1D PHENOMENOLOGICAL MODEL ESTIMATING THE OVERPRESSURE WHICH COULD BE GENERATED BY GAS EXPLOSION IN A CONGESTED SPACE

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ABSTRACT

A phenomenological approach is developed to calculate the velocity of flame propagation and to estimate the value of pressure peak when igniting gaseous combustible mixtures in a congested space. The basic idea of this model is afterburning of the remanent fuel in pockets of congested space behind the flame front. The estimation of probable overpressure peak is based on solution of one-dimensional problem of the piston (having corresponding symmetry) moving with given velocity in polytropic gas. Submitted work is the first representation of such phenomenological approach and is realized for the simplest situation close to one-dimensional.

1. Introduction

The problem of an estimation of hazard and consequences of industrial accidents caused by explosion of combustible gases is crucial. It is now stimulated by the development of new applications of hydrogen as a fuel material. Direct modeling of industrial accidents involves key difficulties, which makes it a real challenge. Though the computational power continuously grows, CFD modeling of such tasks still requires huge resources and cannot guarantee the desired accuracy. In such a situation phenomenological models have their own range of applicability since they are bound with simplified consideration of real processes. The simplification of the physical pattern allows estimating process parameters promptly, and phenomenological models are very useful at the first stage of problem investigation.

Although it is difficult to imagine that essentially new phenomenological approaches could appear for problems investigated for many years, some elements of available models could be developed. For example the phenomenological estimate of the excess pressure due to an explosion is based on a model of burning in an enclosure with a vent hole. It is assumed that the bulk pressure is spatially uniform and the evolution of pressure in time is controlled by burning and by the outlet velocity of the gas in the vent hole. The most known implementations of such approach are the models **SCOPE** (**S**hell **C**ode for **O**verpressure **P**rediction in gas **E**xplosions) and **CLICHE** (**C**onfined **LI**nked **CH**amber **E**xplosion). These models are described, for example, in [1,2] and [3,4].

Prima facie the presence of a vent hole is a key element in these models, and the hole size should be small in a comparison with the total cross-section of the channel, to provide a value of excess pressure about hundreds mbars. In principle explosions in open congested areas cannot be described within this framework. Moreover this approach of an incompressible medium assumes that typical velocities in the considered area are smaller than the speed of sound. This assumption eliminates the opportunity to simulate modes with intensive shock waves, but the presence or absence of a closure and vent holes does not affect the correctness of such approach. It means that as long as the relations for incompressible medium can be applied to determine the position of flame front (and the value front velocity), the model should yield reasonable estimations of flow parameters. It is a motivation to reformulate a phenomenological model.

A basic way to adjust the models **SCOPE** and **CLICHE** consists in tuning the parameters controlling the “velocity of turbulent burning”. As a matter of fact, in a one-dimensional phenomenological

approach, the relations calculating the velocity of turbulent burning are used for model tuning. In such relations the usage of dimensionless criteria of Reynolds, Karlowitz, Markstein, Lewis does not look not so fruitful, especially in the case of a congested space, where the word “turbulence” covers all features of scale and geometry of a congestion.

2. Governing equations

In the work presented here, it is proposed to modify the phenomenological description of burning in a congested space. For this purpose the model of “turbulent burning” is replaced by a model of “afterburning of residual fuel behind flame front”. In such an approach the considered space is separated into two areas: the area behind the flame front and the area ahead of the front. The concepts “behind” and “ahead” are bound with the direction of front propagation. Unburnt fuel remains partially behind the front in stagnant (vortex) areas of congested space as well as in boundary layers in vicinity of solid surfaces (fig. 1).

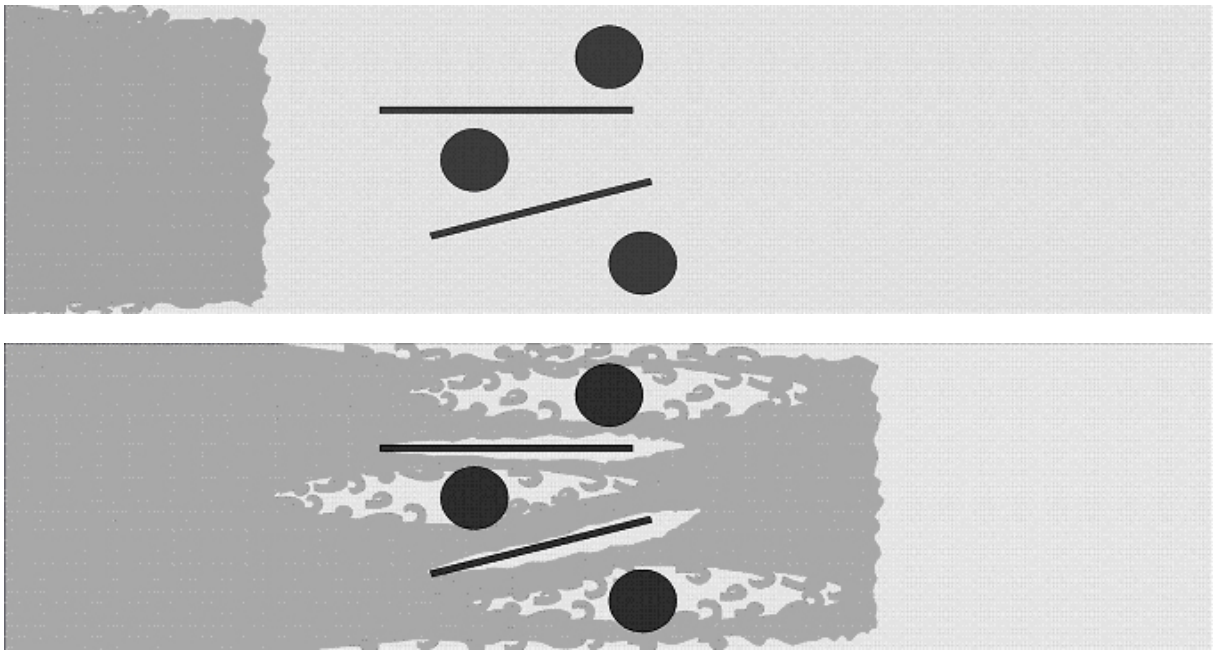

Figure 1. Propagation of flame front through congestion (combustible mixture is shown by grey colour, biscuit one denotes combustion products).

Within such approach the concept of “turbulent combustion regime” is not used at all. The congestion characteristics of the residual fuel have a geometrical explanation, and make more room for phenomenological intuition, than the concept of “velocity of turbulent burning”. The burning velocity in the proposed model differs from the velocity of a laminar flame only by a parameter accounting for the front “wrinkling”. This coefficient usually has value within limits from 2 up to 3, i.e. burning velocity (in air) for different combustibles is within range from ~1 m/s (methane) up to ~7 m/s (hydrogen). Such values considerably differ from the parameters used in conventional approaches, where the velocity of turbulent burning reaches values of tens meters per second.

The acceleration of the flame front happens owing to afterburning of residual fuel behind the front instead of a transition to a turbulent combustion regime. The combustion of this fuel can be rather prompt, as the surface of burning can be very large. In turn, the accelerated front transits bigger volume of congested space igniting residual fuel in it. The process occurs as long as the flame front encounters combustible domains. The combustible mixture leaking in free space is mixed with ambient air and other laws control the burning of this mixture. The processes of «exterior burning» is not considered here.

The assumption of a constant pressure in the considered area means, that gas motion occurs at velocities smaller than the speed of sound. In other words the hot gases have time to extend so to equalize pressure in the area after combustion of the fuel. This approach restricts the range of model applicability to rather weak "explosions". As it is known from the practice of gas-dynamic calculations, when disregarding compressibility effects it is still possible to obtain reasonable computational results up to a characteristic velocity of 70-80% of the sound speed (~ 200-250 m/s). If in the computational domain the velocity of the combustion front exceeds the sound speed, the model is not correct, and another procedure is required to estimate the value of the pressure peak.

In order to describe the kinematics of a motion of flame front let us formulate the continuity equations, energy conservation law, and the state of ideal gas at constant pressure:

$$\begin{aligned} &\frac{\partial \rho}{\partial t} + \left(\nabla, \rho u\right) = 0 \\ &c_p \rho \left[\frac{\partial T}{\partial t} + \left(u, \nabla T\right)\right] = Q \\ &\rho = \frac{A}{T} = \frac{\rho_0 T_0}{T} \end{aligned} \tag{1}$$

Substituting the equation of state, the continuity equation can be written as:

$$-\frac{\partial T}{\partial t} - \left(u, \nabla T\right) + T\left(\nabla, u\right) = 0 \tag{2}$$

The equation combining flow field with heat sources is obtained from equation (2) and the energy conservation law:

$$\left(\nabla, u\right) = \frac{Q}{c_p A} \tag{3}$$

In the one-dimensional case equation (3) allows calculating the dependence of velocity on coordinate using known distribution of heat source. The heat source Q in reduced equations is perceived both as due to burning in flame front and volumetric afterburning of residual fuel. Equation (3) is quasi-stationary, as Q is function of coordinates and time. The value of A also can be function of time, if pressure increase in area behind flame front has to be taken into account (for example the burning in closed volume with a vent hole). In order to determine the flow field in 2D and 3D variants of such model the additional condition of flow potentiality is required. Such requirement (absence of vortexes) does not contradict the previous reasoning about "residual fuel in vortex areas". It is known that the potential solutions with discontinuous flow over obstacles describe well actual streamlines and velocity distributions (excluding alone vortex structures). Earlier we use double term: stagnant (vortex) areas to emphasize that the vortex formations in actual flow is stagnant areas in the potential solution. For the subsequent estimation of pressure peak it is necessary to take into account that such method of modeling approximates well a kinematics of flow pattern, but underestimates its dynamic parameters.

Spatial coordinate in the one-dimensional approach is perceived as a line a perpendicular to a surface of flame front. Such interpretation allows considering more complex situation than one-dimensional geometry. However it is more convenient to present the model at consideration of simple geometry (spherical symmetry, cylindrical symmetry, one-dimensional channel). In case of complex configurations with several vent holes the determination of position of flame front and its velocity becomes an additional problem, which is not considered at the present moment. The experiments with open areas are selected to compare the data with calculations, i.e. at calculation of a kinematics it is

possible to consider that pressure in computational domain is approximately equal to atmospheric pressure and leave out of account the change of A with time. Taking into account pressure increase due to impeded flowing out has not key difficulties, but it is not required for presentation of model.

In proposed model the key element is the amount of unburnt fuel remaining behind flame front. Let us introduce the dimensionless function Ψ_v to describe the evolution of residual fuel. This function characterizes a portion of unburnt fuel behind the flame front. As in considered problems the initiation of "explosion" always happens in some point, it is reasonable to formulate function Ψ_v in form of spatial dependence on distance from this point. The elements creating congestion have own characteristic sizes. Therefore the characteristics of residual fuel should depend on these sizes. Initial value of function Ψ_v, i.e. its value at the moment of transit of flame front depends on properties of congestion and front velocity. The direction of flame propagation is important also, especially when the configuration of congestion is far from isotropic one. The construction of one-dimensional function Ψ_v by given geometry of congestion is a separate task; its successful solution determines the accuracy of estimations made by this model. In this direction the first steps are made only.

Let us accept the following functional dependence $\Psi_v(r, u_f(t_r), t; \alpha_i)$ for this function. Here: r is the distance from a point of mixture ignition, t_r is the time, when the flame front is in the point r, $u_f(t_r)$ is the velocity of flame front at an instant t_r, and α_i are the parameters featuring a congestion. It is clear that the function Ψ_v is determined only for $t \geq t_r$, and describes elementary layer (spherical, cylindrical or plane), i.e. yields averaged characteristic of residual fuel in such layer disposed at a distance r from ignition point.

After transit of the flame front, the residual fuel burns down some time, thus Ψ_v varies from initial value $\Psi_v(r, u_f(t_r), t; \alpha_i)$ down to zero. Let us use two characteristics to describe burning of residual fuel: $S_v(r, u_f(t_r), t; \alpha_i)$ surface area of burning in a unit volume and V_v velocity of flame propagation (relative to motionless gas) for process of an afterburning of residual fuel. Using these characteristics the equation for Ψ_v can be written as:

$$\frac{d\Psi_v}{dt} = -S_v \cdot V_v \tag{4}$$

The equation (4) allows calculating the heat source q_v behind the flame front. The following expression for q_v can be written using ΔT_{ad} of temperature increase at adiabatic - isobaric combustion of the mixture $q_v = -c_p \rho_0 \Delta T_{ad} \frac{d\Psi_v}{dt}$ then $\frac{q_v}{c_p A} \equiv \frac{q_v}{c_p \rho_0 T_0} = -\frac{\Delta T_{ad}}{T_0} \frac{d\Psi_v}{dt} = -(K_{ex} - 1) \frac{d\Psi_v}{dt}$, where K_{ex} is expansion coefficient of mixture after combustion. Fuel burning down in flame front generates a local heat source $q_f = c_p \rho_0 \Delta T_{ad} V_f \delta(r - r_f)$, where V_f burning velocity in flame front (with taking into account "wrinkling" coefficient, r_f is coordinate of flame front, and $\delta(r - r_f)$ is delta function. Thus, the equation (3) can be rewritten in form:

$$(\nabla, u) = (K_{ex} - 1) \left[V_f \delta(r - r_f) - \frac{d\Psi_v}{dt} \right] \tag{5}$$

The equations (4, 5) allow calculating the dependence $u(r,t)$, the position of flame front $r_f(t)$, and the velocity of this front $u_f(t)$. Zero velocity in ignition point is used as initial condition for equation (5).

The estimation of pressure peak by $\rho u_f^2/2$ value is essentially undervalued, as gas acceleration is not taken into account. It is proposed to use the value of pressure calculated at solution of one-dimensional problem of the piston (having corresponding symmetry) moving with given velocity in polytropic gas. Within framework of a considered problem, the "piston" is perceived as propagating flame front, and its velocity is boundary conditions for the problem of the piston. The equations of such model formulated using Riemann invariants R and S is written as (see for example [7]):

$$\begin{aligned}
&\frac{\partial R}{\partial t}+(u+c)\frac{\partial R}{\partial x}=-\kappa\frac{uc}{x},\\
&\frac{\partial S}{\partial t}+(u-c)\frac{\partial S}{\partial x}=-\kappa\frac{uc}{x},\\
&R=\mathrm{P}+u,\quad S=\mathrm{P}-u,\\
&\mathrm{P}=\int_{p_0}^{p}\frac{dp}{\rho(p)\cdot c(p)},\quad \frac{p}{\rho^{\gamma}}=const,\quad c=\sqrt{\gamma\frac{p}{\rho}},
\end{aligned}\tag{6}$$

where c is local sound velocity, and parameter k determines the type of geometry: 0 - flat, 1 - cylindrical, 2 - spherical. It is hardly reasonable to solve the equation (6) together with the equations (4, 5). It is enough to calculate the table distribution of pressure in a subsonic interval of velocities of the piston for three geometries, and further to use these data for pressure estimation. Basically, such three curves can be found and in the textbooks, for example, [8]. The symmetry type selected for pressure estimation should correspond to the conditions of development of actual flow.

3. Description of congested space and construction of functions $\Psi_v(r,u_f(t_r),t_r;\alpha_i)$ and $S_v(r,u_f(t_r),t_r;\alpha_i)$

In a phenomenological approach the information about congestion should correspond to the type of model. For a one-dimensional model one can use only one-dimensional functions, even if the detailed design of all elements of congestion is actually three-dimensional,. The simplest parameter describing congestion is the porosity $por(r)$, i.e. the portion of free space in section r (when referring to experimental situation the blockage ratio $br(r)=1-por(r)$ is often used.). Knowing the congestion geometry and the direction of the flame front propagation, it is basically possible to calculate the function $por(r)$. By implication of the model it is necessary to add stagnant areas to a geometrical porosity. The moving gas stream flows over these stagnant areas has the velocity of the flame front. Let us determine such "effective" porosity as $Por(r,u_f;\alpha_i)$. Additional complexity in the definition of function $Por(r)$ is the influence of congestion element on stream at some distance both downstream and upstream. Such influence depends on flow rate. In other words the function $Por(r,u_f;\alpha_i)$ is not completely determined by the congestion geometry, but it should be defined more exactly iteratively during solution procedure. The model of higher dimensionality (at least 2D) is desirable to improve the function $Por(r,u_f;\alpha_i)$.

If the function of effective porosity is constructed, the function of residual fuel Ψ_v basically is proportional to a difference of geometrical and effective porosity

$\Psi_v(r,u_f(t_r),t_r;\alpha_i) \sim \left[por(r) - Por(r,u_f;\alpha_i) \right]$. Except for stagnant areas taken into account in such way, there is residual fuel in boundary layers of surfaces. It is basic effect at flame propagation in channels without obstacles. The intuition suggests that increasing front velocity leads to increase of volume of stagnant areas, i.e. effective porosity $Por(r,u_f;\alpha_i)$ should have descending behavior.

Another characteristics of congestion elements is the averaged size of these elements $d(r)$ (or even the distribution function on the sizes $f(d,r)$). Basically this parameter determines the maturity of the surface of residual fuel combustion, i.e. the function $S_v(r,u_f(t_r),t;\alpha_i)$. At identical porosity in case of a congestion with small characteristic sizes the surface of residual fuel burning is more developed, i.e. the values of function $S_v(r,u_f(t_r),t;\alpha_i)$ is large. Apparently the maturity of the surface of residual fuel combustion increases with the parameter u_f. When burning the residual fuel its specific surface decreases. The following dependence should be proposed as first approach:

$$S_v(r,u_f(t_r),t;\alpha_i) = \frac{\Psi_v^{\xi}(r,u_f(t_r),t;\alpha_i)}{d(r)} \left\{ S_0 + S_1 \left(\frac{u_f}{c} \right)^{\beta} \right\}, \tag{7}$$

which has dimension (m^{-1}) required for S_v. The sound velocity c is used to make dimensionless variable of velocity. The coefficients S_0, S_1 as well as β, ξ are tuning parameters. All of them have to be positive and the value of ξ has not exceeded 1.

At the present moment it is necessary to limit consideration by arguing about choice of functions Por, Ψ_v and S_v. As the experience in data interpretation will be accumulated, the technique of construction of these functions and the range of variation of their values could be determined more precisely. When 2D model based on the same principles of solving procedure will be developed, the amount of free parameters decreases and the accuracy of taking into account congestion geometry increases.

4. Comparison of simulation results and experimental data

Actual explosion experiments of enough large scales in unclosed congested spaces are not so numerous, and their geometry has no sufficient symmetry to consider a situation as one-dimensional. In essence this experimental activity has not the purpose to approach to such symmetry. Usage of 2D approach would be more preferable, but such version of model is not ready yet. Therefore only the results of 1D modeling are presented.

Experimental data [5] and [6] are used for the comparison. These experiments considerably differ in volume of combustible mixture (4000 and 18 $м^3$ in [5] and [6] correspondingly) as well as in geometry of experimental rig and diameters of tubes creating congestion (0.315 m in [5] and 0.026 or 0.049 m in [6]). Besides the peaks of pressure the maximum velocities of flame front, temporal variation of flame front position and time evolution of signals of pressure sensors are given in [5].

The schematic diagram of experimental rig [5] and position of gates in experiments [6] are given in fig. 2 and 3 correspondingly. The experimental rig [6] comprises a steel lattice framework of 1 -m-cube cells. For the unconfined tests a framework which had 3 m × 3 m footprint, and which was 2 m high is used. The tables 1 and 2 show the data of experiments with natural gas selected from [5] and [6]. These data are supplemented by modeling results.

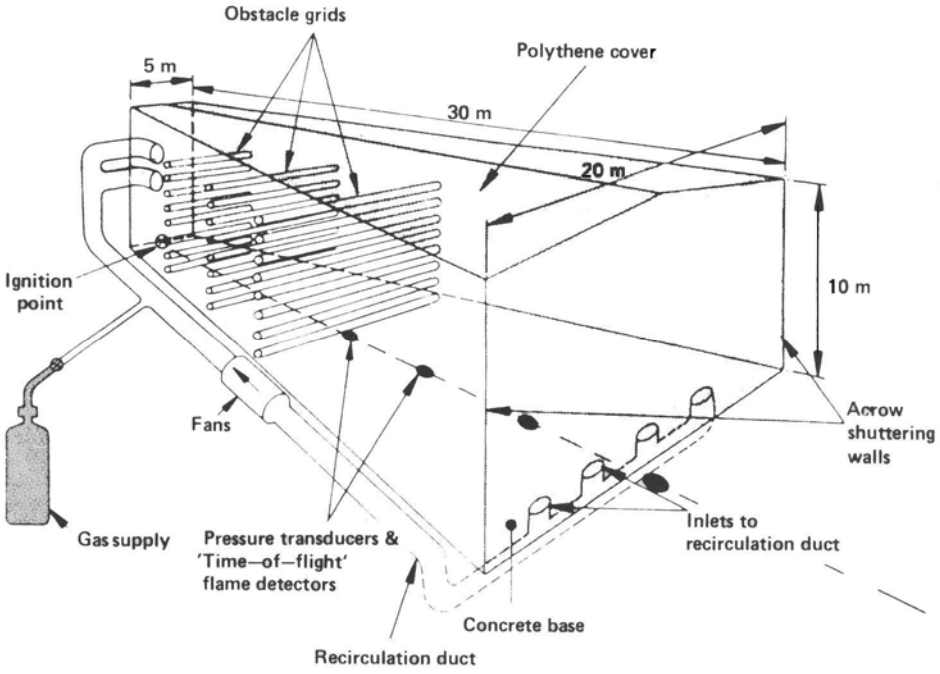

Figure 2. Schematic diagram of experimental rig [5].

The data on position of flame front and its velocity measured by photodiodes are rather useful to tune the parameters of model. They enable to estimate rate and duration of influence of each series of obstacles that allows selecting the parameters of residual fuel and specific surface area of burning. Though such measuring by photodiodes is conducted in both experiments, the relevant data are given in [5] only. Such data set allows better tuning the model. As a matter of fact all procedure of model tuning is based on the analysis of experimental data [5]. The same values of tuned parameters are used when experiments [6] are simulated using geometry from [6].

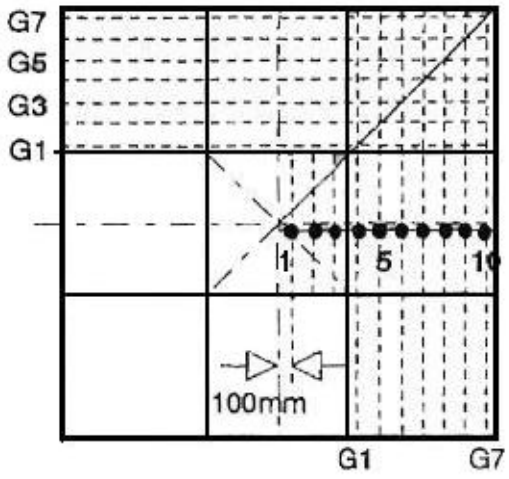

Figure 3. Position of gates in experimental rig [6].

Table 1. Comparison of calculated overpressure and maximum flame speed with experimental data [5].

Gas mixture				Obstacle configuration					Results			
Test	Fuel	Conc. % vol	Stoich.	No of grids	Intergrid spacing m	Blockage ratio %	No of pipes per grid	Grid height m	Max. flame speed exper.	estim.	Overpressure exper.	estim.
2	NG	8.8	0.95	-	-	-	-	-	8	9	5	5
4	NG	9.6	1.06	6	2	40	10	8	119	129	208	216
5	NG	11.6	1.31	3	2	40	10	8	49	35	55	21
6	NG	9.7	1.07	3	4	40	10	8	51	62	63	57
7	NG	10.0	1.11	3	5.8	40	10	8	50	41	30	29
9	NG	10.4	1.16	6	2	20	5	8	43	43	29	33
10	NG	10.2	1.13	6	2	40	5	4	37	43	30	33
13	NG	10.3	1.15	-	-	-	-	-	?	8	4	4

Table 2. Comparison of calculated overpressure with experimental data [6].

Test	Fuel	Gate BR	Gate (N/S)	Gate BR	Gate (E/W)	Gate BR	Gate (UP)	Stoich.	Peak overpressure exper.	estim
		%		%		%			mbar	
G	Methane	10	1,2,3,4	10	1,2,3,4	10	1,2,3,4	1.1	25	10
J	Methane	10	1,2,3,4,5,6	10	1,2,3,4,5,6	10	1,2,3,4,5,6	1.1	55	12
L	Methane	20	1,2,3	20	1,2,3	20	1,2,3	1.09	29	21
N	Methane	20	1,2,3,4	20	1,2,3,4	20	1,2,3,4	1.09	50	30
Q	Methane	20	1,2,3,4,5,6	20	1,2,3,4,5,6	20	1,2,3,4,5,6	1.1	109	63
BB*	Methane	20	1,2,3,4	20	1,2,3,4	20	1,2,3,4	1.1	45	15
DD*	Methane	20	1,3,5,7	20	1,3,5,7	20	1,3,5,7	1.09	37	32
DDD	Methane	20	1,3,5,7	20	1,3,5,7	20	1,3,5,7	1.1	80	12
FFF	Methane	30	1,3,5,7	30	1,3,5,7	30	1,3,5,7	1.1	154	215

* all obstacle diameters = 26mm except tests BB and DD (d=49mm)

Though exterior geometry of experiment [5] is similar to a spherically symmetric case, the geometry of set obstacles is closer to cylindrical symmetry. The attempts to simulate these experiments in spherically symmetric approach have not yielded to reasonable results. It could be explained that the actual flow pattern (and burning of residual fuel) is set by blockage and its symmetry. Therefore all reduced simulation data are obtained using cylindrical symmetry. Only initial stage of flame propagation (up to the first series of obstacles) is considered as spherically symmetric.

Except for relations reduced above, at model operation the experimental data on velocity of laminar flame propagation depending on stoichiometric ratio of mixture $v_{lam}(St)$ and similar dependence $\Delta T_{ad}(St)$ (or $K_{ex}(St)$) obtained from thermodynamic calculation are used.

Coincidence of calculated and experimental data for [5] (table 1) could be considered as good enough, while the modeling is not so successful in case of [6] (table 2).

Principal explanation of such situation is the absence of sufficient symmetry in congestion of experiments [6]. Among 9 inferior cubic cells four of them do not contain lattices at all, four cells have an identical blockage ratio, and lost one has doubled blockage ratio. Such construction is far from cylindrical symmetry as well as from spherical one. The most essential moment is the double density of obstacles in an angular cube. This cube will determine maximum peak of pressure, especially at low

blockage ratio. Certainly, within the framework of the one-dimensional approach it is impossible to take into account such design features. Since the model tuned on experiment of a large scale has not given senseless results at simulation of small scale experiments, it could be considered as the positive moment.

5. Conclusions

The phenomenological approach presented here eliminates the concept of "turbulent combustion regime" from physical model of flame propagation. In co-ordinates bound with flame front position the burning occurs at rather low speeds, namely with velocity of a laminar flame typical for considered mixture multiplied by wrinkling coefficient of a surface of flame front. An acceleration of the flame front and generated peak of pressure arise because of an afterburning of residual fuel behind the flame front in stagnant areas and boundary layers.

Testing of the model has shown reasonable coincidence with experimental data [5] that is not surprising, as the model was tuned by these experiments. There is a considerable discrepancy between simulation results and data [6] that could be explained by applying of one-dimensional modeling to the experiments, which have not right symmetry. In order to verify proposed approach, it is necessary to analyze much more experimental data.

Though 1D approach of developed model is presented here, kinematic calculation based on potential model of gas flow could be implemented for higher dimensionality. The procedure determining the position of flame front should be the basic additional unit of models of higher dimensionality. Even a 2D version of this model could essentially clarify the mechanism of residual fuel formation.

A number of experiments and actual situations should be considered with taking into account vent holes. Unconditionally such modification of the model will extend the range of its applicability. However it is necessary to keep in mind that merely deflagration situations can be modeled at used assumption of medium incompressibility. Nevertheless such restriction remains broad enough range of actual situations, where such estimations are valid.

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