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# Mathematical and numerical modeling of transfer processes in the cleaning of exhaust gases in an automobile neutralizer

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Every year, the atmosphere in Kazakhstan is polluted approximately 5-7 million tons of pollutants, about a third of which belong to the vehicle. Also excess pollution of the air basin of the cities of the Republic is caused by pollution of pollutants by metallurgy, oil refining and chemical industry factories, automobile and railway transport. The harmful substances emitted by motor transport adversely affect the air, water reservoirs, soil and the planet's biosphere. At Nowadays car engine consumes about 3 kilogram of atmospheric oxygen when liters of gasoline per 1 kg are burned. Every car delivers 60 $m^3$ of gas per hour, and the truck produces 120 $m^3$ of gas. These substances are very dangerous for living organisms and finding solution for the problem of cleaning exhausted gases is very actual.

The purpose of this article is mathematical and numerical modeling on transfer processes in motor-car neutralizer with usage modern programming language and modern computing technologies. The solution of such a problem brings a certain contribution to the protection of the environment from automobile exhaust gases. The task of cleaning at exhaust gases is investigated, that is to say catalytic oxidation of exhausted gases automobile neutralizer . The mathematical model there is a system of differential equations warm and mass transfer including heat generation from the chemical reaction. The equation system is solved through numerical methods and to create and develop an algorithm of computing the task of cleaning exhaust gases in automobile neutralizer.

**Key words**: neutralizer, catalytic neutralizer, iterative numerical method.

## Автомобильді нейтрализаторда пайдаланылған газдарды тазалау кезінде тасымалдау процестерін математикалық және сандық модельдеу

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Қазақстанда жыл сайын атмосфераны 5-7 млн. тонна төңірегінде зиянды заттар ластайды, оның үштен бір бөлігі көлікке тиесілі. Республика қалалары әуе бассейнінің тым ластануы - ластаушылардың металлургия, мұнай өңдеу және химия өнеркәсібі кәсіпорындарының, автомобиль және теміржол көлігінің зиянды заттарды шығаруынан туындап отыр. Автомобиль көлігі бөліп шығаратын зиянды заттар ауаға, су қоймаларына, топыраққа түсіп планетамыздың биосферасына кері әсер етеді. Қазіргі кезде автомобиль қозғалтқышында 1 килограм бензин жанғанда 3 килограм атмосфералық оттегі шығындалады. Әрбір автомобиль ауаға сағат сайын 60 $м^3$ газ, ал жүк машинасы 120 $м^3$ газ бөліп шығарады. Бұл заттар тірі организмдер үшін өте қауіпті және таусылған газдарды тазарту проблемасын шешу өте өзекті.

Осы мақаланың мақсаты - заманауи программалау тілі мен заманауи есептеу техникасын қолдана отырып, автокөлік құралдарын бейтараптандырудағы көшіру процестеріндегі математикалық және сандық моделдеу. Осындай мәселені шешу қоршаған ортаны автокөлік газдарынан қорғауға белгілі бір үлес қосу болып табылады. Пайдаланылған газдарда тазалау жұмысы зерттелді, яғни автокөлік бейтараптандырғышының пайдаланылған газдарының катализдік тотығуы. Математикалық модельде дифференциалдық теңдеулер жүйесі жылу мен масса алмасу бар, оның ішінде химиялық реакциядан жылу таралады. Теңдеулер жүйесі сандық әдістер арқылы шешіледі және автокөлік бейтараптандырғышында таусылған газдарды тазарту міндетін есептеудің алгоритмі құрылып дамытылады.

**Түйін сөздер**: нейтрализатор, катализдік нейтрализатор, итерация әдісі, қуалау әдісі.

**Математическое и численное моделирование процессов переноса при очистке выхлопных газов в автомобильном нейтрализаторе**

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Ежегодно в Казахстане выделяется в атмосферу около 5-7 миллионов тонн загрязняющих веществ, около трети из которых относятся к транспортному средству. Кроме того, избыточное загрязнение воздушного бассейна городов республики вызвано загрязняющими веществами металлургическими, нефтеперерабатывающими и химическими заводами, автомобильным и железнодорожным транспортом. Вредные вещества, выделяемые автотранспортом, отрицательно влияют на воздух, водохранилища, почву и биосферу планеты. В настоящее время автомобильный двигатель потребляет около 3 килограммов атмосферного кислорода при сжигании литров бензина на 1 кг. Каждый автомобиль доставляет 60 м$^3$ газа в час, а грузовик производит 120 м$^3$ газа. Эти вещества очень опасны для живых организмов и решения проблем.

Целью данной статьи является математическое и численное моделирование процессов переноса в нейтрализаторе автомобилей с современным языком программирования и современными вычислительными технологиями. Решение такой проблемы вносит особый вклад в автомобильные выхлопные газы. Задача очистки выхлопных газов состоит в том, чтобы исследовать, то есть каталитическое окисление выхлопных газов в автомобильном нейтрализаторе. Математическая модель представляет собой систему дифференциальных уравнений. Система уравнений решается с помощью вычислительной машины в автомобильном нейтрализаторе.

**Ключевые слова**: нейтрализатор, каталитический нейтрализатор, итерационный метод, метод прогонки.

## 1 Introduction

Automobiles are the main sources which pollutes the atmosphere. Automobile car is in the first location by transportation volume among the all developed countries. However, due to the increased speed and volume of automation, there are number of important issues related to the environment and society's vulnerability to this process. Every year, the atmosphere in Kazakhstan is polluted about 5-7 million tons of pollutants, about a third of which belong to the vehicle. Also excess pollution of the air basin of the cities of the Republic is caused by pollution of pollutants by metallurgy, oil refining and chemical industry factories, automobile and railway transport. The harmful substances emitted by motor transport adversely affect the air, water reservoirs, soil and the planet's biosphere. At the present car engine consumes about 3 kilogram of atmospheric oxygen when liters of gasoline per 1 kg is burned. These substances are very dangerous for living organisms. Most of them are gases, oil products and dust that emit toxic and non-toxic components containing organic and inorganic substances, chlorides, wastes in the use and production of cars. In this way, due to the increase in traffic, in the environment harmful components are constantly accumulating and increasing its impact. Combustion products of automobile oil are collected on the Earth's surface and spread to the whole territory of the community and enter the body of people's respiratory tract. It is a very difficult task to ensure that the toxicity of spent gases is low. To address it, it is necessary to mobilize joint efforts of industrial operation and traffic regulation services.

The initial state of pollution reduction is the technical condition of the engine. The heavily engineered engine consumes less fuel and also reduces the air pollution level. However, focus

should be on proper functioning of the fuel equipment and the connecting system.

## 2 Review of literature

Currently, research and experimental works on the improvement of engines are carried out in the following areas: improvement of the combustion system, change of the fuel cycle in the engine cylinder, installation of additional equipment, reduction of harmful particles in the extracted gases. In this regard, the use of electronic ignition, which is characterized by high stability and high degree of ignition burner, makes significant changes (Yershin, 1997: 5-9).

The most effective way to reduce atmospheric emissions is the creation of closed, non-waste technological cycles, including the circulation of gases. Iodine wasteless, technology; is understood; ideal model, which in most cases can not be fully realized, but with the development of technical progress, it is possible to approach it more and more. Now, a waste-free technological cycle represents a combination of organizational and technical measures, technological processes, equipment, materials that ensure maximum and comprehensive use of raw materials and allow minimizing the negative impact of: waste on the environment. Currently, such events are often associated with enormous technological complexity and high costs, therefore, one of the main directions is the development and implementation of gas purification systems. At the same time, the main task of gas purification is to bring the content of toxic impurities to the maximum permissible concentrations established by sanitary standards, by separating it from gas or turning into a harmless condition of the pollutant.

Methods for reducing the intoxication can be divided into 4 major groups: special regulation and modification of their systems of design, work process, production technology and internal combustion engines; use of another type of fuels or change of physical and chemical properties of fuels and lubricants; purification of exhaust gases from toxic components; replacement of engines with less toxicity.

Bearing in mind the good qualities of all of the above structural changes, it is important to recognize that they do not effective solve the problem. Therefore, it is very important to use different types of neutralizers to clean the toxicity of the exhaust gases.

Neutralizer is a small reactor for combustion of flammable products to reduce the emissions of extracted gases and to separate nitrogen oxides, nitrogen and oxygen. It is possible to note the thermal, catalytic, liquid, mechanical and compound types of neutralizer. The process of turning into carbon dioxide in the thermoelectric is accompanied by the combustion of unsaturated hydrocarbons and aldehydes in the cylinder. Oxidation reaches 500-6000 $^{\circ}$ C and double hydrocarbon, while carbon dioxide decreases 2-3 times (Yershin, 1997: 10-11).

## 3 Materials and methods

### 3.1 Mathematical model

There will be considered the system of non-stationary temperature and concentration equations in partial derivatives, that describes the processes of warm and mass transfer in of motor-car neutralizer:

$$\begin{cases} \frac{\partial T}{\partial t} + \frac{U}{\varepsilon}\frac{\partial T}{\partial x} = a\frac{\partial^2 T}{\partial x^2} + Q \\ \frac{\partial C}{\partial t} + \frac{U}{\varepsilon}\frac{\partial C}{\partial x} = a\frac{\partial^2 C}{\partial x^2} - \rho\beta aC \end{cases} \quad (1)$$

$T$ - temperature, $C$ - concentration, $a$ - thermal conductivity coefficient, $\rho$ - density, $\varepsilon$ - characteristic of a porous enviroment.

$$Q = q\rho\beta aC$$

Initial conditions:

$$T|_{t=0} = 0,\ C|_{t=0} = 1$$

Boundary conditions:

$$T|_{x=0} = 1,\ C|_{x=0} = 1$$

$$\frac{\partial T}{\partial x}T|_{x=L} = 0,\ \frac{\partial C}{\partial x}T|_{x=L} = 0$$

### 3.2 The numerical method of task solution

To solve numerically the equation system by iterative method there is used the explicit scheme (Samarskiy, 1989: 38-47):

$$\frac{C_i^{n+1} - C_i^n}{\Delta t} + \frac{U}{\varepsilon}\frac{C_{i+1}^n - C_{i-1}^n}{2\Delta x} = D\frac{C_{i+1}^n - 2C_i^n + C_{i-1}^n}{\Delta x^2} - \rho\beta aC_i^n$$

$$C^{n+1} = C_i^n + \Delta t\left(D\frac{C_{i+1}^n - 2C_i^n + C_{i-1}^n}{\Delta x^2} - \rho\beta aC_i^n - \frac{U}{\varepsilon}\frac{C_{i+1}^n - C_{i-1}^n}{2\Delta x}\right)$$

$$i = \overline{1, L-1}$$

$C_i^n = 1$ - initial condition for concentration.
$C_0^{n+1} = 1$ - the first boundary condition for concentration.

$$\frac{C_L^n - C_{L-1}^n}{\Delta x} = 0$$

$C_L^n = C_{L-1}^n$ - the second boundary condition for concentration.

$$\frac{T_i^{n+1} - T_i^n}{\Delta t} + \frac{U}{\varepsilon}\frac{T_{i+1}^n - T_{i-1}^n}{2\Delta x} = a\frac{T_{i+1}^n - 2T_i^n + T_{i-1}^n}{\Delta x^2} + q\rho\beta aC_i^n$$

$$T_i^{n+1} = T_i^n + \Delta t + \left(a\frac{T_{i+1}^n - 2T_i^n + T_{i-1}^n}{\Delta x^2} + q\rho\beta aC_i^n - \frac{U}{\varepsilon}\frac{T_{i+1}^n - T_{i-1}^n}{2\Delta x}\right)$$

$$i = \overline{1, L-1}$$

$T_i^n = 1$ - initial condition for temperature.
$T_0^{n+1} = 1$ - the first boundary condition for temperature.

$$\frac{T_L^n - T_{L-1}^n}{\Delta x} = 0$$

$T_L^n = T_{L-1}^n$ - the second boundary condition for temperature.

## 4 Results and discussion

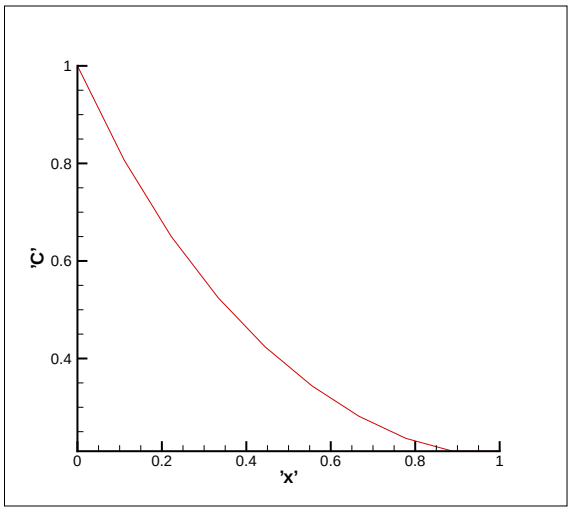


**Figure 1** – Concentration profile (explicit scheme, the iterative method)

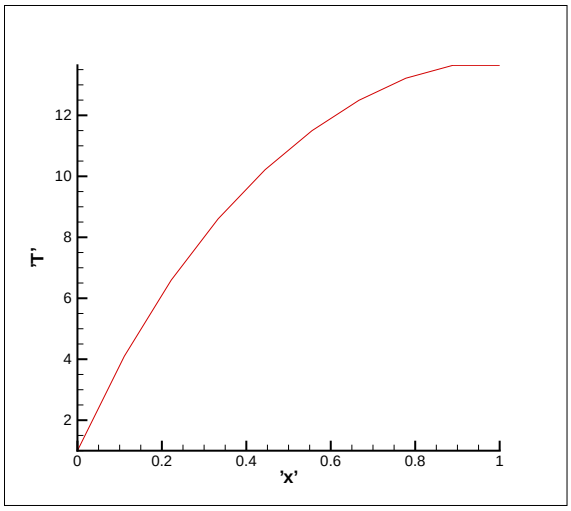


**Figure 2** – Temperature profile (explicit scheme, the iterative method)

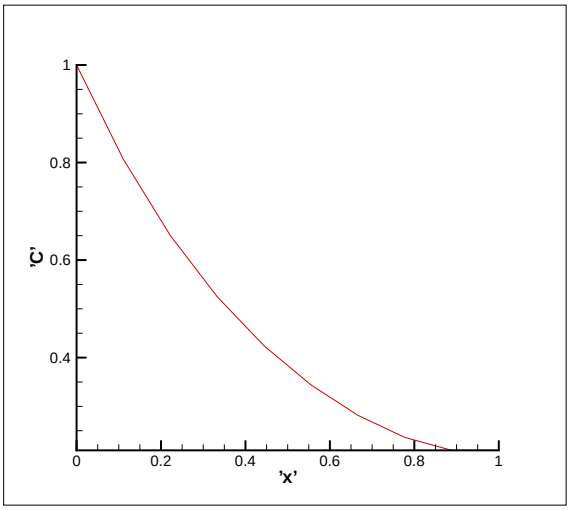


**Figure 3** – Concentration profile (implicit scheme, the raising method)

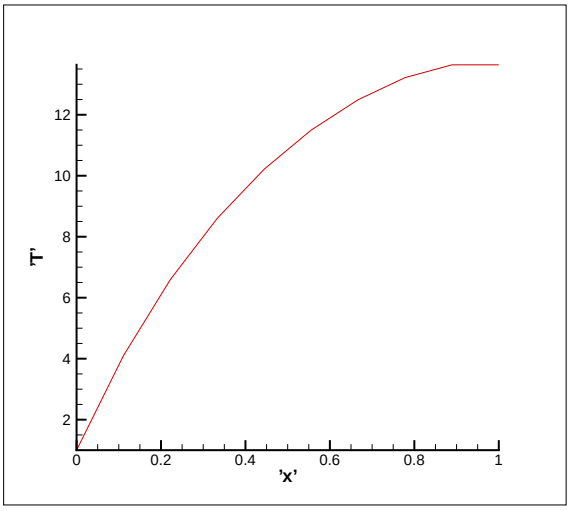


**Figure 4** – Temperature profile (implicit scheme, the raising method)

Based on the difference schemes and methods described above, numerical calculation algorithms have been developed:

- according to the explicit scheme

- according to the implicit scheme

Numerical calculation programs are developed in the modern C ++ programming language.

The results of the numerical calculations shown in the figures indicate a good qualitative and quantitative correspondence. Thus, the constructed mathematical and numerical simulation showed the correct results.

## 5 Conclusion

To make the usual human living environment, not to let the negative anthropogenic influence, it is necessary to ensure of normal ecological status in the country And then there is possible to make decision based on regulation of environment's quality.

In this article is to study the mathematical and numerical modeling of car exhausting gas cleaning processes, to create and develop an algorithm of computations, to make program code in the C ++ programming language (Lee, 1999: 168-199).

The result of the work is the program code written in the programming language C ++, most explicitly describing the process of gas purification. All modules are debugged, compiled and implemented in a single environment.

The given numerical solution of equation system was implemented on C++ programming language and the result was taken in TECPLOT graphical editor.

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