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Satbayev University

# Х А Б А Р Л А Р Ы

# ИЗВЕСТИЯ

НАЦИОНАЛЬНОЙ АКАДЕМИИ НАУК
РЕСПУБЛИКИ КАЗАХСТАН
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# CREATION OF MATHEMATICAL AND COMPUTER MODELS OF THE DYNAMICS OF FLAME PROPAGATION OF AIR-SUSPENDED SOLIDS IN VARIOUS ROCKS USING MATLAB ENVIRONMENT

**Abstract.** The propagation of transient, air-suspended solids in a vented explosion chamber is numerically investigated by a dynamic formulation for the Concentration Limit of Flame Propagation (CLFP) with the GUI MATLAB environment. The geomechanics is modeled by a one-step overall reaction, which simulates the reaction of a stoichiometric propane– air-suspended solids. The CLFP modeling in the reaction rate model is numerically employed with mathematical models on basis Antoine's equation. This is based on an empirical correlation of the velocity fluctuations and implemented as interface with input-output data with graphic realization. The computer modeling show that the dynamic CLFP models provide superior results as general implementation of physical process of flame propagation and could be used for different rocks (f.e. granite, limestone, sandstone etc).

**Key words:** GUI MatLab, flame propagation, dynamic CLFP, air-suspended solids, equation of Antoine, rocks.

**Introduction.** Flame propagation investigation is widely used in different fields of industry as mining, tube construction, building construction and so on. In emergency gas explosions, the damage caused by pressure resulting from gas or air-suspended solids propagation and interaction with them depends on many conditions, such as the initial conditions, the operating environment, and the properties and mechanical, physical and chemical characteristics of the obstacles [1,2].

Computational fluid dynamics (CFD) and computer modeling using different special software can offer potentially cost-effective design solutions for such complex gas explosion scenarios. Such kind of scenario could be dangerous, time-limited, and expensive for experimental research. Many researches were bounded with classical approaches, e.g. such as research using the Reynolds-averaged Navier-Stokes method (RAEN). Such kinds of research were implemented by many authors [3,4]. We use here known approach based on equation of Antoine which describes flame propagation of different physical and chemical substances. It could be solved taking into consideration mechanical, physical and chemical properties of substances, in our case there are air-suspended solids in different rocks. It is supposed that the composition is known, and the user can use known set of definite rocks characteristics for calculation. Knowing them, and pressure and heat of combustion of definite air-suspended solids as well, created interface reproduce the graphical implementation and several numerical results using GUI MatLab interface. Thus, the graphical results of lower and upper concentration limits of flame propagation could be calculated, and the graphical representation is animated also. These studies confirmed the high accuracy of MatLab with a graphical interface in predicting the key characteristics of propagated flames.

**Mathematicalmodel.** In order to calculate certain processes of flame propagation for the construction of various structures of underground structures in different rocks (f.e. granite, limestone, sandstone etc.), the construction of pipelines or during the construction of gas storages, various storages of minerals and so on, especially for construction in the rocks. Main combination of mechanical characteristics of rocks were taken from mining of Kazakhstan [5]. One of the most important characteristics of flame propagation is the calculations of the lower and upper concentration limits of flame propagation. In order to calculate them, the classical theories of the theory of heat transfer are used, in particular, one of the Antoine equation, which describes the dependence of the pressure of saturated vapors of liquids on atmospheric pressure and on the characteristics of the medium itself. Thus, the temperature can be calculated, that is, the heat of combustion and the lower and upper concentration limit of flame propagation. This research used several definite air-suspended of saturated vapors of liquids that propagate in different rocks (e.g. along a certain pipes). Here, the interface developed by the authors in the MatLab environment, provides the possibility of knowing certain input parameters, such as the characteristics and the A, B, C of the Antoine equation constants, knowing the atmospheric pressure in kPa, allows you to calculate the flame propagation temperature and thus calculate the lower and upper concentration limit of flame propagation. Naturally these limits depend on the heat of combustion in each specific environment.

*The calculation of the lower concentration limit of the flame propagation of air suspensions.*

The value of the lower concentration limit of the flame propagation (CLFP) of air-suspended particles (g/m3) for organic compounds (not applicable for calculating the combustion of metals):

$$CFLP = \frac{100 \cdot M}{a_1 \cdot \beta \cdot b_1 \cdot (\Delta H_i - \sum V_i \cdot \Delta H_{i1000})} \qquad (1)$$

$M$ – is the molecular weight of the dust; $\beta$ – is the stoichiometric coefficient of oxygen in combustion reactions; $\Delta H_i$ – heat of combustion; $V_i$ – is the stoichiometric coefficient of combustion products; $\Delta H_{i1000}$ – heat content of combustion products (enthalpy) when heated from 298 to *1000 K*; $a_1$ and $b_1$ are empirical coefficients for a given class of combustible materials.

Formula for calculating the lower concentration limit for organic compounds:

$$CFLP = a - \frac{b}{\Delta H_i} \qquad (2)$$

where *a* and *b* are empirical coefficients.

$$CFLP = \frac{8 \cdot 10^5}{-\Delta H_{cm}^0} \qquad (3)$$

Here $H_{cm}^0$ is heat combustion. The relative root-mean-square error of calculation by formula (3) is 15%.

*Dynamic concentration limit of the flame propagation (CLFP) model.*

To create certain mathematical models, the proposed dynamic formulation for the lower and upper concentration limits of flame propagation was used here. For this purpose, some experimental data obtained from measurements of flame propagation in various mixed mixtures were used to develop a conceptual model of the similarity of the lower concentration. The created application package has been successful in predicting the operation of certain industrial structures, where the contribution of mathematical and computer modeling is the simplest and most viable for numerical implementation.

*Temperature limits of flame propagation of individual liquid substances.*

If the dependence of the saturated vapor pressure of a liquid on temperature is known, then the value of the lower or upper temperature limit of flame propagation $t_n$ (°C) can be calculated using the corresponding value

$$t_n = \frac{B}{A - \lg(\varphi_n \cdot P_0 / 100)} - C_A, \qquad (4)$$

where $A$, $B$, $C_A$ – are the constants of the Antoine equation expressing the dependence of the pressure of saturated vapors of liquids, $\varphi_n$ – the proportion of the gas phase.

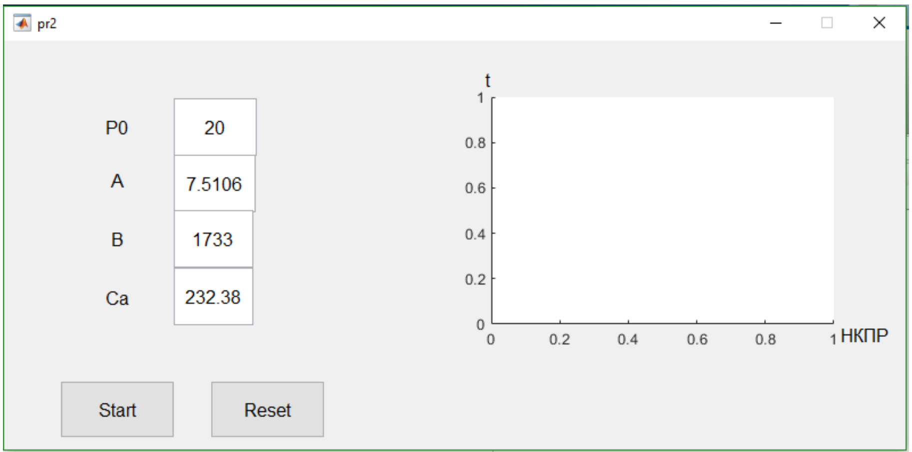
**Numerical procedure.** In order to create mathematical models and construct corresponding models of the present study, the following tasks were performed [6-8]:

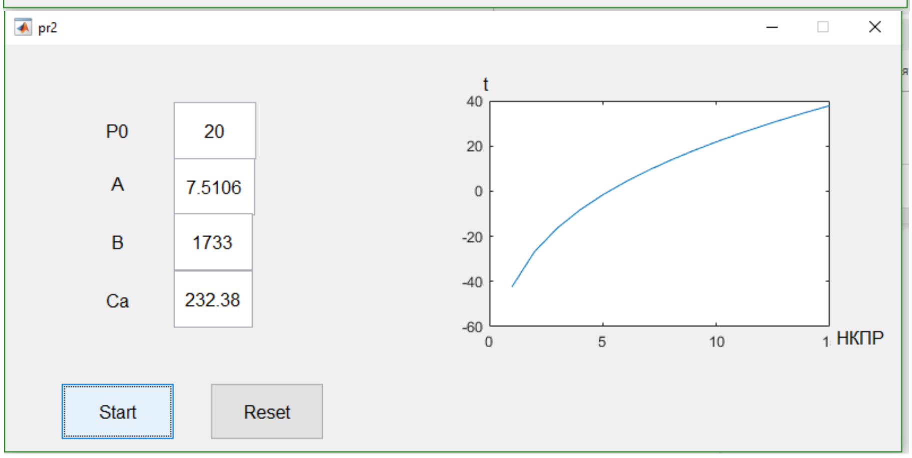
1. to calculate the Antoine equation and the upper concentration limits of the propagation of the flame of air-suspended of varying structures.

2. based on mathematical models developed by authors, computer models were developed. They were used for the corresponding parameters of the Antoine equation' constants and current atmospheric pressure, the known heat of combustion of air-suspensions.

3. a corresponding interface was created using the named input parameters, calculated the numerical values of the lower and upper concentration limits of flame propagation and the temperature. Flame concentration limits propagated by this definite temperature in certain directions. In this case, the corresponding built-in MatLab library was naturally used for calculations, the value of analytical and special functions of Bessel were displayed, the result was displayed both in numerical form and in graphical form (2D graphs). This plot represents the dependence of the lower concentration limit on time of flame propagation. Thus, a created interface was presented various structures of the flame beams of isopropyl alcohol, whose limit varies from 1 to 12%, while the corresponding Antoine's equation constants are taken as A = 7,5106, B = 1733,0, CA = 232,38. Concentration of atmospheric pressure is P0 =20 kPa.

The model described in this study is created using GUI MatLab. It solves fully compressible interdependent comparisons written in Cartesian coordinates and discretized and using the finite element method. Discretization is based on the formulation of the control volume of a homogeneous Cartesian grid. The first-order central difference approximation is used for the diffusion terms pulse pressure for the gradient in the pressure correction equation. The equation advances in time is fractional steps. We take several iterations of linking the equations to each other. Used boundary conditions for compressible flow is used to prevent bolt pressure at this boundary. Model is implemented by setting a variable at the lower center of the chamber to achieve an initial quasi-laminar phase match most experiments.

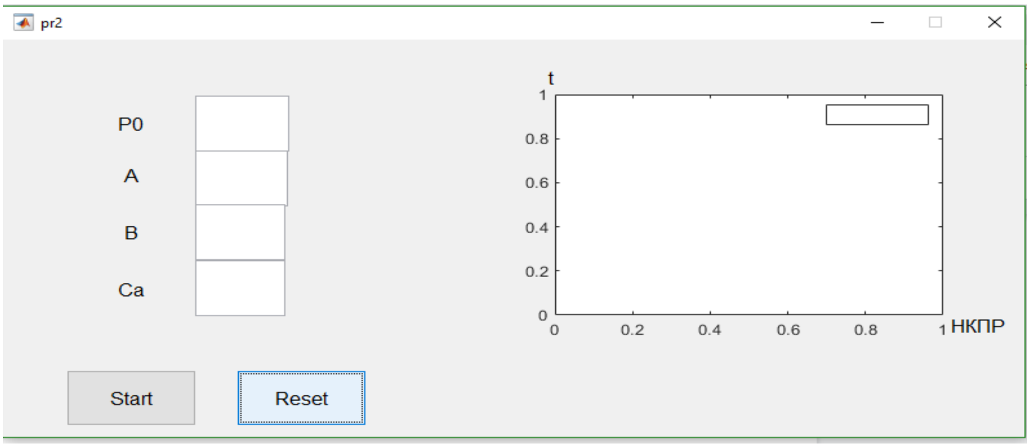



Modeling in the MatLab environment at start screen presents several forms with initial parameters and empty fields for answers. After entering the initial data, pressing the start button, the program starts calculating the unknown's values. Here is a code snippet that allows you to calculate and see how the lower boundary limits of certain substances were set.

When launched, the user sees several forms with initial parameters and an empty chart.

After you have entered the values and clicked on the “Start” button, the program will calculate the value of the unknowns and build a graph.




After pressing Reset, the program deletes the values of the variables and the graph.

p=get (handles.edit1,’string’); % value PO
p= str2double (p);
a=get (handles.edit2,’string’); % constant value A
a= str2double (a);
b=get (handles.edit3,’string’); % value B
b= str2double (b);
c=get (handles.edit4,’string’); % value Ca
c= str2double (c);
n=1:1:15;% CFLP
t=b./(a-log(n*p./100) ) | ¯c
plot (t)

Code snippet is responsible for the operation of the 'start' button, calculations and for the construction of the graph.

```
set(handles.edit1,'string', '');
set(handles.edit2,'string', '');
set(handles.edit3,'string', '');
set(handles.edit4,'string', '');
axes(handles.axes1)
cla;
legend('');
```

Thus, the interface in GUI MatLab was created and it helps to model several simple calculations and demonstrate the numerical calculation of CLFP for different rocks.

**Conclusion.** Predictions of possible explosions or fires in the combustion chamber can be presented for different models of the rate of mechanical and chemical reactions. Here, as we have already noticed, a dynamic model of the lower and upper concentration limits of flame propagation on base of Antoine’s equation was used. This task was carried out using an empirical model and a dynamic model, and the finite element method was used in MatLab modeling [9-13]. A close comparison of the existing model by the existing developed model by other models was not carried out due to the lack of data in the existing one, if, however, the created dynamic model in the form of an interface can be used for general prediction of turbulent and weakly turbulent air-suspensions showing a clear interaction between the air flow of suspensions and possible solid obstacles. The animation interface will show the time of the peak pressure occurrence, which can probably improve the errors associated with the calculation and modeling of flame propagation in various media, in pipes. Further studies are planned to evaluate the predictability of this model over a wide range of flow configurations.

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## MATLAB ОРТАСЫНДА ӘРТҮРЛІ ҚАТТЫ ТАУ ЖЫНЫСТАРЫНАН БӨЛІНЕТІН ГАЗ ҚАЛҚЫМАЛАРЫНЫҢ ЖАЛЫНЫ ТАРАЛУЫНЫҢ МАТЕМАТИКАЛЫҚ-КОМПЬЮТЕРЛІК МОДЕЛЬДЕРІН ЖАСАУ

**Аннотация.** MATLAB GUI графикалық ортасында жалынның концентрациялық таралу шегіне (CLFP) динамикалық тұжырымды қолдану арқылы желдетілетін жарылыс камерасында ауада тоқтатылған өтпелі бөлшектердің таралуы сандық тұрғыда зерттелді. Геомеханикалық және стехимиялық үдерістер стехиометриялық пропан-ауа арқылы тоқтатылған қатты денелер реакциясын имитациялайтын біратылы жалпы реакциямен модельденеді. Реакция жылдамдығы моделіндегі CLFP моделі Антуан теңдеуіне негізделген математикалық модельдермен сандық түрде қолданылады. Бұл жылдамдық ауытқуының эмпирикалық корреляциясына негізделген және графикалық іске асырумен енгізу-шығару деректерімен интерфейс ретінде жүзеге асырылады. Компьютерлік модельдеу CLFP динамикалық модельдері жалын таралуының физикалық үдерісінің жалпы жүзеге асыру арқылы жақсы нәтиже беретіндігін және түрлі тау жыныстарына қолдануға болатындығын көрсетті.

**Түйін сөздер:** MATLAB, графикалық интерфейс, жалынның таралуы, динамикалық CLFP, ауа-өлшенген зат, Антуан теңдеуі, жартас.

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## СОЗДАНИЕ МАТЕМАТИЧЕСКО-КОМПЬЮТЕРНЫХ МОДЕЛЕЙ ДИНАМИКИ РАСПРОСТРАНЕНИЯ ПЛАМЕНИ АЭРОВЗВЕСЕЙ ТВЕРДЫХ ВЕЩЕСТВ В РАЗЛИЧНЫХ ГОРНЫХ ПОРОДАХ В СРЕДЕ MATLAB

**Аннотация.** Распространение переходных, взвешенных в воздухе твердых веществ в вентилируемой взрывной камере численно исследуется с помощью динамической формулировки для концентрационного предела распространения пламени (CLFP) в среде GUI MATLAB. Геомеханика моделируется одностадийной общей реакцией, которая имитирует реакцию стехиометрического пропан – воздух– взвешенные твердые вещества. Моделирование CLFP в модели скорости реакции численно используется с математическими моделями на основе уравнения Антуана. Это основано на эмпирической корреляции флуктуаций скорости и реализовано в виде интерфейса с данными ввода-вывода с графической реализацией. Компьютерное моделирование показало, что динамические модели CLFP дают превосходные результаты в качестве общей реализации физического процесса распространения пламени и могут быть использованы для различных горных пород (например, гранита, известняка, песчаника и др.).

**Ключевые слова:** MATLAB, графический интерфейс, распространение пламени, динамический CLFP, воздух-взвешенные вещества, уравнение Антуана, скалы.

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