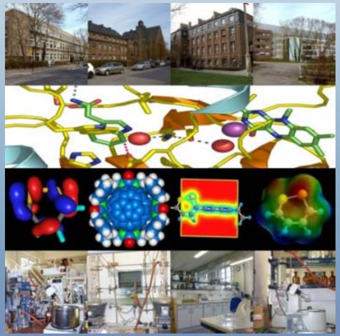
National Technical University of Ukraine "KPI"

"Kyiv Polytechnic Institute"

Cybernetics of Chemical Technology Processes Department

# DEVELOPMENT OF TECHNOLOGICAL BASES OF USING ZEOLITES FOR DENITRATION OF EXHAUST GASES



Institut für Technische Chemie

Technisch Universität Dresden

TECHNISCHE UNIVERSITÄT DRESDEN

# Framework Structure

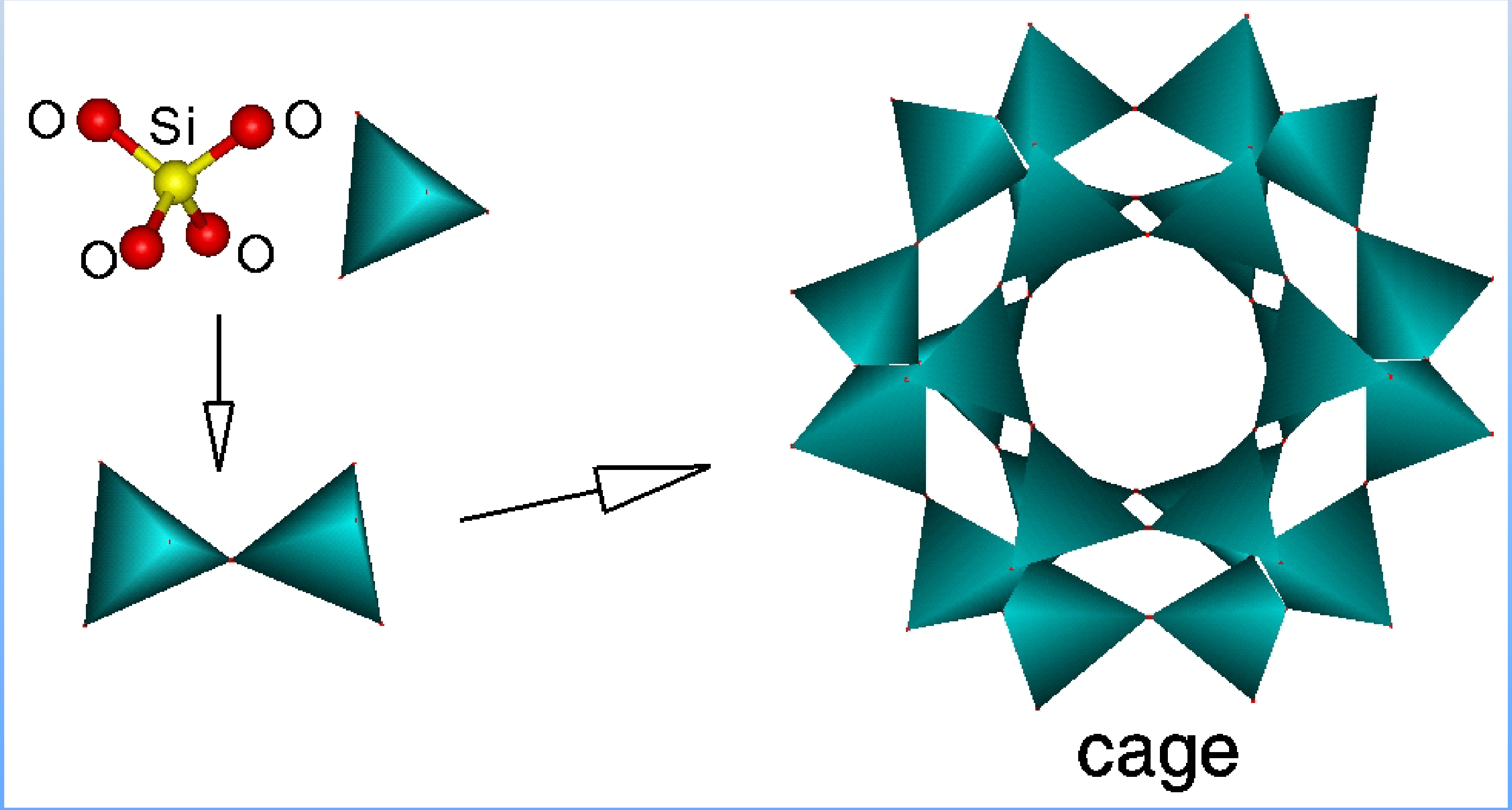
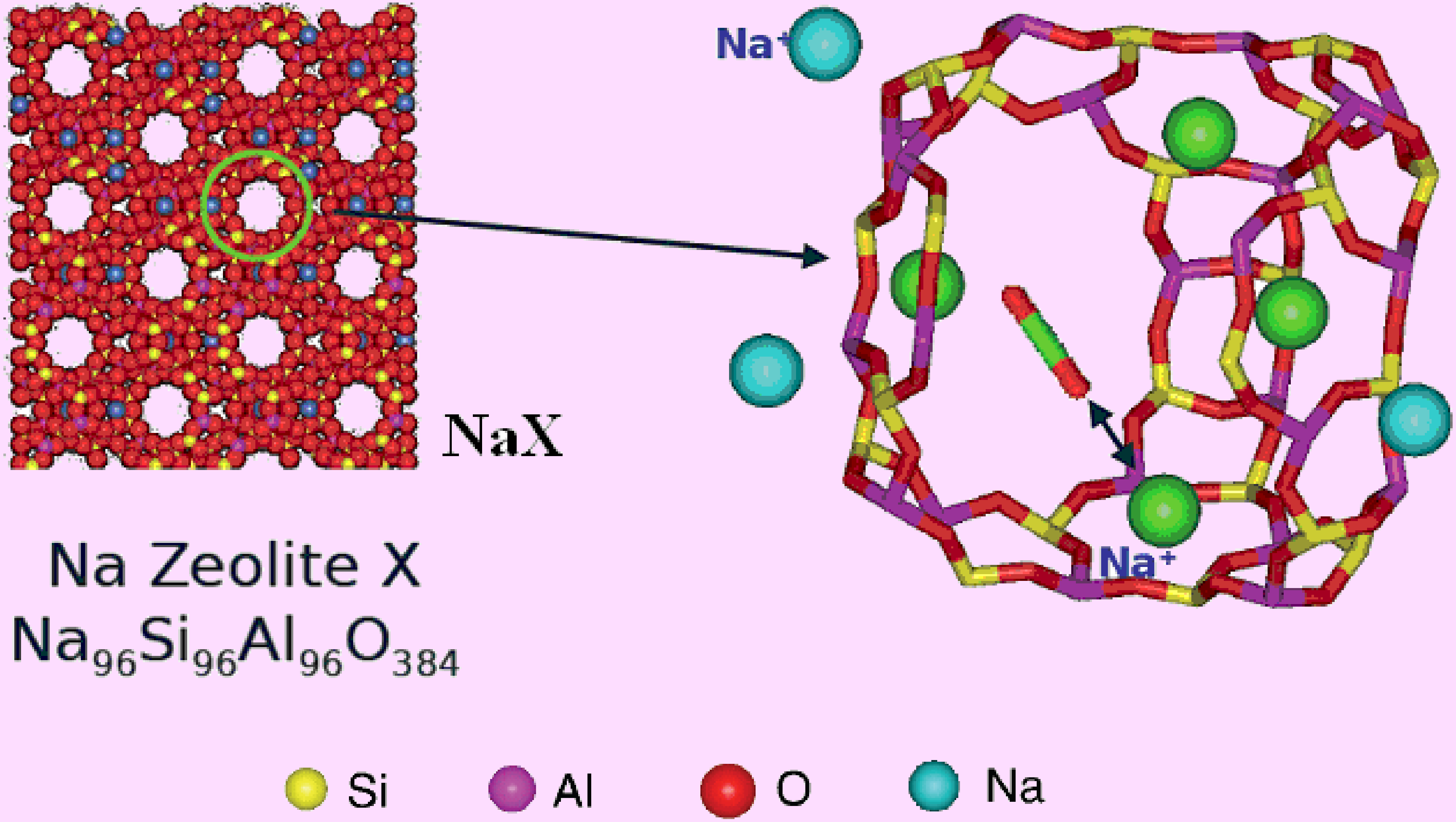



Figure 1. Framework structure

# Zeolites as Adsorbents



# Properties of some zeolites

| Name | Crystal structure | Chemical compound |
|---|---|---|
| A | Cubic, a=12,3 | $Na_{12}Al_{12}Si_{12}O_{48}*27H_2O$ |
| Chabazite | Rhombiedrichna, a=9,4 | $(Ca,Na_2)_{\sim 2}Al_4Si_8O_{24}*13H_2O$ |
| Eronit | Hexagonal, a=13,3 | $(Ca, K_2, Na_2)_{\sim 4}Al_8Si_{28}O_{72}*27H_2O$ |
| Faujasite | Cubic, a=24,7 | $Na_{13}Ca_{11}Mg_9K_2Al_{55}Si_{137}O_{384}*235H_2O$ |
| X | Cubic, a=25,0 | $Na_{86}Al_{86}Si_{106}O_{384}*264H_2O$ |
| Y | Cubic, a=24,7 | $Na_{56}Al_{56}Si_{136}O_{384}*250H_2O$ |
| Gmelinit | Hexagonal, a=13,7 | $(Na)_8Al_8Si_{16}O_{48}*24H_2O$ |
| L | Hexagonal, a=18,4 | $K_2Al_9Si_{27}O_{72}*22H_2O$ |
| Mussit | Hexagonal, a=18,4 | $K_{2,5}Mg_{2,1}Ca_{1,4}Na_{0,3}Al_{10}Si_{26}O_{72}*28H_2O$ |
| Ω | Hexagonal, a=18,2 | $(Na)_8Al_8Si_{28}O_{72}*21H_2O$ |
| Mordenit | Rhombic, a=18,1 b=20,5 | $Na_8Al_8Si_{40}O_{96}*24H_2O$ |
| Ofretit | Hexagonal, a=13,3 | $KCaMgAl_5Si_{13}O_{36}*15H_2O$ |

# Experimental Equipment

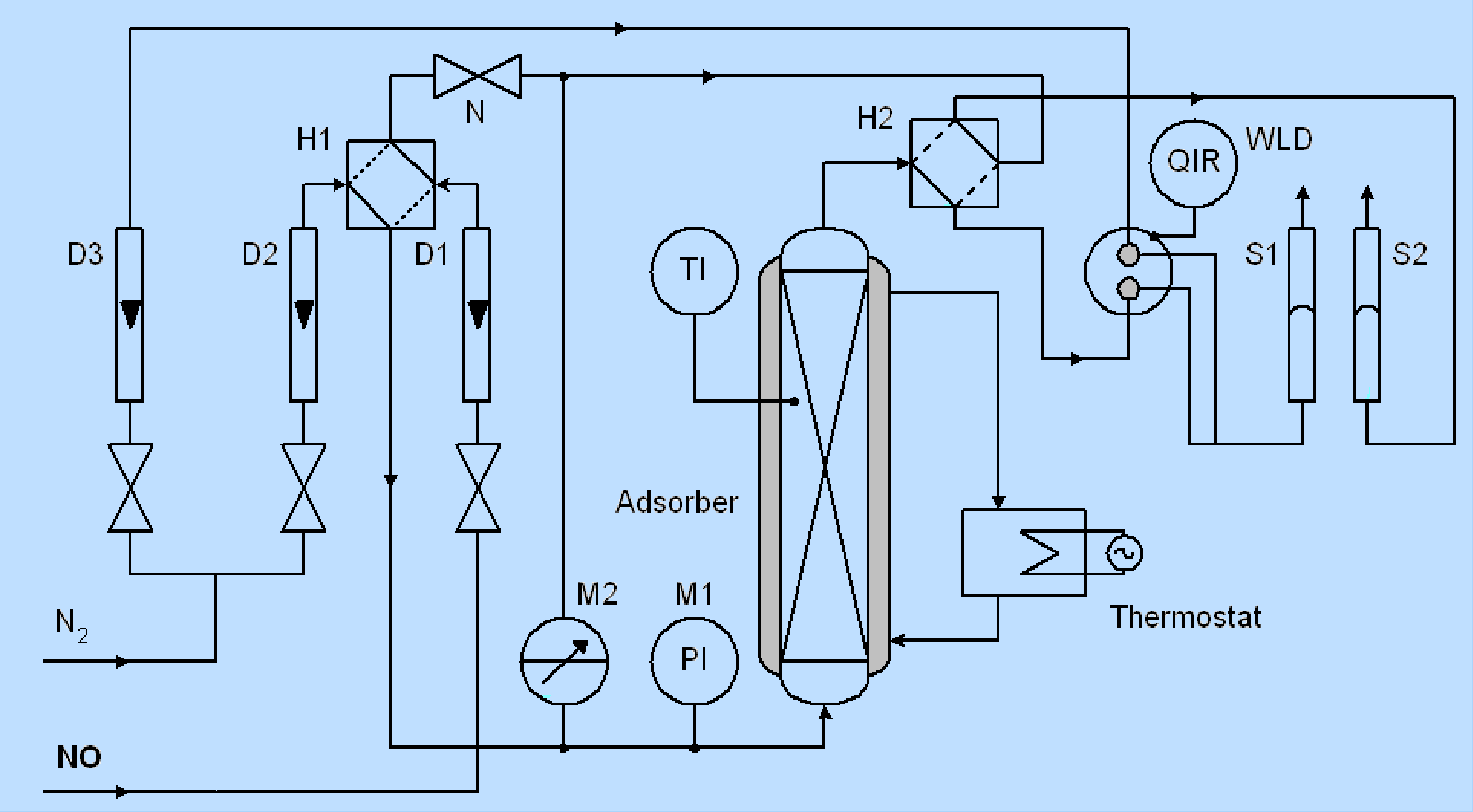



**Figure 3. Flow diagram of experimental equipment**

# Experimental curves of NO adsorption/desorption on 13X zeolite

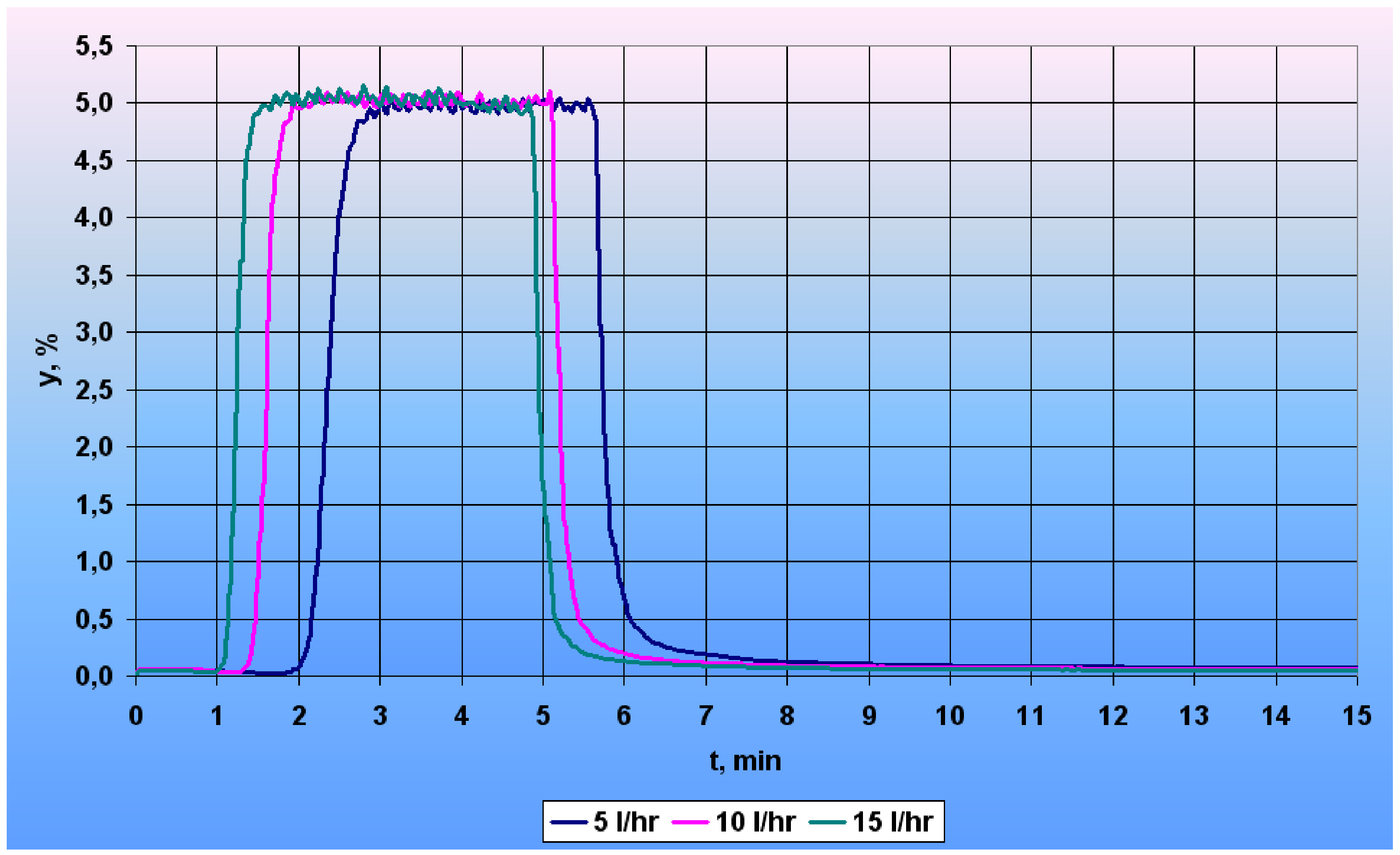



**Figure 4. NO concentration vs. time for adsorption-desorption on 13X zeolite at 25 $^{0}$C depending on the gas flow rate.**

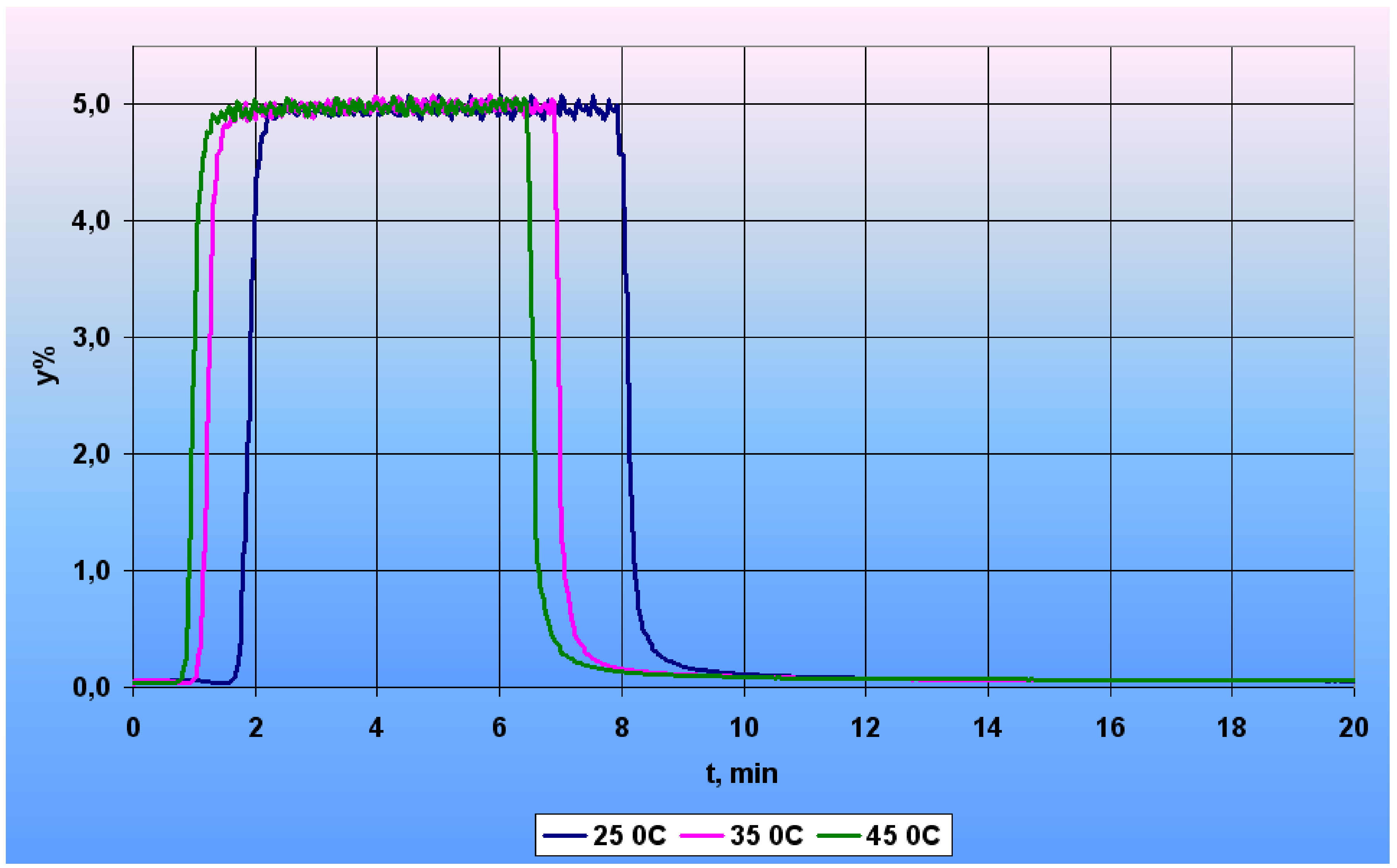



**Figure 5. NO concentration vs. time for adsorption-desorption on 13X zeolite depending on the temperature.**

# Experimental curves of NO adsorption/desorption on LiLSX zeolite

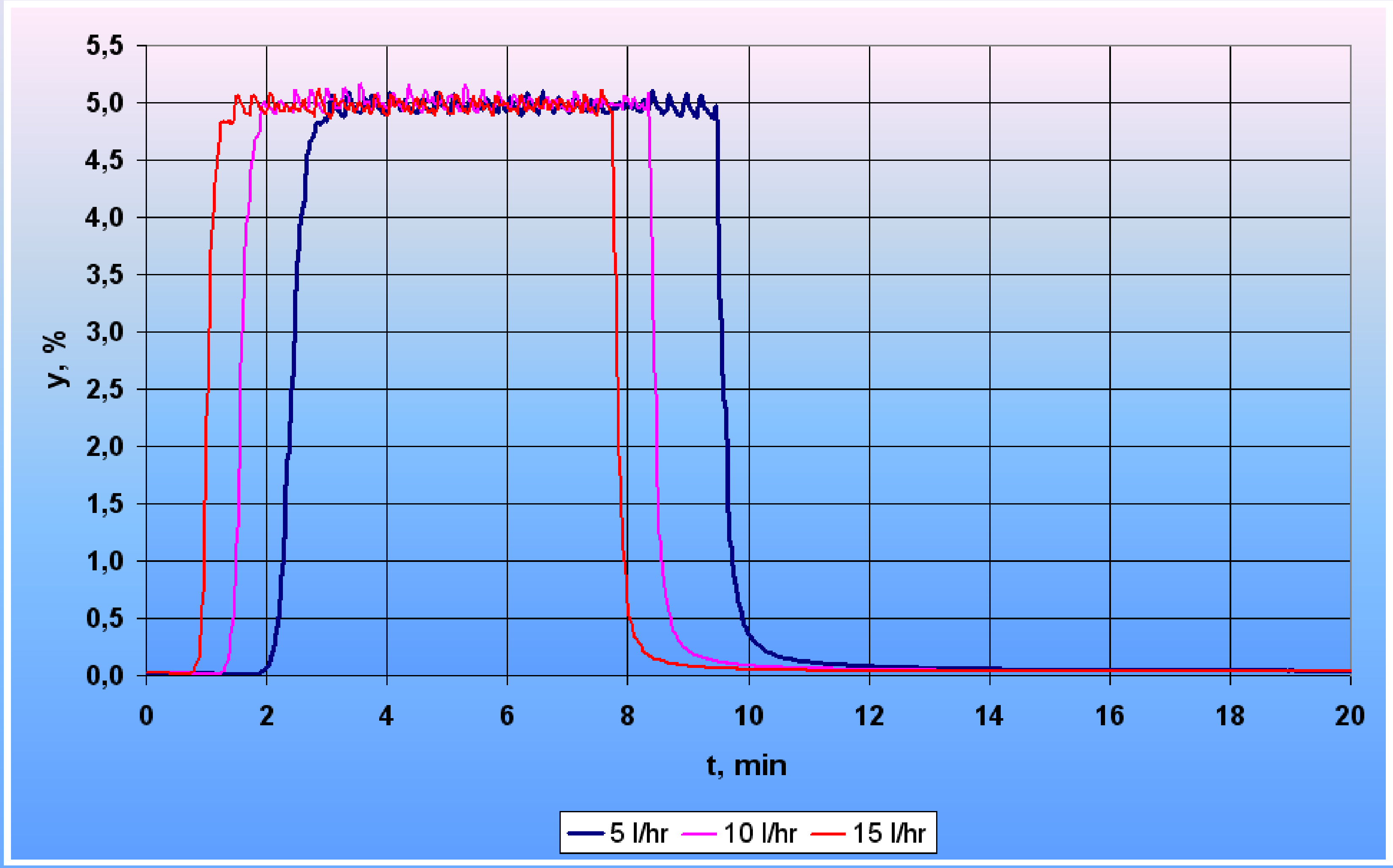



**Figure 6. NO concentration vs. time for adsorption-desorption on LiLSX zeolite depending on gas flow rate.**

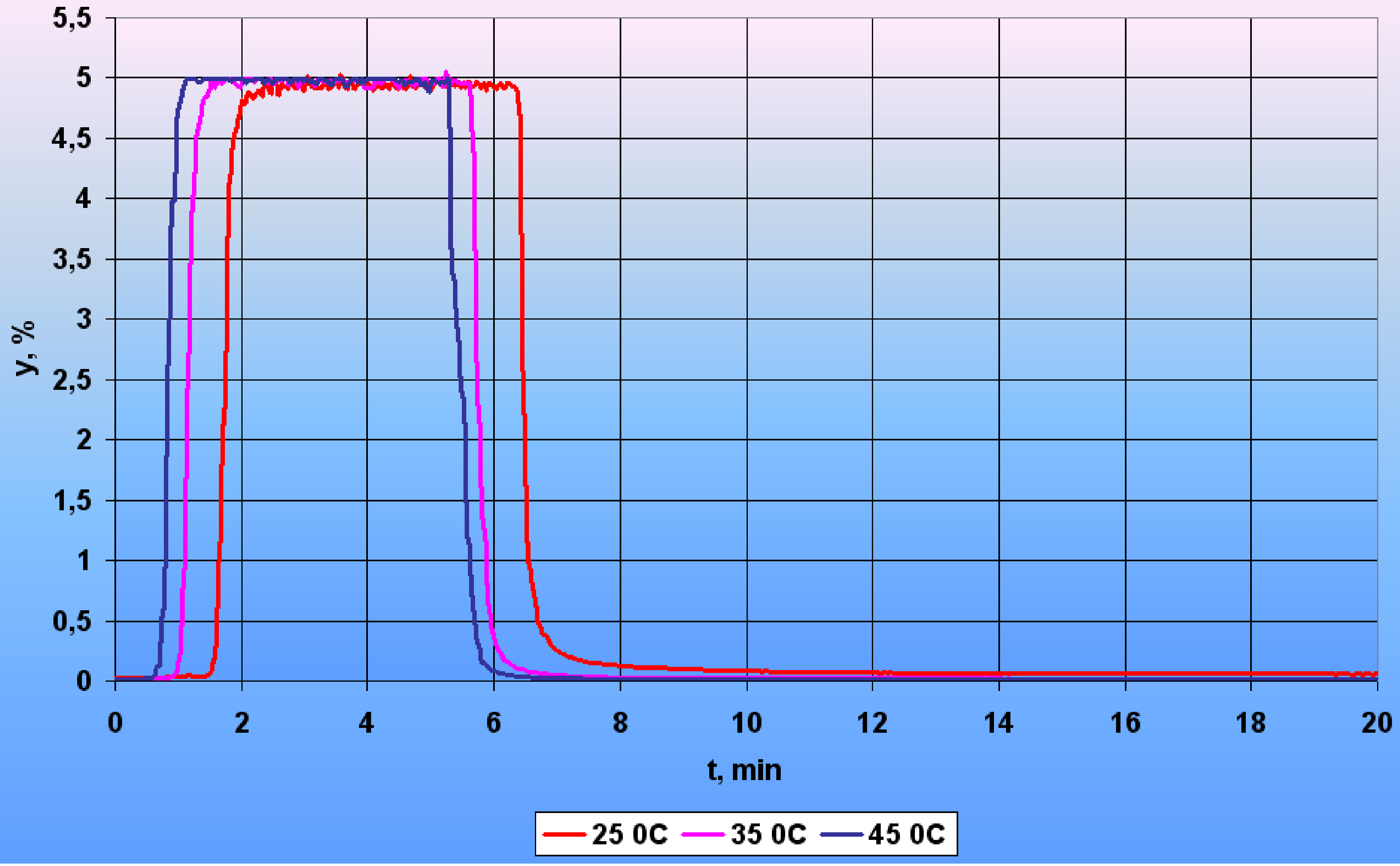



**Figure 7. NO concentration vs. time for adsorption-desorption on LiLSX zeolite depending on temperature**

# THE Techniques of gas purification process

# Development of the mathematical model of adsorption/desorption process of $NO_x$ over zeolites

The mathematical model of $NO_x$ adsorption/desorption over zeolites based on the mass balance in the i-th layer within the gas and the solid phase with corresponding initial conditions.

**Initial conditions:**

$t = 0, y(0) = y_0;$

$\theta_v(0) = 0$

## The hypotheses for the modeling were as follows:

- Mass transfer rate is represented by a linear driving force.
- There are no radial concentration and temperature gradients.
- The diffusion of the gas species is negligible.
- There is no deactivation of the adsorbent during the experiments.

$$\frac{dy_{out,i}}{dt} = \frac{2RT}{\varepsilon V_i P_t}\left[\frac{FP_t}{RT}(y_{in,i} - y_{out,i}) - k \cdot \overline{y_i} \cdot \theta_{V,i} \cdot q_0 \cdot w_i\right]$$

$$\theta_{V,i} = y_{in,i}\frac{dF}{dt}\frac{P_t M_{NO_x}}{RT}(t_s - \sum_0^{t_s}\frac{\overline{y_i}}{y_{in,i}}dt)$$

**where**

$F$ - gas flow rate, [l/h]

$y_{in}$, $y_{out}$ - inlet and outlet mole fractions of adsorbate, [-]

$P_t$ - total pressure, [Pa]

$\overline{y_i}$ - the average gas mole fraction in the i layer, [-]

$V_i$, $w_i$ - volume and weight of the layer, [l, kg]

$k$ - rate constant, [$s^{-1}$]

# Comparison the modeling and experimental results

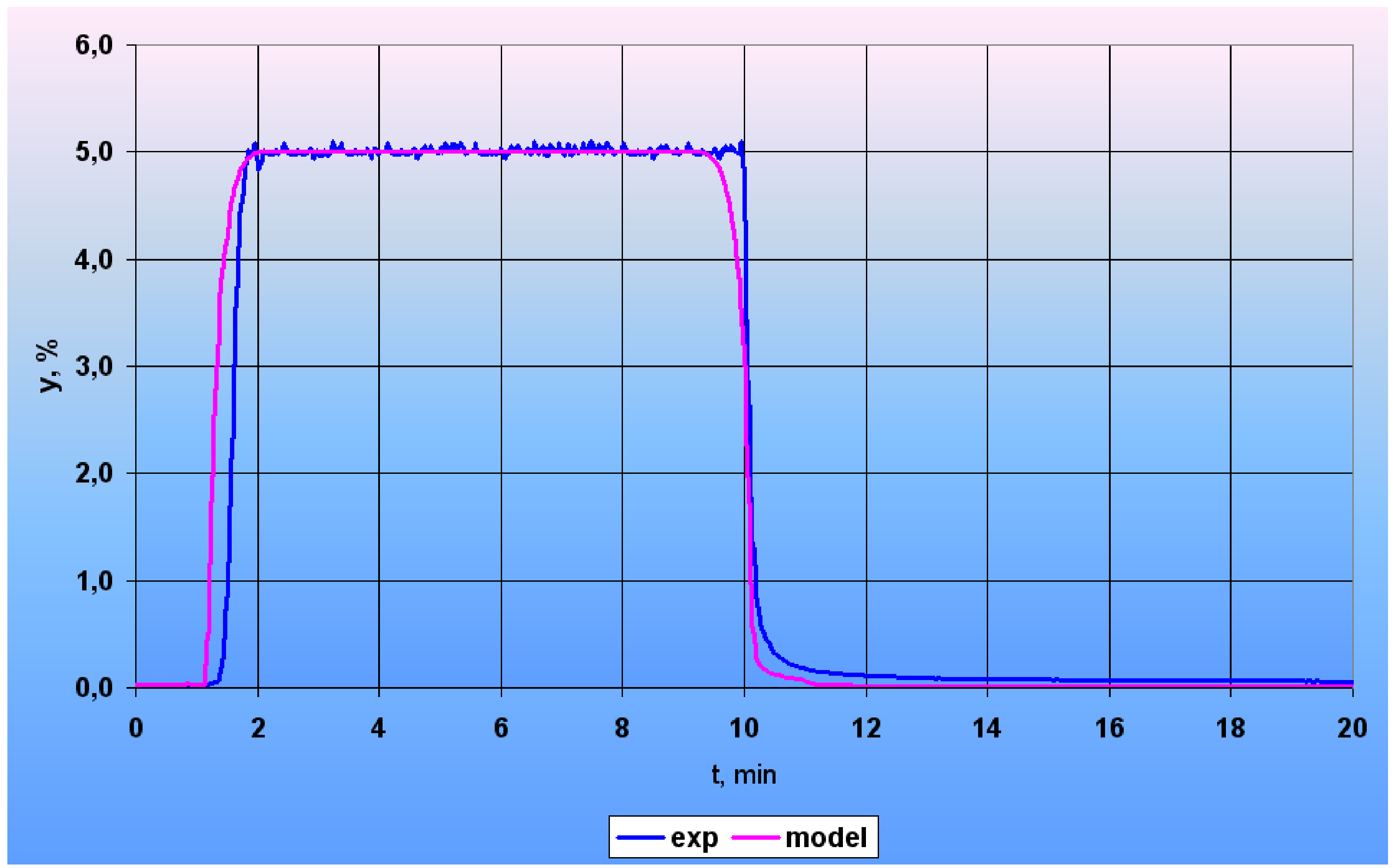



**Figure 8. Experimental and modeling curves of NO vs. time obtained for the adsorption-desorption on 13X zeolite at 25 $^{0}$C.**

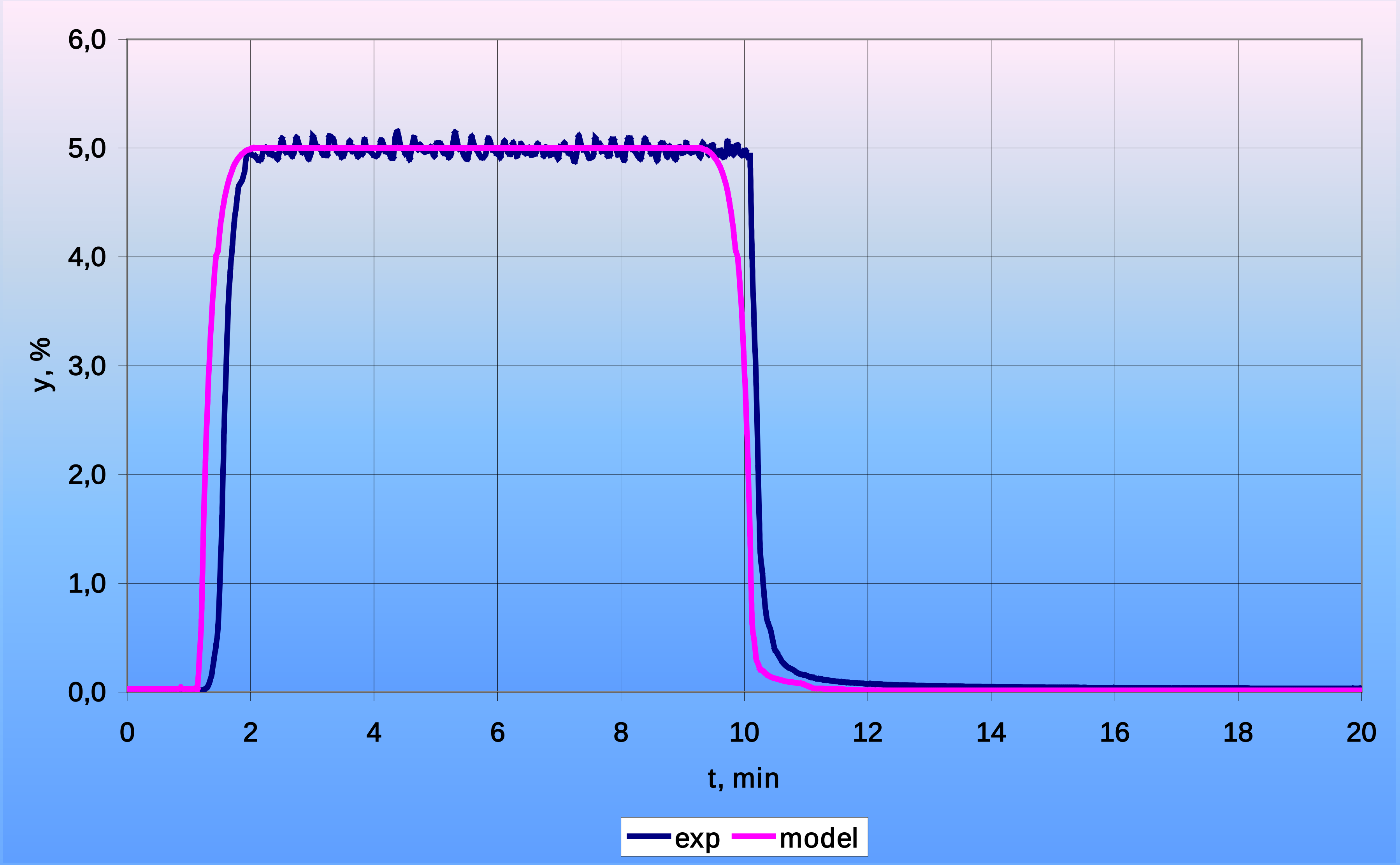



**Figure 9. Experimental and modeling curves of NO vs. time obtained for the adsorption-desorption on LiLSX zeolite at 25 $^{0}$C.**

# Summary

· The experiments of $NO_x$ adsorption/desorption over 13X and LiLSX zeolites were conducted.

· The column dynamics (the breakthrough curves under specific operating conditions) was reported.

· The one-dimensional mathematical model has been developed for a isothermal fixed-bed adsorption/desorption process.

· The adsorption and desorption $NO_x$ concentration profiles on 13X and LiLSX zeolites particles were reasonably well reproduced by the models.

· The optimal operating conditions and key parameters (the gas flow rate, the temperature) for the certain equipment were determined.

· The method of mathematical modeling is a potentially effective technique for the reduction of energy and economic charges.

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# DEVELOPMENT OF TECHNOLOGICAL BASES OF USING ZEOLITES FOR DENITRATION OF EXHAUST GASES

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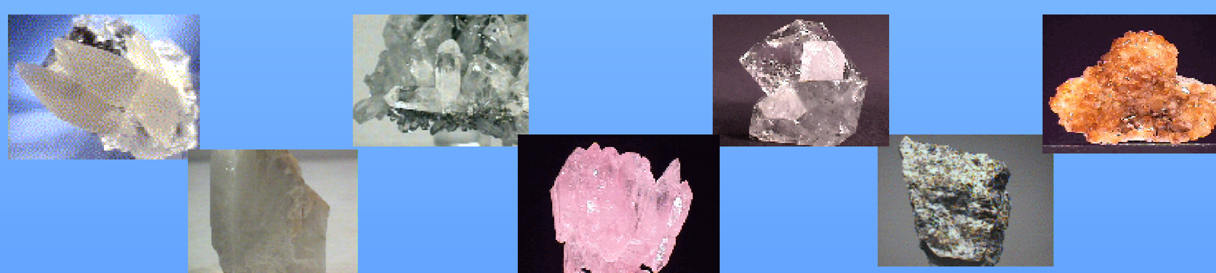



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