

Modeling of carbon monoxide oxidation process on the two-dimensional catalyst surface

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In this paper the two-dimensional mathematical model for carbon monoxide (CO) oxidation on the surface of Platinum (Pt) catalyst is investigated accounting for the processes of the catalyst surface reconstruction and the effect of the substrate temperature. It is shown that the stability region for reaction of CO oxidation changes in two-dimensional case.

Keywords: *reaction of catalytic oxidation, reaction-diffusion model, mathematical modelling of reaction-diffusion processes.*

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UDC: 538.9

1. Introduction

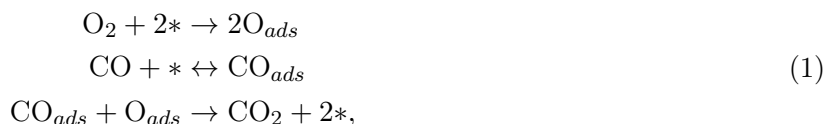
Studies of the catalytic oxidation of carbon monoxide is one of the most important problems in modern science [1]. Technologically, this process is vital for many applications: car exhaust emissions control, air purification, carbon dioxide lasers and sensors etc. Theoretically, it is one of the simplest catalytic reactions and is widely used as a model system in understanding heterogeneous catalysis.

The problem of efficiency of chemical reactions on the surfaces of metal catalysts covers quite a wide range of scientific problems. Unfortunately, there are still no physical models that can both accurately and adequately associate the results of theoretical and practical studies.

Obviously, it is impossible to build a model for a quantitative description of carbon monoxide (CO) catalytic oxidation without understanding the mechanisms of this process. One of the mechanisms of catalytic CO oxidation on the platinum (Pt) catalyst surface is the Langmuir-Hinshelwood (LH) mechanism, studied by Baxter and others [2].

In the Langmuir-Hinshelwood (LH) mechanism, the two reacting species CO and oxygen (O) have to adsorb on the catalytic surface (onto places called active adsorption sites) before the reaction takes place. Then adsorbed CO_{ads} and O_{ads} (subscript ‘ads’ denotes an adsorbed state) react under thermodynamically favourable conditions. The product of reaction carbon dioxide (CO_2) desorbs from the catalytic surface immediately.

Chemical reactions, that may proceed during CO oxidation on the catalytic surface via (LH) mechanism, are described with the following chemical equations:



where ‘*’ denotes an empty adsorption site on the catalytic surface.

When modelling the reaction of CO oxidation within chemical kinetics equations we assume that reaction takes place only on the catalyst surface. That is, the interactions can occur only between particles adsorbed on the catalyst surface. In order for oxygen to adsorb, a molecule breaks up into two

atoms near the catalyst surface and then each atom absorbs onto distinct empty site independently [3]. CO molecules adsorb onto surface and stay on it without breaking up into atoms. The transformation of particles is possible only in the adsorbed layer. During adsorption O₂ molecules rapidly dissociate into atoms. Oxygen desorption is very unlikely to occur in the range of temperatures at which experiments are conducted and therefore desorption is neglected. Since diffusion coefficient of adsorbed oxygen is 3–4 orders of magnitude smaller than CO diffusion coefficient [4], adsorbed oxygen is considered to be immobile.

The processes of surface reconstruction of the catalyst atoms play a crucial role in heterogeneous catalysis. The clean Pt(110) surface is reconstructed and has a (1×2) structure [5]. During reaction oxygen and CO adsorb on the Pt surface. If CO coverage exceeds specific critical value the surface reconstructs into (1×1) bulk structure [6]. When oxygen and CO react, carbon dioxide is formed and surface returns to its initial configuration. Such structural changes influence the rates of other elementary processes therefore should be taken into account when developing a mathematical model of reaction.

For thin plate catalysts heat generated in the chemical processes may dynamically change the temperature T of the catalyst. Even small changes may alter the CO oxidation dynamics dramatically. It is therefore also relevant to analyze the heat balance conditions and try to understand the characteristic time and space scales of the temperature field that may influence the chemical reaction.

2. Description of mathematical model

We consider a model for catalytic CO oxidation that accounts for diffusion of molecules of CO on Pt(110) surface. Assume that catalytic surface is flat with a given Cartesian coordinate system XOY . The time evolution of CO and O coverages on the catalyst surface is determined by the following kinetic equations [7, 8]:

$$\frac{\partial u}{\partial t} = \overbrace{p_u \kappa_u s_u (1 - (u/u_{sat})^q)}^{\text{adsorption}} + \overbrace{k_{des} u}^{\text{desorption}} + \overbrace{k_r uv}^{\text{reaction}} + \overbrace{D_x \frac{\partial^2 u}{\partial x^2} + D_y \frac{\partial^2 u}{\partial y^2}}^{\text{diffusion}}, \quad (2)$$

$$\frac{\partial v}{\partial t} = \overbrace{p_v \kappa_v s_v (1 - u/u_{sat} - v/v_{sat})^2}^{\text{adsorption}} + \overbrace{k_r uv}^{\text{reaction}}. \quad (3)$$

Here u and v denote CO and O surface coverages, respectively; p_u , p_v are the partial pressures of species; κ_u , κ_v are the impingement rates; s_u , s_v are the sticking coefficients; u_{sat} , v_{sat} refer to the maximal coverages namely the saturation coverages; k_r , k_{des} are the rates of reaction and CO desorption; D_x , D_y are CO diffusion coefficients in x and y directions, respectively. The factor $q = 3$ models the precursor-type kinetics [9] of CO adsorption, since the inhibition of CO and O₂ adsorption is asymmetric and adsorbed CO blocks oxygen adsorption stronger.

The structural phase transition $(1 \times 2) \leftrightarrow (1 \times 1)$ on Pt(110) surface is modeled by the following law [10, 11]:

$$\frac{\partial w}{\partial t} = \overbrace{k_{ph} (f(u) - w)}^{\text{reconstruction}}, \quad (4)$$

where variable w denotes the fraction of the surface in the nonreconstructed (1×1) state, coefficient k_{ph} is a rate of structural phase transition and

$$f(u) = \frac{1}{1 + \exp\left(\frac{u_0 - \frac{u}{u_{sat}}}{\delta u}\right)} \quad (5)$$

is a nondecreasing smooth function of the interval $[0, 1]$. Parameter u_0 determines the threshold value above which adsorbed CO molecules significantly influence the structure of the surface and δu determines the stepness of the threshold.

The sticking coefficient s_v is modified in equation (3) and can be rewritten as a linear combination of the values for the $(1 \times 2) - (1 \times 1)$ structures:

$$s_v = s_v^{1 \times 1} w + s_v^{1 \times 2} (1 - w), \quad (6)$$

where $s_v^{1 \times 1}$, $s_v^{1 \times 2}$ are oxygen sticking coefficients in (1×1) and (1×2) phases, respectively.

The rates of reaction, desorption and phase transition are temperature dependent and are determined by the Arrhenius equations [12]:

$$k_r [T] = k_r^0 \exp(-E_r/RT), \quad (7)$$

$$k_{des} [T] = k_{des}^0 \exp(-E_{des}/RT), \quad (8)$$

$$k_{ph} [T] = k_{ph}^0 \exp(-E_{ph}/RT). \quad (9)$$

Here k_r^0 , k_{des}^0 , k_{ph}^0 are temperature independent coefficients; E_r , E_{des} , E_{ph} are the activation energies; R is the universal gas constant.

To complete the model thermal processes generated in chemical reactions should be taken into account. In phenomenological definition [13] the heat balance equation includes thermal conductivity and heat of reaction of oxidation and may be written as:

$$\begin{aligned} c_p \rho \frac{\partial T}{\partial t} = & \overbrace{\kappa_{cond} \left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right)}^{\text{conduction}} - \overbrace{2n_{sites} \Delta H_{u,ads} p_u \kappa_u s_u (1 - (u/u_{sat})^q)}^{\text{CO adsorption}} \\ & - \overbrace{2n_{sites} \Delta H_{v,ads} p_v \kappa_v s_v (1 - u/u_{sat} - v/v_{sat})^2}^{\text{O adsorption}} - \overbrace{2n_{sites} \Delta H_{des} k_{des} u}^{\text{CO desorption}} - \overbrace{2n_{sites} \Delta H_r k_r uv}^{\text{reaction}}, \end{aligned} \quad (10)$$

where c_p is the heat capacity, ρ is the density, κ_{cond} is the thermal conductivity of the catalyst.

The number of sites in 1 cm^2 of Pt(110) surface is modeled by the following expression [13]:

$$n_{sites} = \frac{1}{\sqrt{2} d^2 L N_A}, \quad (11)$$

where d is the size of a side of an elementary cube in the Pt crystal lattice; L is the plate thickness; N_A is the Avogadro's constant.

The last term of equation (10) contains the heat of reaction ΔH_r that can be estimated as follows [13]. The adsorbed energy of an atom of oxygen is half the heat of adsorption of a molecule $\Delta H_{O_2,f}$, namely $\Delta H_{O,ads} = -54 \text{ kcal/mol}$ [13, 14]. For carbon monoxide, the heat of formation is $\Delta H_{CO,f} = -26.42 \text{ kcal/mol}$ and the heat of adsorption coincides with the desorption activation energy $\Delta H_{O,ads} = -E_{CO,des} = -38 \text{ kcal/mol}$. The heat of reaction can be estimated by the difference between the enthalpy of the adsorbed species and the enthalpy of the carbon dioxide in its gaseous phase:

$$\begin{aligned} \Delta H_r = & \overbrace{\Delta H_{CO_2,f}}^{\text{CO}_2(\text{gas})} - \overbrace{\left(\frac{1}{2} \Delta H_{O_2,f} + \Delta H_{CO,f} + \Delta H_{CO,ads} + \Delta H_{O,ads} \right)}^{\text{CO(ads)+O(ads)}} \\ = & -(94.05) - (0 + (-26.42) + (-38.00) + (-54.00)) = 24.37 \text{ kcal/mol}. \end{aligned}$$

Equations (2)–(4), (10) compose the mathematical model of carbon monoxide catalytic oxidation process.

3. Numerical analysis of the mathematical model

For numerical analysis, equations (2)–(4), (10) are transformed into dimensionless form by substituting:

$$u = u_{sat}U, \quad v = v_{sat}V, \quad T = T_0\tilde{T}, \quad (12)$$

$$x = l_0\tilde{x}, \quad y = l_0\tilde{y}, \quad t = t_c\tilde{t}, \quad (13)$$

where

$$t_c = v_{sat}/p_u\kappa_u s_u. \quad (14)$$

Parameter l_0 is chosen according to experimental data for the size of Pt-crystal $l_0 = 10^{-3}$ cm [15]. $T_0 = 540$ K is a temperature at which the reaction of CO oxidation has the maximal CO_2 output.

In dimensionless form equations (2)–(4), (10) compose a mathematical model of catalytic CO oxidation on the Pt surface:

$$\begin{cases} \frac{\partial U}{\partial \tilde{t}} = \frac{v_{sat}}{u_{sat}}(1 - U^q) + \tilde{k}_{des}U + \tilde{k}_r v_{sat}UV + \tilde{D}_x \left(\frac{\partial^2 U}{\partial \tilde{x}^2} + D_0 \frac{\partial^2 U}{\partial \tilde{y}^2} \right), \\ \frac{\partial V}{\partial \tilde{t}} = \tilde{p}_v s_v (1 - U - V)^2 + \tilde{k}_r u_{sat}UV, \\ \frac{\partial w}{\partial \tilde{t}} = \tilde{k}_{ph} \left\{ \left[1 + \exp \left(\frac{u_0 - U}{\delta u} \right) \right]^{-1} - w \right\}, \\ \frac{\partial \tilde{T}}{\partial \tilde{t}} = \tilde{\kappa}_{cond} \left(\frac{\partial^2 \tilde{T}}{\partial \tilde{x}^2} + \frac{\partial^2 \tilde{T}}{\partial \tilde{y}^2} \right) - \Delta \tilde{H}_{u,ads} v_{sat} (1 - U^q) - \Delta \tilde{H}_{v,ads} \tilde{p}_v s_v (w) v_{sat} (1 - U - V)^2 \\ - \Delta \tilde{H}_{des} \tilde{k}_{des} u_{sat} U - \Delta \tilde{H}_r \tilde{k}_r u_{sat} v_{sat} UV. \end{cases} \quad (15)$$

Here

$$\tilde{k}_{des} = k_{des} t_c, \quad \tilde{k}_r = k_r t_c, \quad \tilde{k}_{ph} = k_{ph} t_c,$$

$$\tilde{p}_v = \frac{p_v \kappa_v t_c}{v_{sat}}, \quad \tilde{\kappa}_{cond} = \frac{\kappa_{cond} t_c}{c_p \rho l_0^2}$$

$$\tilde{D}_x = \frac{D_x t_c}{l_0^2}, \quad D_0 = \frac{D_y}{D_x},$$

$$\Delta \tilde{H}_{u,ads} = \frac{2n_{sites}}{L c_p \rho T_0} \Delta H_{u,ads}, \quad \Delta \tilde{H}_{v,ads} = \frac{2n_{sites}}{L c_p \rho T_0} \Delta H_{v,ads},$$

$$\Delta \tilde{H}_{des} = \frac{2n_{sites}}{L c_p \rho T_0} \Delta H_{des}, \quad \Delta \tilde{H}_r = \frac{2n_{sites}}{L c_p \rho T_0} \Delta H_r.$$

System (15) is a system of four coupled nonlinear partial differential equations. It can be solved numerically with the software Matlab [16].

Explanation and parameter values used in numerical calculations are given in Table 1 [7, 11, 13].

The results of numerical analysis of two-dimensional mathematical model (15) of CO oxidation on Pt catalyst surface are presented in Figs. 1–8.

Fig. 1 shows the computed dynamics of CO surface coverage dependence $U(\tilde{x}, \tilde{y}, \tilde{t})$ at a given ratio of the components of tensor of diffusion coefficients $\hat{D} = \begin{pmatrix} D_x & 0 \\ 0 & D_y \end{pmatrix}$, namely $\frac{D_x}{D_y} = 10$ (D_x is CO diffusion coefficient along OX -axis and D_y is CO diffusion coefficients along OY -axis, which are assumed to be constant). This ratio corresponds to actually observed [15, 17]. The dynamics of CO surface coverage $U(\tilde{x}, \tilde{y}, \tilde{t})$ exhibits clear oscillatory behaviour with the period of oscillations $\tau_0 = 5$, which has a weak

Table 1. Parameters of mathematical model.

CO ₂	Partial pressure	p_u	2.25×10^{-5} Torr
	Impingement rate	κ_u	4.2×10^5 1/s Torr
	Sticking coefficient	s_u	1
	Saturation coverage	u_{sat}	1
	Diffusion coefficient	D_x	1.2×10^{-7} cm ² /s
O ₂	Partial pressure	p_v	5.08×10^{-5} Torr
	Impingement rate	κ_v	7.8×10^5 1/s Torr
	Sticking coefficient	$s_v^{1 \times 1}; s_v^{1 \times 2}$	0.6; 0.4
	Saturation coverage	v_{sat}	0.8
Rates	Reaction	k_r^0	3×10^6 1/s
	Desorption of CO	E_r	10 kcal/mol
		k_{des}^0	2×10^{16} 1/s
		E_{des}	38 kcal/mol
	Phase transition	k_{ph}^0	2×10^{-2} 1/s
		E_{ph}	7 kcal/mol
Pt(110)	Thickness	L	1.0×10^{-5} cm
	Density	ρ	21.45 1/cm ³
	Heat capacity	c_p	0.00003107 kcal/g K
	Thermal conductivity	κ_{cond}	0.00017113 kcal/s K
	Lattice constant	d	392.42×10^{-10} cm
Energetics	Heats of formation	$\Delta H_{CO,f}$	-26.42 kcal/mol
		$\Delta H_{CO_2,f}$	-94.05 kcal/mol
		$\Delta H_{O_2,f}$	0 kcal/mol
	Heats of adsorption	$\Delta H_{u,ads}$	-38 kcal/mol
		$\Delta H_{v,ads}$	-54 kcal/mol
	Enthalpy of reaction	ΔH_r	24.37 kcal/mol
Other	Temperature	T_0	540 K
	Avogadro's constant	N_A	6.0221367×10^{23} 1/mol
	Gas constant	R	0.001987 kcal/mol K
	Model parameter of diffusion	D_0	0.1–1
	Parameters of phase transition	$u_0; \delta u$	0.35; 0.05

dependence on coordinates. At the same time the amplitude of oscillations of $U(\tilde{x}, \tilde{y}, \tilde{t})$ depends on y -coordinate and changes from 0.05 (for $\tilde{y} = 0.1$) to 0.1 (for $\tilde{y} = 1.0$), i.e., doubles. This shows the effect of diffusion along OY -axis despite the fact, that diffusion coefficient along OY -axis is $D_y = 0.1D_x$.

The oscillatory behaviour of $U(\tilde{x}, \tilde{y}, \tilde{t})$ has a strong dependence on the $\frac{D_x}{D_y}$ ratio (see Fig. 5) as well as on the initial values of the partial pressures p_u and p_v . In contrast to the one-dimensional model [18], the oscillatory region (the stability region) of reaction of CO oxidation is more narrow (see Fig. 10) and matches the experimentally obtained stability region for reaction of CO oxidation more realistically [19].

The results of numerical analysis of oxygen surface coverage $V(\tilde{x}, \tilde{y}, \tilde{t})$ at a given ratio of diffusion coefficients $D_y = 0.1D_x$ are depicted in Fig. 2. The graph shows that the dynamics of $V(\tilde{x}, \tilde{y}, \tilde{t})$ dependence exhibits clear oscillatory behaviour with the period of oscillations $\tau_0 = 5$ (similarly to $U(\tilde{x}, \tilde{y}, \tilde{t})$), which changes little with a change of y . The oscillations of coverage $V(\tilde{x}, \tilde{y}, \tilde{t})$ are in antiphase with the oscillations of $U(\tilde{x}, \tilde{y}, \tilde{t})$, namely, the maximum u_{max} of CO coverage correspond to minimum v_{min} of O coverage. This is physically understandable, since CO oxidation requires atomic oxygen. This behaviour of oxygen coverage is experimentally observed. Similarly to the $U(\tilde{x}, \tilde{y}, \tilde{t})$

dependence, the $V(\tilde{x}, \tilde{y}, \tilde{t})$ behaviour changes much with a change of $\frac{D_x}{D_y}$ ratio (see Fig. 6). That is, the amplitude values vary considerably at a constant period of oscillation. This is associated with the fact that adsorbed CO can diffuse along both coordinate axes.

Fig. 3 shows the results of numerical analysis of model (15) regarding the fraction of surface in the nonreconstructed (1×1) state $w(\tilde{x}, \tilde{y}, \tilde{t})$. It can be seen that the dynamics also exhibits oscillatory behaviour. The period of oscillations is $\tau_1 \approx 7 \div 8$ and has a weak dependence on y -coordinate but differs from the period of change for $U(\tilde{x}, \tilde{y}, \tilde{t})$ and $V(\tilde{x}, \tilde{y}, \tilde{t})$. This is understandable, since the relaxation of the catalyst surface structure occurs later than the change of $U(\tilde{x}, \tilde{y}, \tilde{t})$, because the change of CO surface coverage is a factor that causes the reconstruction of catalytic surface. Similarly to the previous cases, the period of oscillations has a weak dependence on y -coordinate, but the amplitude values depend on y .

The results of numerical investigation of the catalyst surface temperature $\tilde{T}(\tilde{x}, \tilde{y}, \tilde{t})$ are depicted in Fig. 4. The behaviour of $\tilde{T}(\tilde{x}, \tilde{y}, \tilde{t})$ has an oscillatory character with the period of oscillations, that coincides with the period of change for $U(\tilde{x}, \tilde{y}, \tilde{t})$ and $V(\tilde{x}, \tilde{y}, \tilde{t})$ coverages. The $\tilde{T}(\tilde{x}, \tilde{y}, \tilde{t})$ dependency on coordinate y is weak and changes little depending on the $\frac{D_x}{D_y}$ ratio (see Fig. 8).

Fig. 9 shows the results of numerical analysis of model (15) for $D_y \equiv 0$ (one-dimensional case) without taking an equation for the change of catalyst temperature into account. The results of calculations coincide with the results of paper [18].

A comparison of stability regions (oscillatory behaviours) for model (15) and one-dimensional model [18] is shown in Fig. 10. It can be seen that the stability region for reaction of CO oxidation on the catalyst surface in two-dimensional case is more narrow than the stability region for one-dimensional model and correlates better with the stability region experimentally obtained [19].

4. Conclusions

In this paper the two-dimensional mathematical model of carbon monoxide oxidation for the Langmuir-Hinshelwood mechanism is developed and investigated. It is shown that the stability region for reaction of CO oxidation changes when two dimensions are taken into account. Similarly to the one-dimensional model [18], the reaction of CO oxidation on Pt-catalyst surface is periodic in the stability region with the period of $\tau_0 = 5$ (that differs slightly from the one-dimensional case) and matches the experimentally observed [15]. The amplitude values of the partial pressures p_u and p_v depend on the models dimension as well as on the $\frac{D_x}{D_y}$ ratio (D_x is the component of tensor of diffusion coefficients along OX -axis and D_y is the component of tensor of diffusion coefficients along OY -axis).

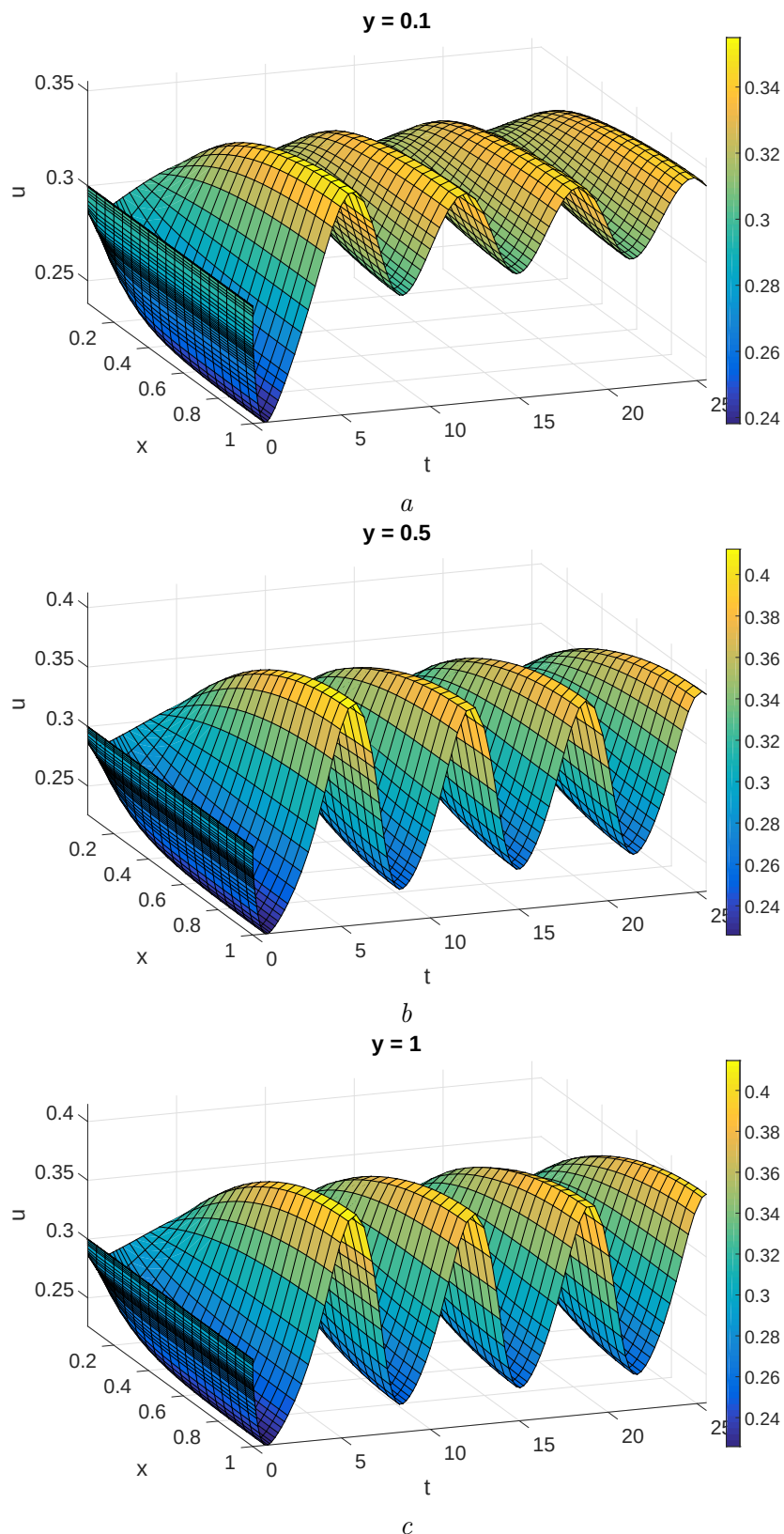


Fig. 1. Dependency of CO surface coverage $U(\tilde{x}, \tilde{y}, \tilde{t})$ for $\frac{D_x}{D_y} = 10$, $l_0 = 10^{-3}$ cm, partial pressures $p_u = 2.25 \times 10^{-5}$ Torr, $p_v = 5.08 \times 10^{-5}$ Torr and certain value of y -coordinate: a) $\tilde{y} = 0.1$; b) $\tilde{y} = 0.5$; c) $\tilde{y} = 1$.

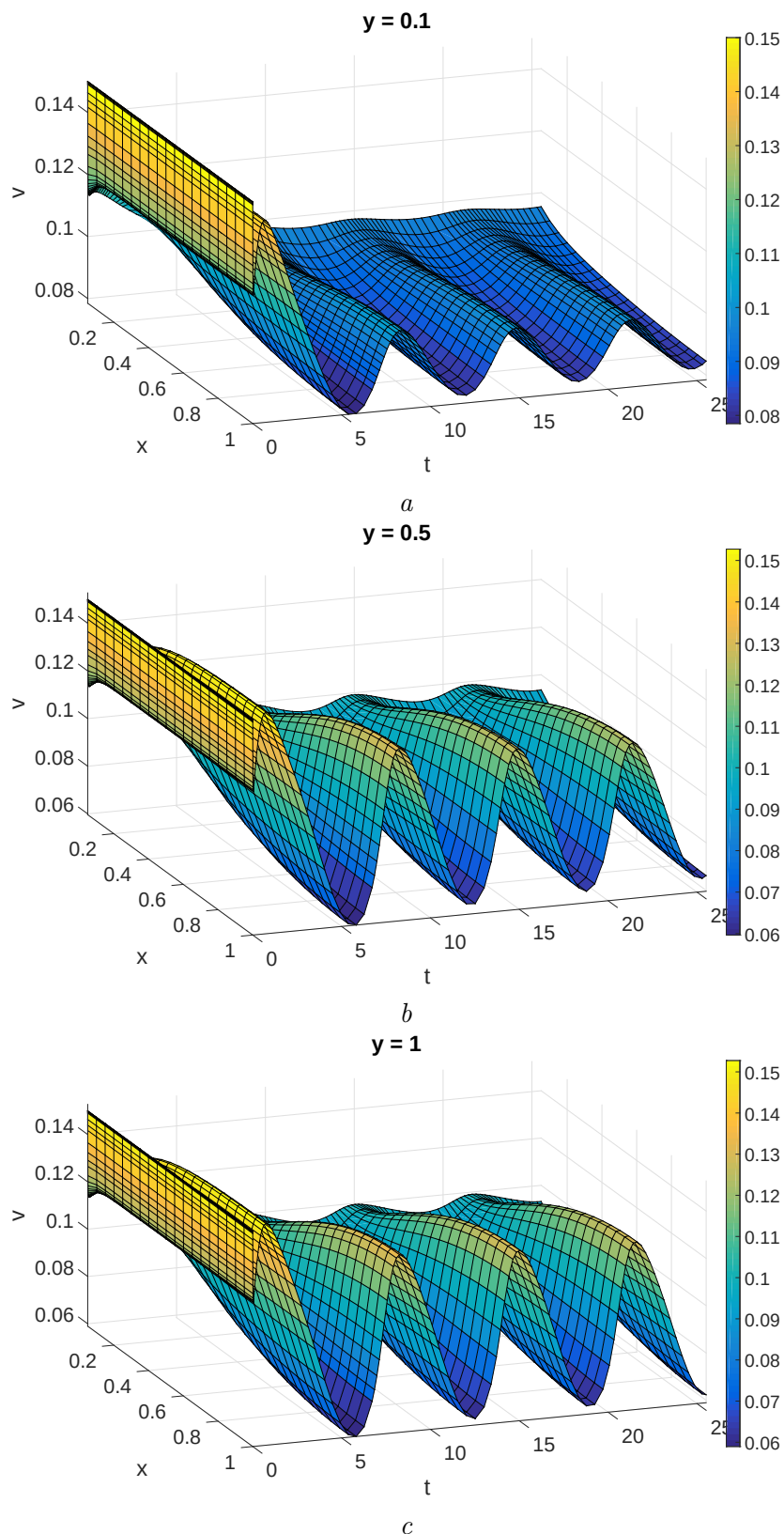


Fig. 2. Dependency of O surface coverage $V(\tilde{x}, \tilde{y}, \tilde{t})$ for $\frac{D_x}{D_y} = 10$, $l_0 = 10^{-3}$ cm, partial pressures $p_u = 2.25 \times 10^{-5}$ Torr, $p_v = 5.08 \times 10^{-5}$ Torr and certain value of y -coordinate: a) $\tilde{y} = 0.1$; b) $\tilde{y} = 0.5$; c) $\tilde{y} = 1$.

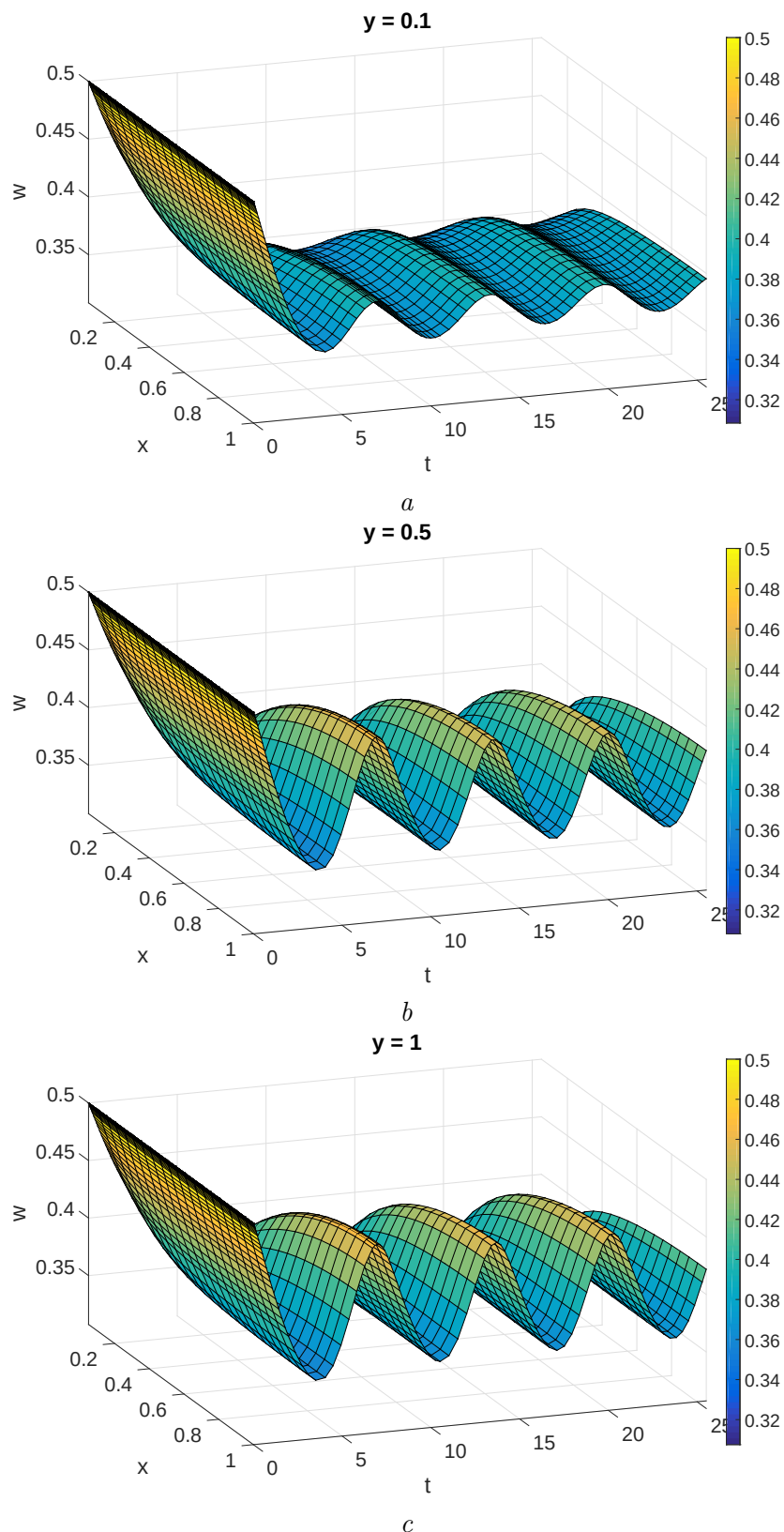


Fig. 3. Dependency of fraction of surface in the nonreconstructed (1×1) -state $w(\tilde{x}, \tilde{y}, \tilde{t})$ for $\frac{D_x}{D_y} = 10$, $l_0 = 10^{-3}$ cm, partial pressures $p_u = 2.25 \times 10^{-5}$ Torr, $p_v = 5.08 \times 10^{-5}$ Torr and certain value of y -coordinate: a) $\tilde{y} = 0.1$; b) $\tilde{y} = 0.5$; c) $\tilde{y} = 1$.

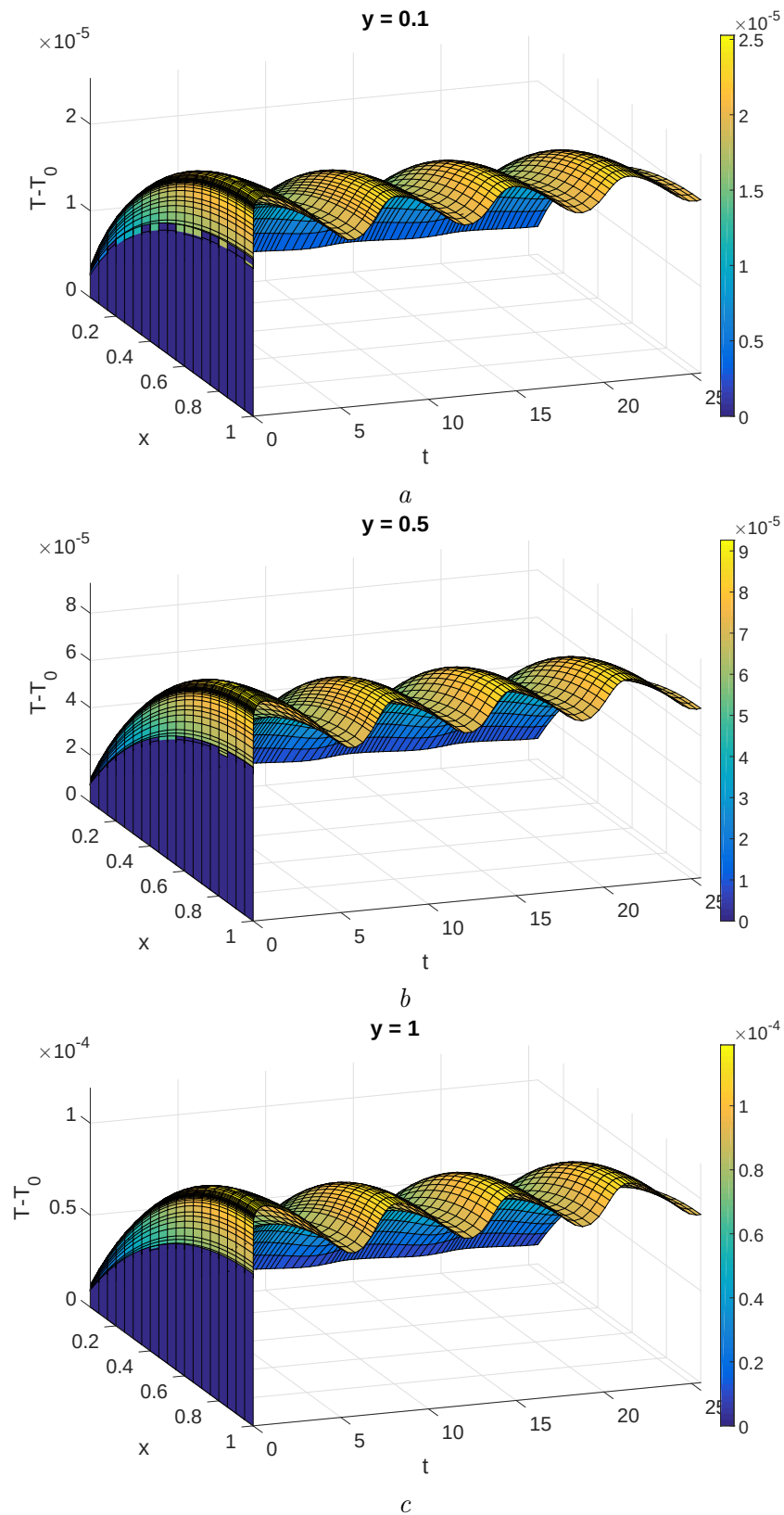


Fig. 4. Dependency of temperature $\tilde{T}(\tilde{x}, \tilde{y}, \tilde{t}) - T_0$ for $\frac{D_x}{D_y} = 10$, $l_0 = 10^{-3}$ cm, partial pressures $p_u = 2.25 \times 10^{-5}$ Torr, $p_v = 5.08 \times 10^{-5}$ Torr and certain value of y -coordinate: a) $\tilde{y} = 0.1$; b) $\tilde{y} = 0.5$; c) $\tilde{y} = 1$.

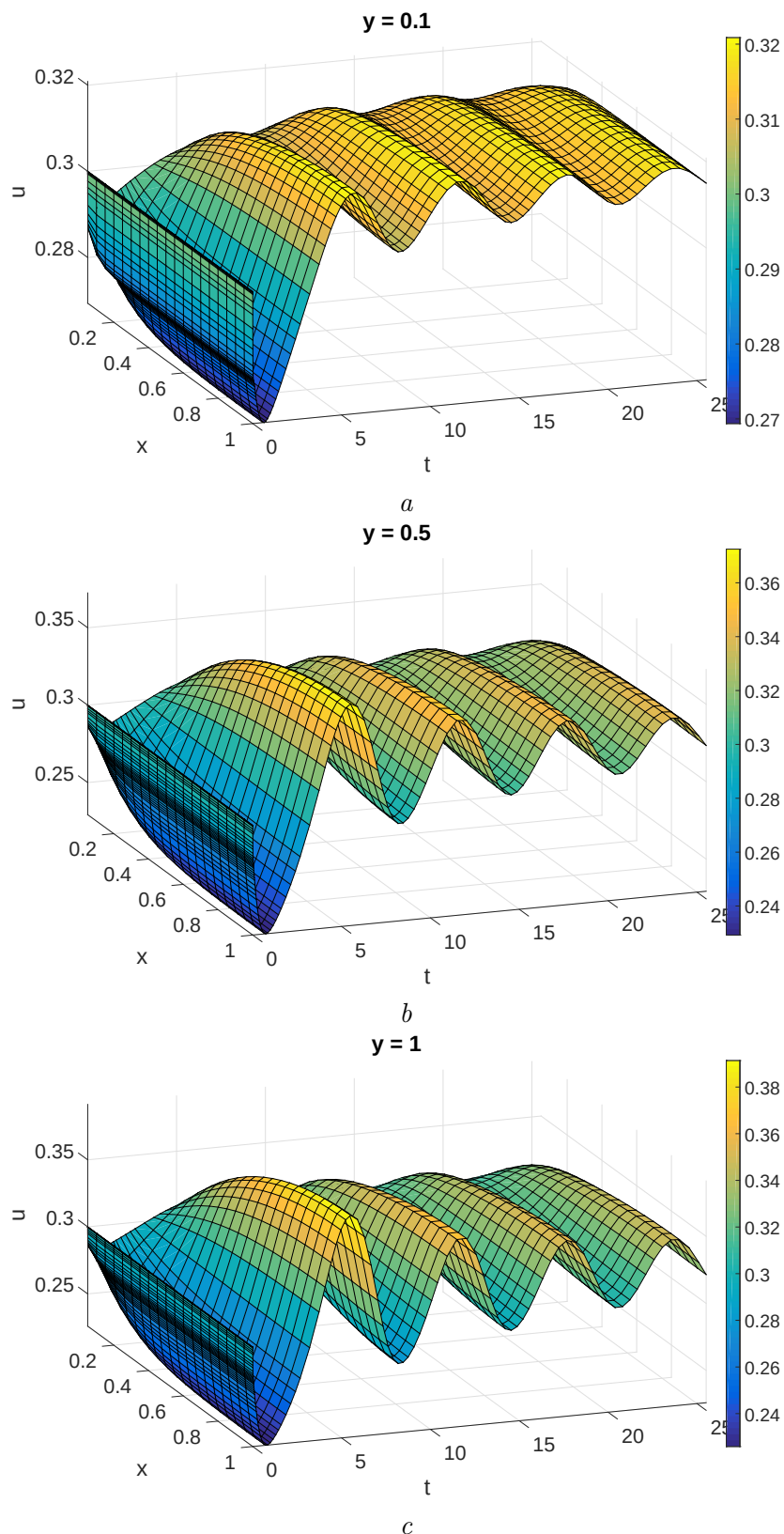


Fig. 5. Dependency of CO surface coverage $U(\tilde{x}, \tilde{y}, \tilde{t})$ for $\frac{D_x}{D_y} = 1$, $l_0 = 10^{-3}$ cm, partial pressures $p_u = 2.25 \times 10^{-5}$ Torr, $p_v = 5.08 \times 10^{-5}$ Torr and certain value of y -coordinate: a) $\tilde{y} = 0.1$; b) $\tilde{y} = 0.5$; c) $\tilde{y} = 1$.

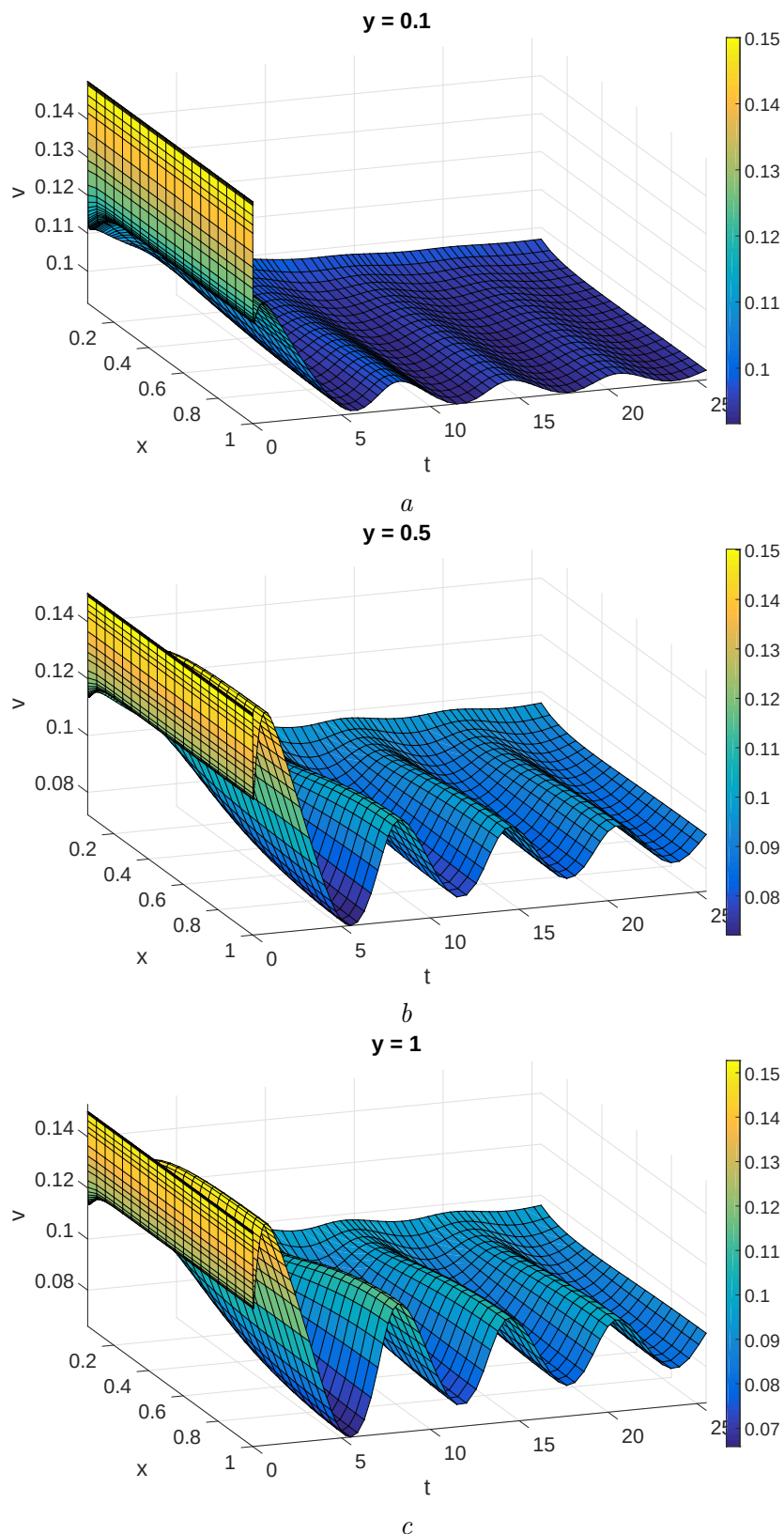


Fig. 6. Dependency of O surface coverage $V(\tilde{x}, \tilde{y}, \tilde{t})$ for $\frac{D_x}{D_y} = 1$, $l_0 = 10^{-3}$ cm, partial pressures $p_u = 2.25 \times 10^{-5}$ Torr, $p_v = 5.08 \times 10^{-5}$ Torr and certain value of y -coordinate: a) $\tilde{y} = 0.1$; b) $\tilde{y} = 0.5$; c) $\tilde{y} = 1$.

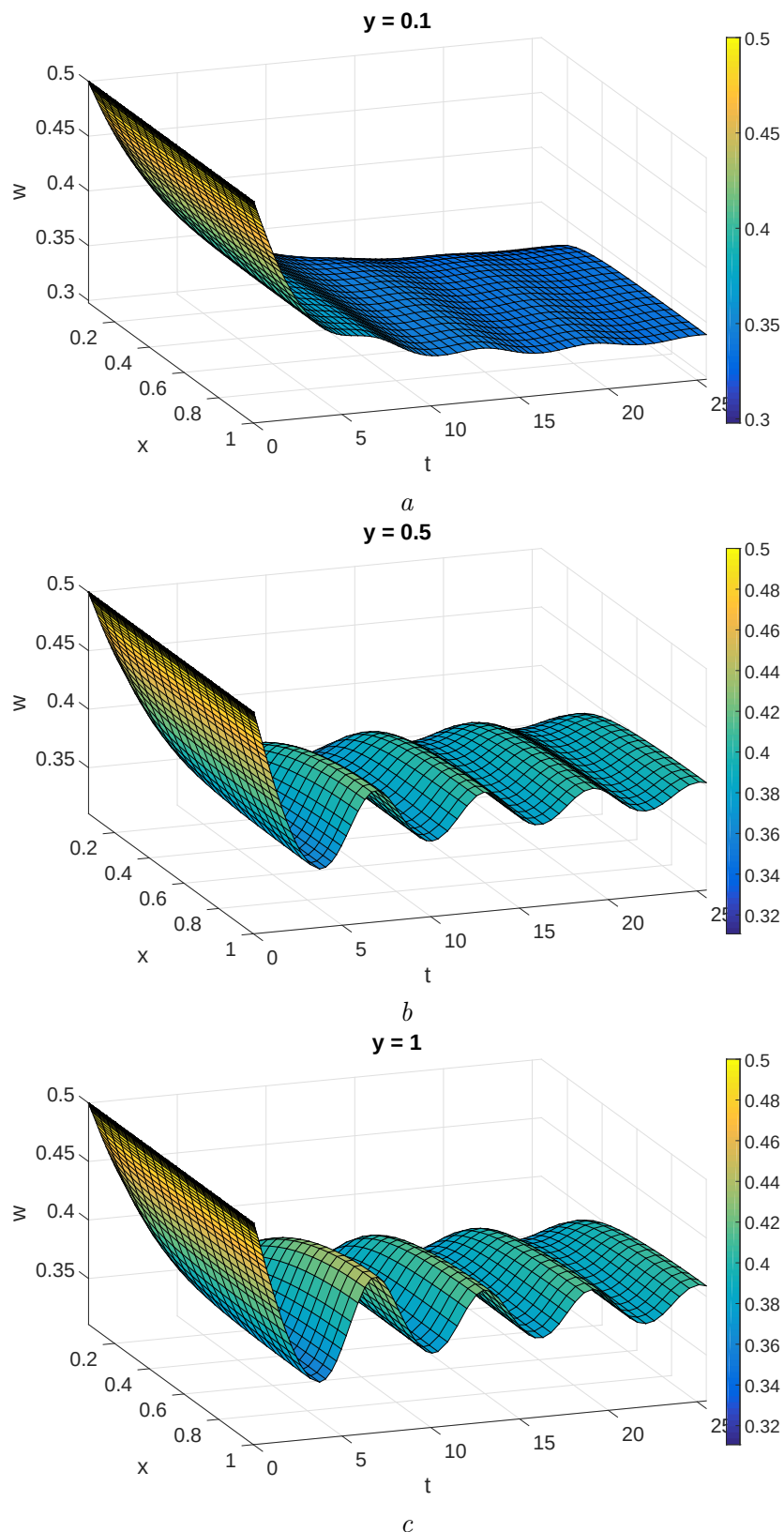


Fig. 7. Dependency of fraction of surface in the nonreconstructed (1×1) -state $w(\tilde{x}, \tilde{y}, \tilde{t})$ for $\frac{D_x}{D_y} = 1$, $l_0 = 10^{-3}$ cm, partial pressures $p_u = 2.25 \times 10^{-5}$ Torr, $p_v = 5.08 \times 10^{-5}$ Torr and certain value of y -coordinate: a) $\tilde{y} = 0.1$; b) $\tilde{y} = 0.5$; c) $\tilde{y} = 1$.

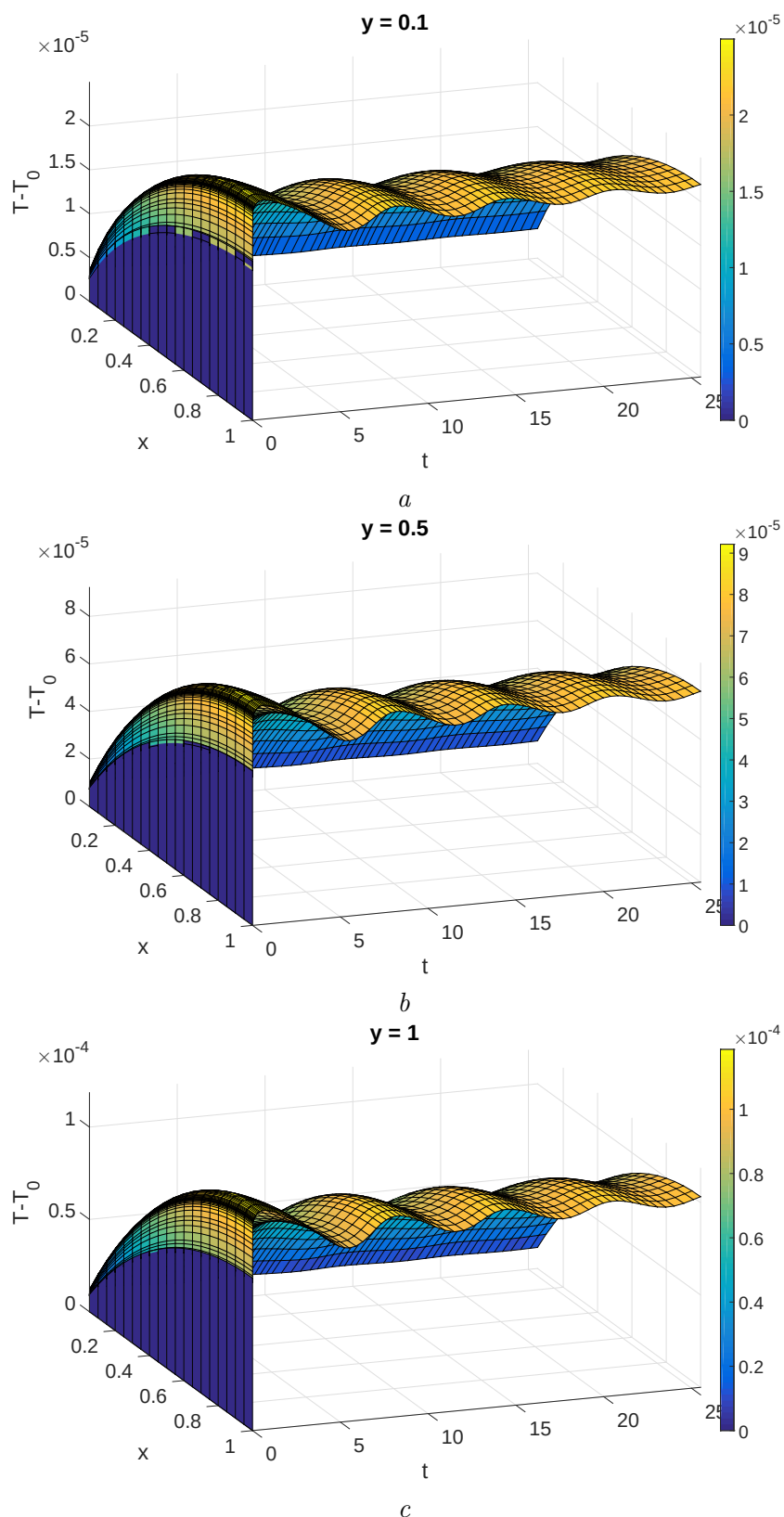


Fig. 8. Dependency of temperature $\tilde{T}(\tilde{x}, \tilde{y}, \tilde{t}) - T_0$ for $\frac{D_x}{D_y} = 1$, $l_0 = 10^{-3}$ cm, partial pressures $p_u = 2.25 \times 10^{-5}$ Torr, $p_v = 5.08 \times 10^{-5}$ Torr and certain value of y -coordinate: a) $\tilde{y} = 0.1$; b) $\tilde{y} = 0.5$; c) $\tilde{y} = 1$.

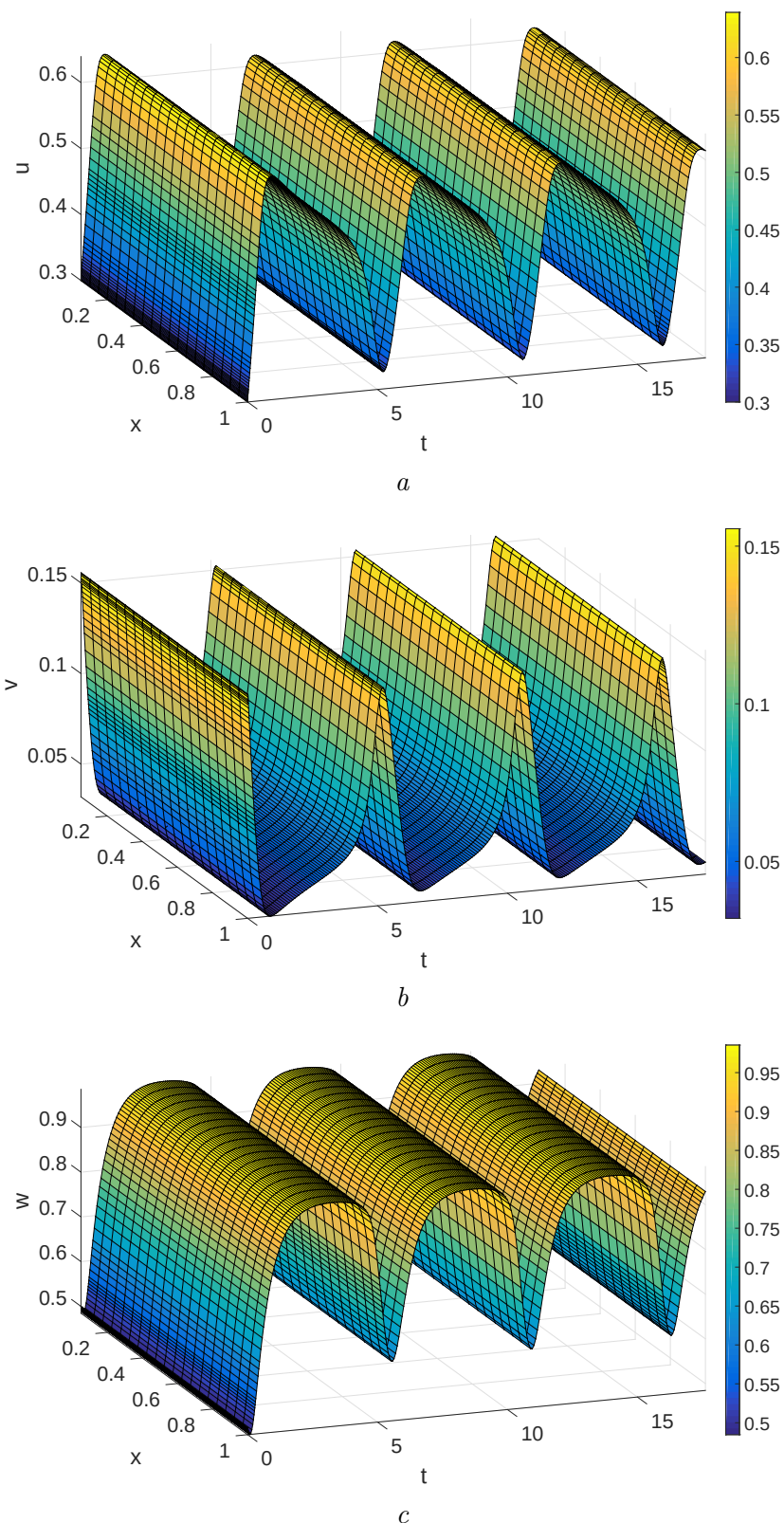


Fig. 9. Dependency of CO (a) and O (b) surface coverages and fraction of surface in the nonreconstructed (1×1) state (c) without taking an equation for temperature into account for $\tilde{D}_y = 0$, $l_0 = 1$ cm, partial pressures $p_u = 3.6 \times 10^{-5}$ Torr, $p_v = 9.75 \times 10^{-5}$ Torr.

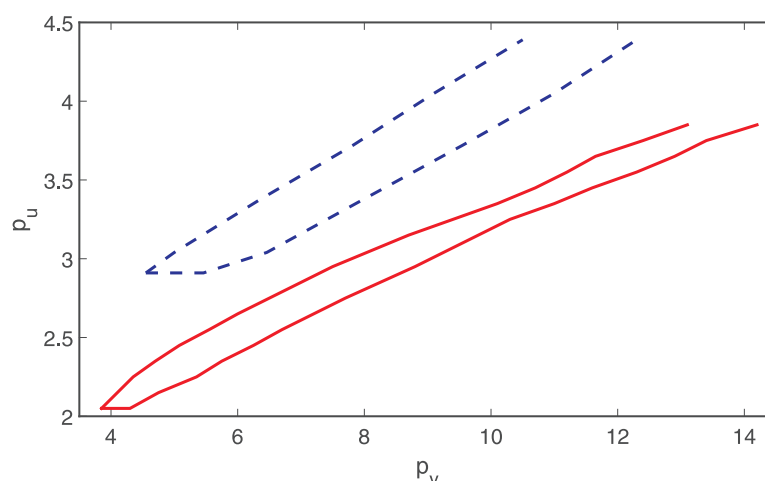


Fig. 10. Stability diagram for reaction of CO oxidation in the (p_v, p_u) parameter plane for model (15) (solid lines) and one-dimensional model [18] (dashed lines).

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Моделювання процесу оксидації чадного газу на двовимірній поверхні каталізатора

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Досліджено двовимірну математичну модель оксидації чадного газу (СО) на поверхні платинового каталізатора з урахуванням процесів перебудови поверхні каталізатора та впливу температури підложки. Показано, що в двовимірному випадку область стійкості реакції окислення СО змінюється.

Ключові слова: каталітична реакція окислення, реакційно-дифузійна модель, математичне моделювання реакційно-дифузійних процесів.

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