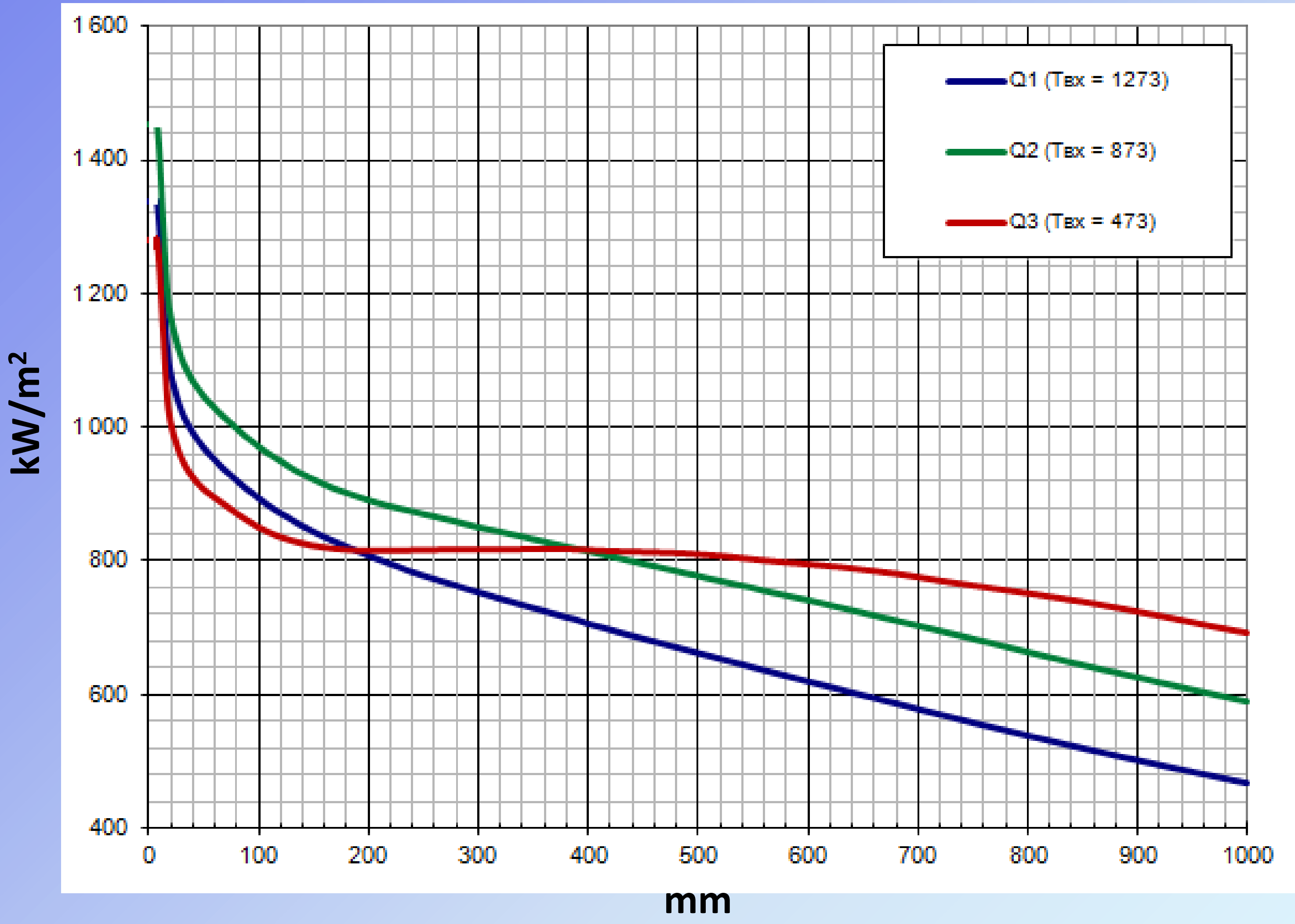
$$i=1-N_k,$$

$$\rho u\frac{\partial H}{\partial x}+\rho v\frac{\partial H}{\partial y}=-\frac{1}{\Pr y^{\alpha}}\frac{\partial}{\partial y}(y^{\alpha}q_{\Sigma})+\frac{M_0^2(\gamma-1)}{y^{\alpha}}\frac{\partial}{\partial y}(y^{\alpha}u\tau_{\Sigma}),$$

$$\frac{\partial p}{\partial y}=0,\qquad p=\frac{\rho T}{m},\quad \frac{1}{m}=\sum_{i=1}^{N_k}\frac{c_i}{m_i},$$

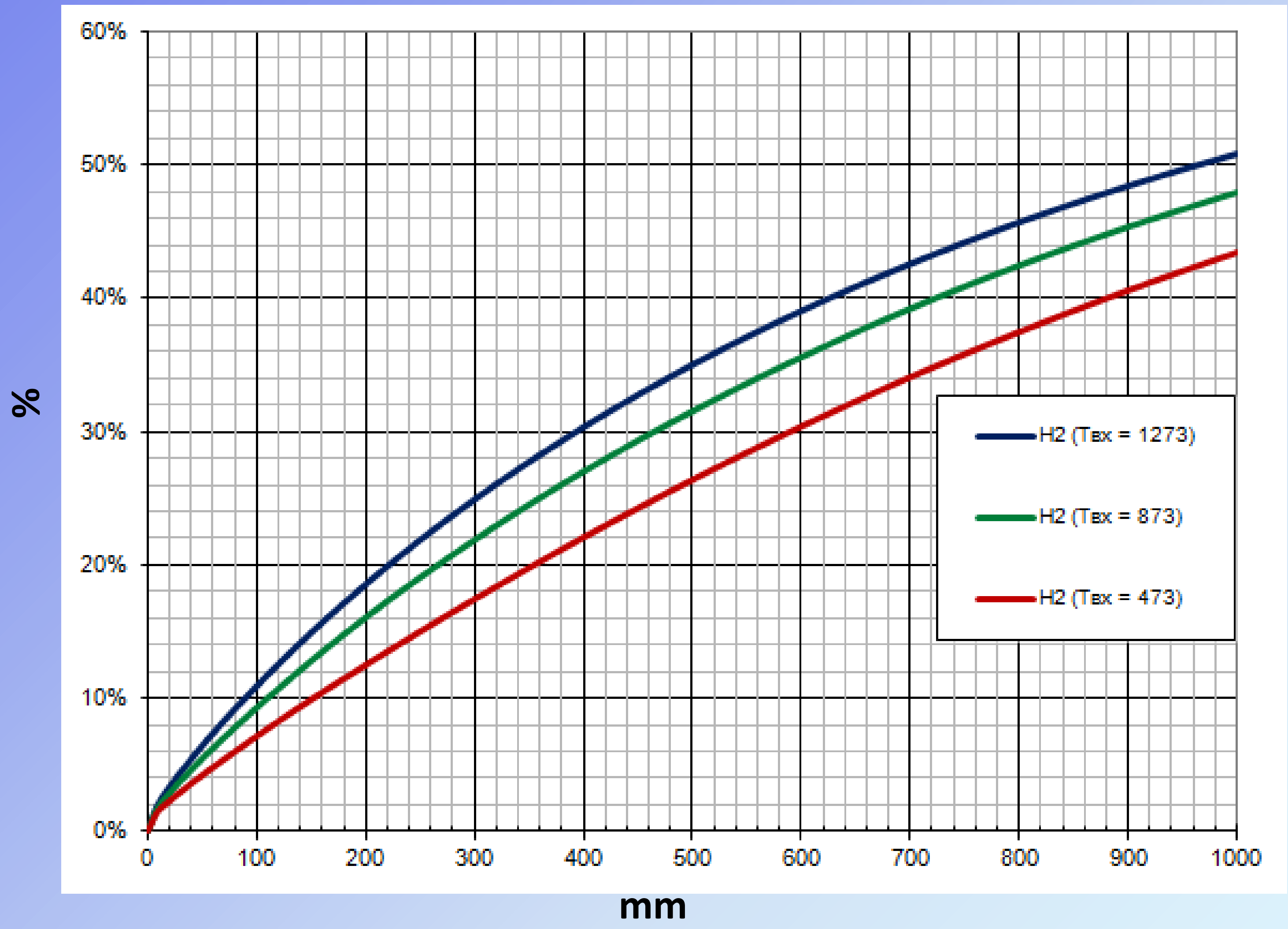
# INFLUENCE OF INLET TEMPERATURE ON THE HEAT FLOW RATE

P = 5 atm; $T_w$ = 1273 K; g = 0,2 kg/sec



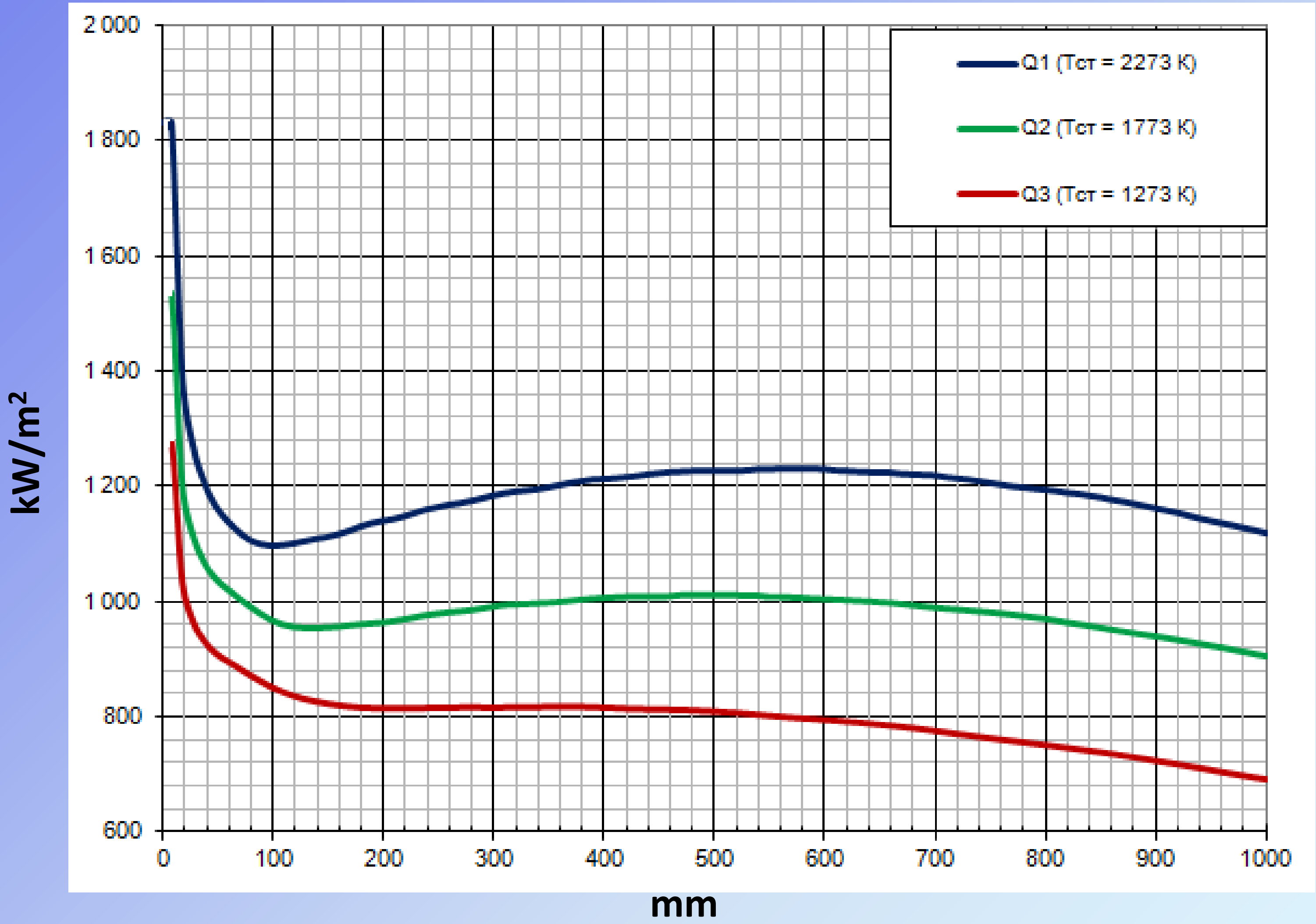
# INFLUENCE OF INLET TEMPERATURE ON THE MOLAR CONCENTRATION OF $H_2$

P = 5 atm; $T_w$ = 1273 K; g = 0,2 kg/sec



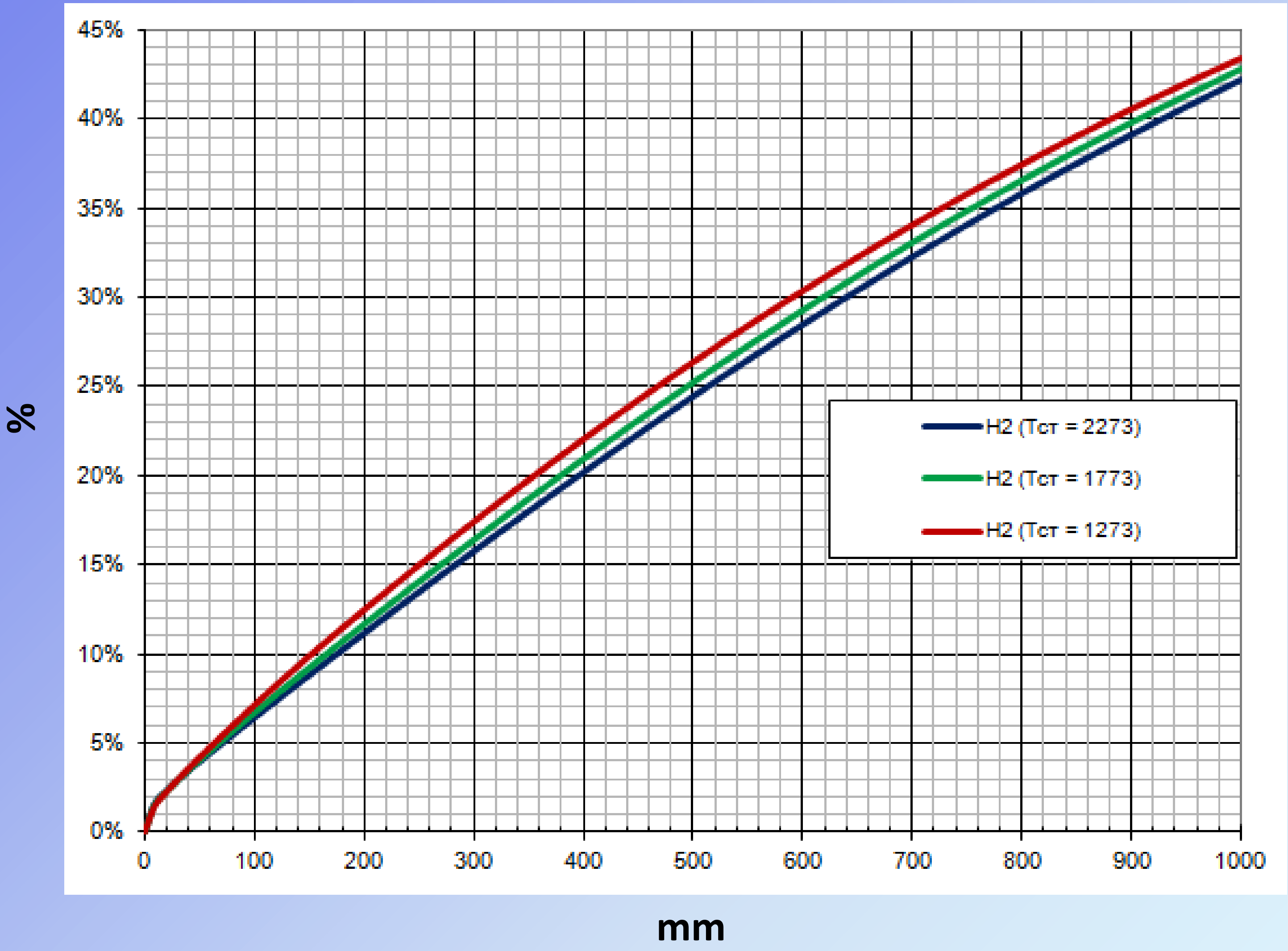
# INFLUENCE OF TEMPERATURE AT TCR' WALL ON THE HEAT FLOW RATE

P = 5 atm; $T_{in}$ = 473 К; g = 0,2 kg/sec



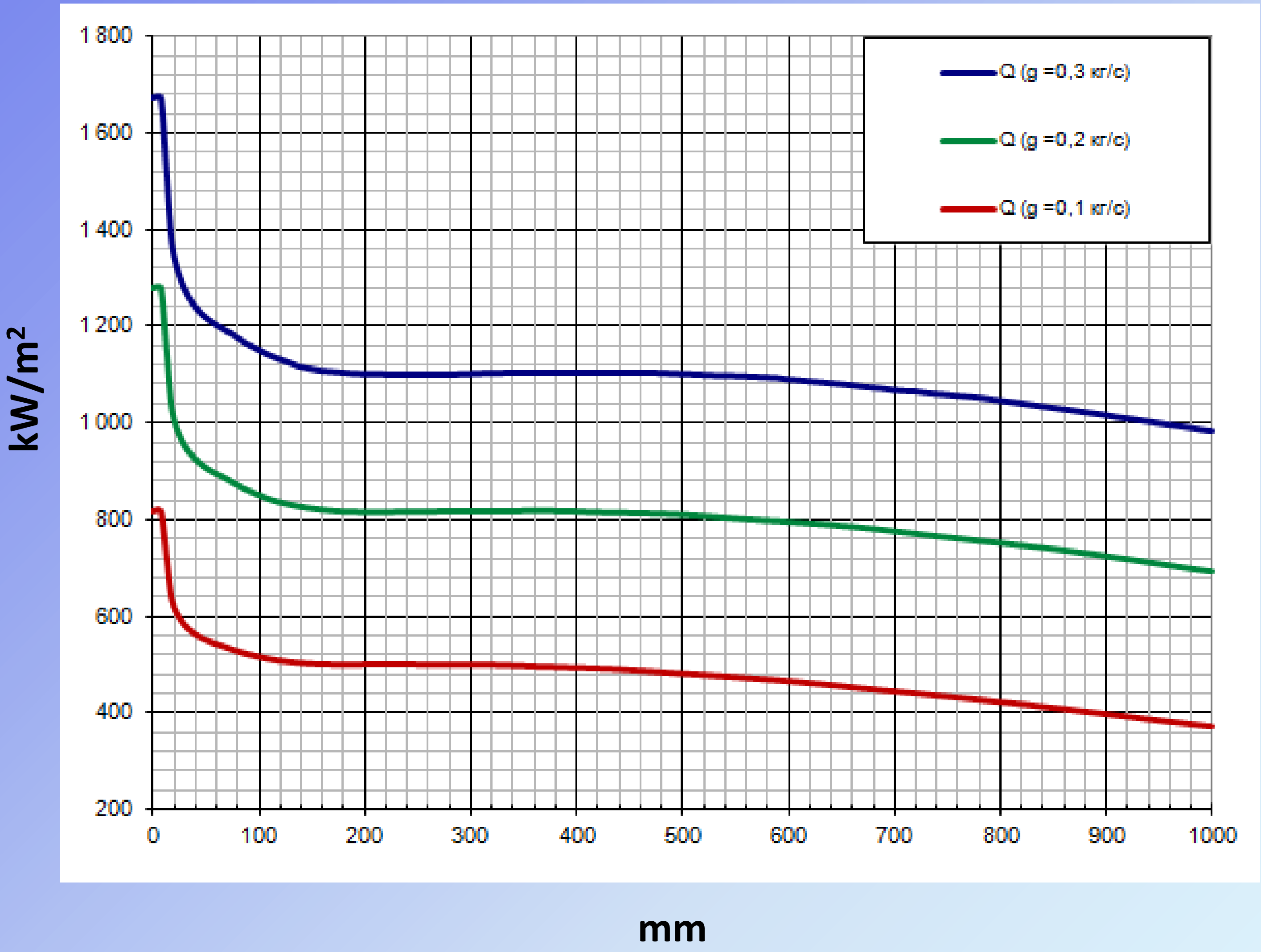
# INFLUENCE OF TEMPERATURE AT TCR' WALL ON THE MOLAR CONCENTRATION OF $H_2$

P = 5 atm; $T_{in}$ = 473 K; g = 0,2 kg/sec



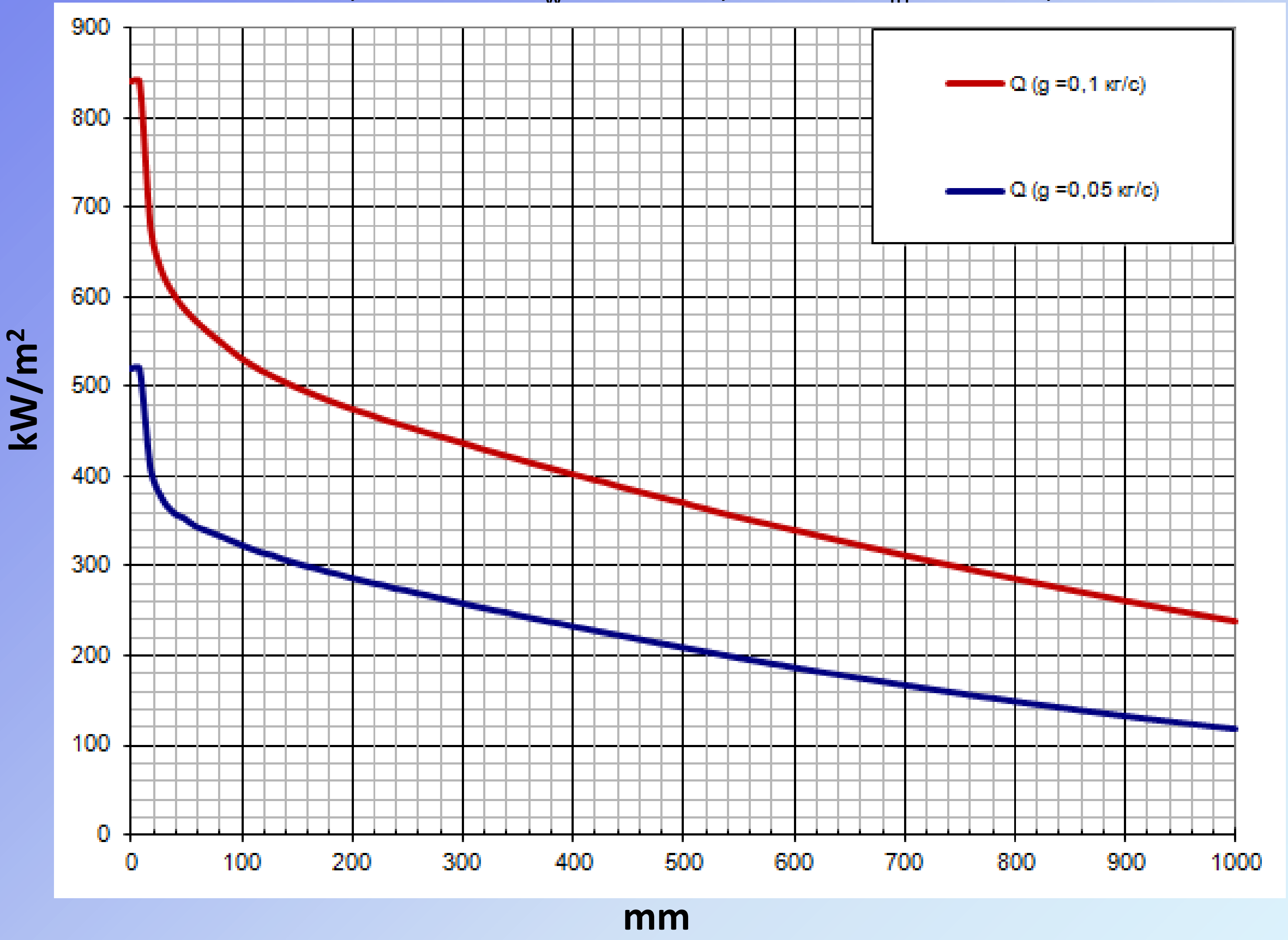
# INFLUENCE OF MIXTURE CONSUMPTION ON THE HEAT FLOW RATE

P = 5 atm; $T_w$ = 1273 К; $T_{in}$ = 473 К;



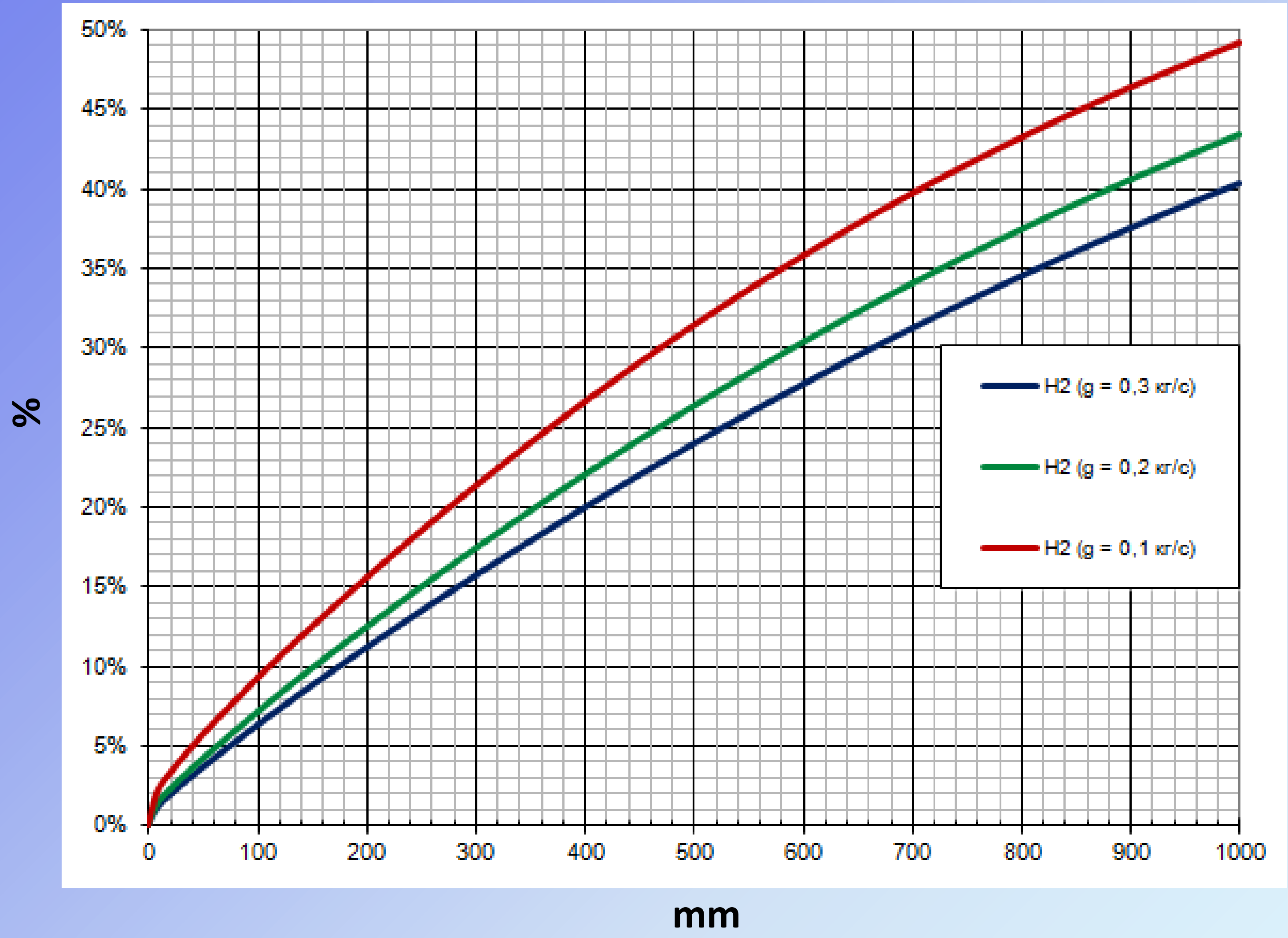
# INFLUENCE OF MIXTURE CONSUMPTION ON THE HEAT FLOW RATE

P = 5 atm; $T_w$ = 1273 К; $T_{in}$ = 473 К;



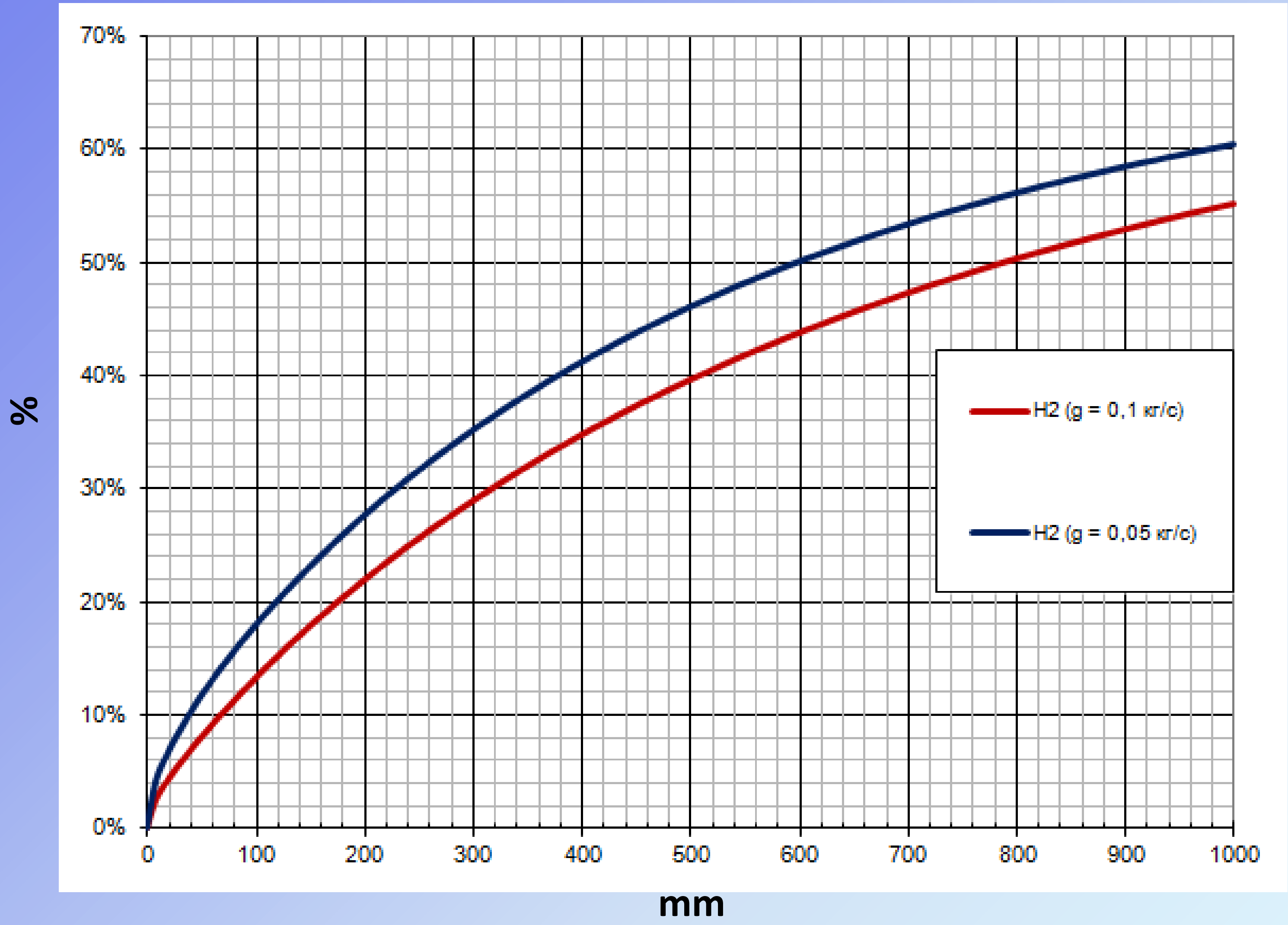
# INFLUENCE OF MIXTURE CONSUMPTION ON THE MOLAR CONCENTRATION OF $H_2$

$P = 5$ atm; $T_w = 1273$ K; $T_{in} = 473$ K;



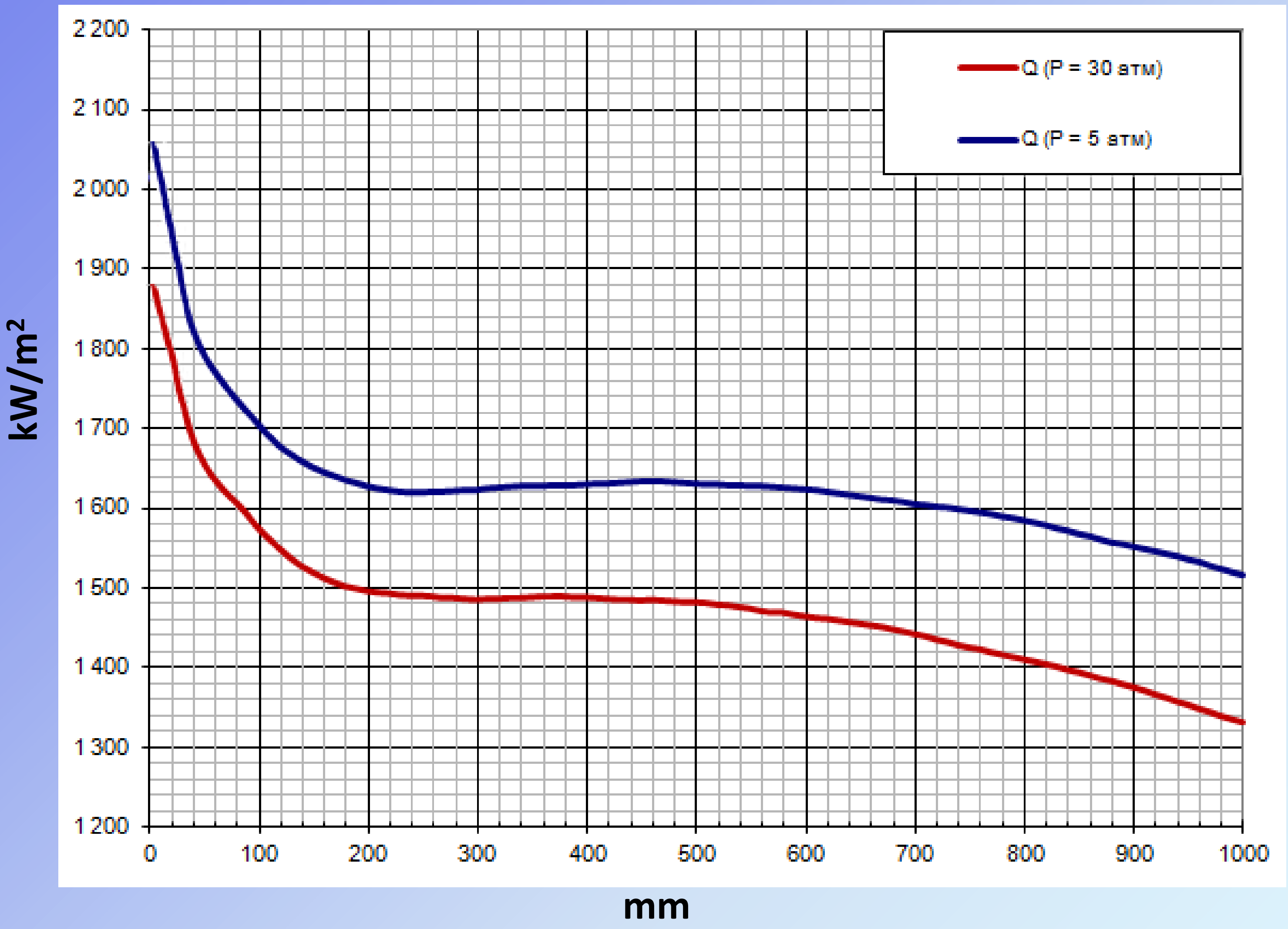
# INFLUENCE OF MIXTURE CONSUMPTION ON THE MOLAR CONCENTRATION OF $H_2$

P = 5 atm; $T_w$ = 1273 К; $T_{in}$ = 473 К;



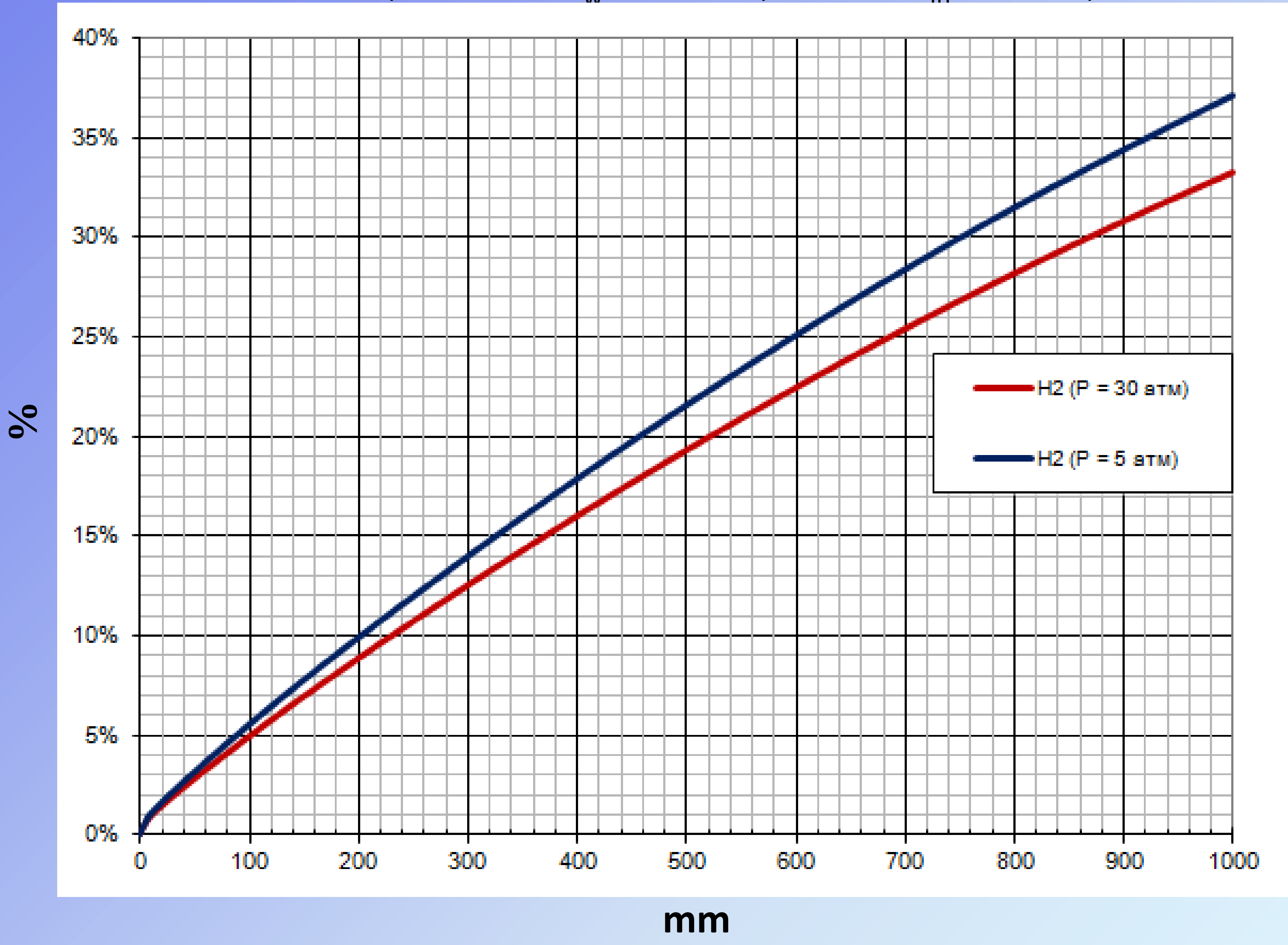
# INFLUENCE OF PRESSURE ON THE HEAT FLOW RATE

$T_w$ = 1273 K; $T_{in}$ = 473 K; g = 0,5 kg/sec



# INFLUENCE OF PRESSURE ON THE MOLAR CONCENTRATION OF $H_2$

P = 5 atm; $T_w$ = 1273 К; $T_{in}$ = 473 К;



# CONCLUSION

Performed computer simulations of equilibrium flows allowed:

- ➢ to give an upper-bound estimate of the recoverable (utilizable) heat flow rate and concentrations of hydrogen H2 and carbon monoxide CO derived from the thermochemical conversion of hydrocarbon fuel;
- ➢ to define the basic relationship between changes in the input parameters (inlet temperature, temperature at TCR’ wall, mixture consumption, pressure) and the molar concentration of hydrogen and heat flow rate obtained by calculation.

The results of computer simulation are in good agreement with the results of experimental research.