

Initiation and its Optimization

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Abstract. The critical initiation energy E_* for detonation wave (DW) is used as the base parameter of detonation hazards. The spatial–time history of initiator energy–release is required for correct experimental determination of critical initiation energy. An influence of spatial factor of initiator energy–release is not similar to time factor: the optimal configuration exists when initiation is more effective. The blast explosion approximation is more preferable for correct experimental determination of E_* . The similar method is identically suitable both to the various initiators with of large distinctions in the spatial–time characteristics of energy–input (flame igniters, electrical or laser spark, exploding wire, high explosive, high-speed bullet...), and to various fuel–oxygen and fuel–air mixtures. The ways of optimisation of critical energy are discussed. Code SAFETY was used for calculation of cell size, critical initiation energy, critical diameter, etc. Calculated results are well correlated with experimental data.

The scientific, practical, hazardous and ecological aspects of large-scale accidental explosions of gaseous fuels attract attention of the researches from many countries. The determination of the critical initiation energies for detonation and combustion processes is the fundamental scientific and practical problem.

In this report the contemporary state of experimental and theoretical aspects of initiation problem are discussed. Calculated results are compared with experimental data.

The excitation of detonation or combustion regimes has a threshold character (“yes” – “no”, “go” – “no go”) for any initiator types. The minimal energy ensuring 100% initiation (“yes”, “go”) for given conditions is named traditionally as the critical energy. Usually the critical energy is characterized by some curve traced on boundary of “go” – “no go” areas on diagram of the initiator energy in dependence of some parameter (initial pressure or temperature, discharge duration, electrodes gap, etc.). For example, the critical initiation energy of spherical detonation (the area I higher continuous curve) and critical ignition energy

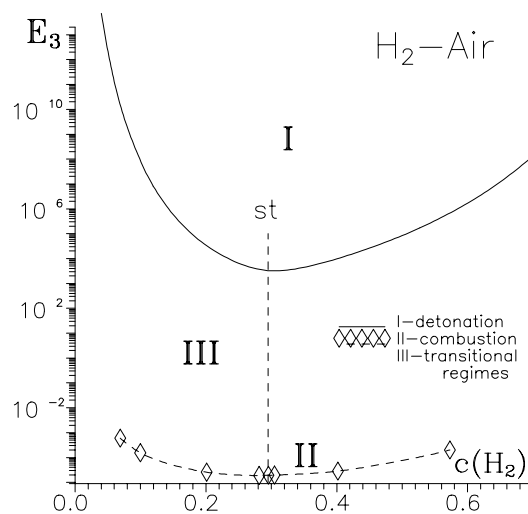


Fig. 1.

(dotted curve II) on molar hydrogen concentration in hydrogen-air mixtures is demonstrated on Fig.1 (similar graphs exist for any fuel-oxygen or fuel-air systems), $E_3 - J$.

According to modern classification the excitation of fast chemical reaction in combustible mixture is carried out by three basic ways: 1) – ignition (weak initiation), when a laminar flame with velocities about some cm/s is initiated only; 2) – (ignition + DDT) case (intermediate initiation), when mixture is fired only on initial stage, and then because of natural or artificial acceleration of the flame front the subsequent transition from deflagration to detonation (DDT) can be observed; 3) – strong initiation, when self-sustaining detonation wave (DW) is formed in neighbouring area with initiator.

In the first case the critical ignition energy E_{flame} acts as the main hazard parameter traditionally. For second case the quantitative criterion of DDT conditions, which be useful for practical applications, is not formulated up till now by virtue of multi-parametric of DDT-phenomenon. In third case the DW- initiation is multi-parametric process too, but for «ideal» initiators only one parameter – the critical initiation energy E^* – may be acts as a measure of explosion hazard: the E^* is less, the combustible mixture is dangerous. The area III on Fig.1 corresponds to transitional regimes with possibility of DDT.

The correct experimental measurement of the E^* (the criterion of the «ideality» of initiator) is important for uniform description of detonation safety problem. And the spatial-time characteristics of energy–release must be taken in account for correct experimental comparison of energy reserves of various initiators.

The E^* value for different initiators (electrical or laser sparks, high explosive, exploding wire, etc...) can be defined experimentally by the trajectory $r(t)$ of blast wave from initiator on initial stage, when the $r(t)$ -law is self-similar in accordance with the strong point blast model (*Sedov, Korobeinikov, Sakurai*) and depends on only an energy release. The similar method is identically suitable both to the various initiators with of large distinctions in the spatial–time characteristics of energy-input, and to various mixtures. Such procedure of determination of the experimental values of E^* for cylindrical symmetry was checked for different initiators and it was demonstrate well correlation with the correct experimental data of other investigators (*Lee, Matsui, Ramamurthi, Vasil'ev*).

The spatial–time history of initiator energy–release is required for correct experimental determination of critical initiation energy and its optimisation (Fig.2 – nondimensional initiation energy on discharge duration). An influence of spatial factor of initiator energy–release is not similar to time factor: the optimal configuration exists when initiation is more effective (lines E_t and E_r on Fig.3).

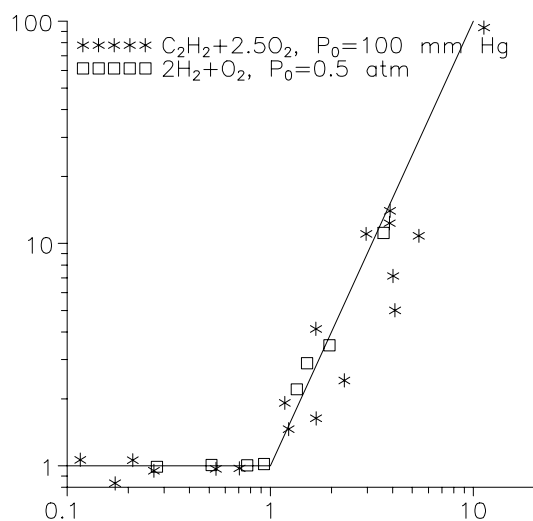


Fig.2.

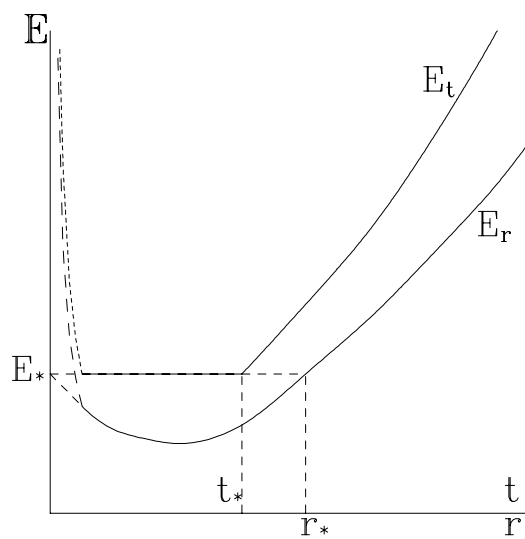


Fig.3.

Known theoretical models of DW-initiation were analyzed and classified on three types: 1) – numerical models: system of one-dimensional gas-dynamic and kinetic equations; 2) – approximate models for DW with one-dimensional smooth front; 3) – approximate models for real multifront DW (*Vasil’ev-Grigor’ev-Nikolaev-Uljanitsky.*).

The hydrodynamic system of the one-dimensional conservation laws for initiation problem with some kinetic model for induction and reaction zone describes in detail the qualitative picture of simultaneous initiation (*Chernij-Korobejnikov-Levin-Markov-Osinkin, He-Clavin, Eckett,...*). But for determination of E_* -value a few variants of long computation procedures are needed for each mixture. Up to now only a little quantity of gaseous mixtures was analyzed, for practice the hundreds mixtures are interesting at widest variation of the main parameters.

Practically all approximated initiation models (about 20: *Zeldovich-Kogarko-Simonov, Lee-Ramamurthi-Matsui-Bach-Knystautas-Guirao-Benedick-Sulmistras, Edwards-Hooper-Morgan, Sichel, Nicholls, Urtiew-Westbrook, Zhdan-Mitrofanov, Uljanitsky, Shulenin-Bohon, Borisov-Zamansky-Lisjansky-Skachkov-Troshin, Vasil’ev,...*) are based on one-dimensional conception of DW with smooth front.

But the real DW is non-one-dimensional and DW front represents the periodic pulsating complex from the shock and transverse waves (TW), contact discontinuous and local chemical reaction zones. The areas of TW collision are similar to “hot spots” or local micro-explosions. Such micro-explosions play an important role in propagation of multifront DW and especially in initiation process: multi-dimensional collisions of TWs of real detonation front noticeably lower the level of critical initiation energy. Only the model of micro-explosions initiation (*Vasil’ev - 1977, Vasil’ev-Nikolaev-Ulyanitsky - 1979, Vasil’ev-Grigor’ev - 1980*) takes into account the real structure of DW (it was named as MultiPoints Initiation (MPI) model). In accordance with MPI-model the critical energy E_* for initiation of multifront DW is proportional to the energy E_0 in area of TW collision - $E_* = n E_0$. The E_0 value for different symmetries may be calculated with the model of Detonation Cell (DC) (*Vasil’ev-Nikolaev -1976, 1978*). In accordance with DC-model the energy E_0 is proportional to the characteristic scale of multifront DW - the longitudinal size of individual cell b (or traditional cell size a). The coefficient $n = F(E, Q, \gamma, \nu)$, ..where E is the effective activation energy for induction period, Q - the chemical energy release in DW, γ - the specific heat ratio (or adiabata index), ν - symmetry index.

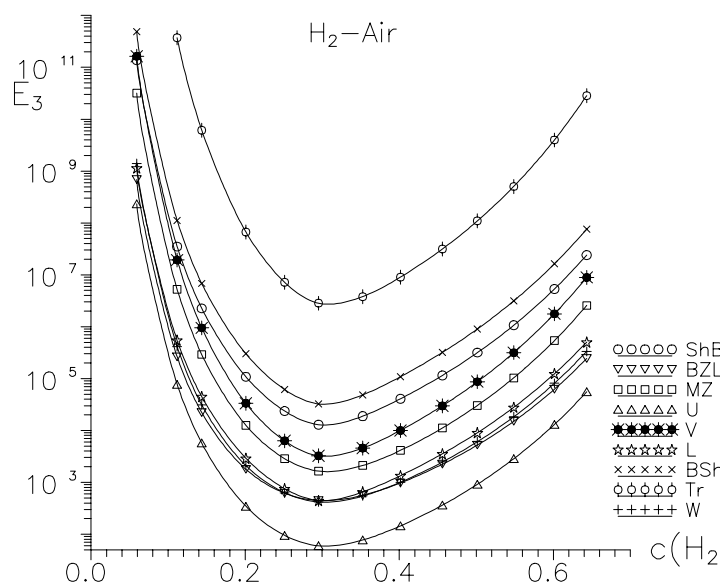


Fig.4.

The MPI-model is allowed to calculate the critical initiation energies for plane, cylindrical and spherical symmetries for any gaseous mixtures. The DC-model and MPI-model are common basic in Code “SAFETY” for calculation of the main parameters of combustion and detonation. The critical initiation energy of spherical detonation, calculated with the help of different initiation models for hydrogen-air mixtures at identical conditions (pressure, temperature, composition, kinetics coefficients, ...), is presented on Fig.4 as example. One can see great discrepancies among different models and only some individual models predict the initiation energy, which correspond to experimental data.

This information may be used for determination of detonation hazard of different mixtures at great variations of the basic parameters: initial pressure and temperature, mixture composition (from lower to upper concentration limits), adding of inert gases, replacing of oxygen on air or any other oxidizer... For example, data about critical initiation energy of spherical detonation on molar fuel concentration is present on Fig.5 for some typical gaseous fuels. Similar graph allow to compare the hazard of different systems. The main detonation parameters (pressure and temperature of products, critical diffraction diameter, critical diameter of gaseous charge, diameter of high-speed piston, size of forming zone...) are calculated also with the help of Code “SAFETY”.

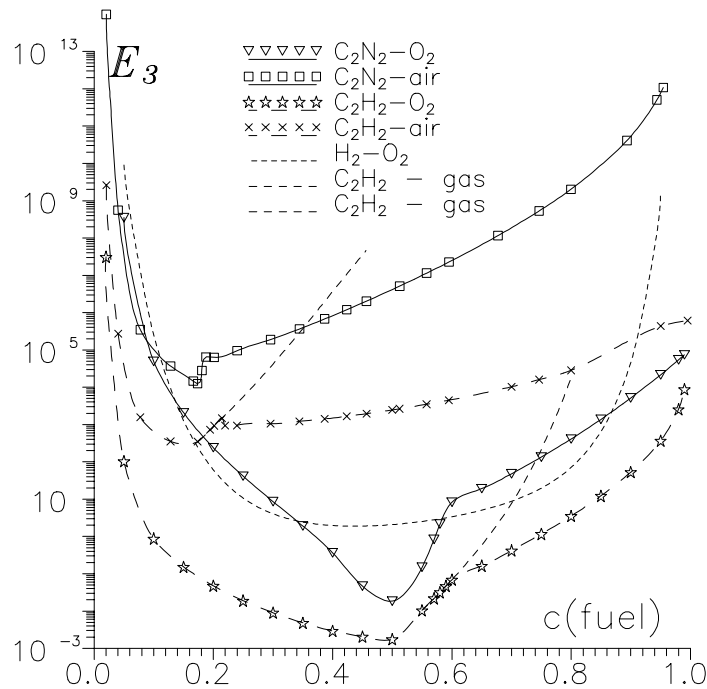


Fig.5. Duplication of lines for C2H2 and C2N2 systems is connected with carbon condensation.

All available experimental results on initiation of different gaseous fuels obtained in research centers of Russia, Canada, USA, France, Norway, Great Britain, Germany, etc., are examined in this report as a basis (*Zeldovitch, Kogarko, Simonov, Adushkin, Ljamin, Freiwald, Koch, Lee, Knystautas, Guirao, Benedick, Moen, Murray, Bull, Elsworth, Shuff, Methalfe, Bjerketvedt, Thibault, Edwards, Thomas, Nettleton, Stroganov.... and many-many others*).

The comparison of the calculated (with the help of MPI-model) results with the experimental data demonstrates their well correlation for different fuel-oxygen and fuel-air mixtures at variation of pressure, temperature, concentration, symmetry, etc. (Figs.6-11). The

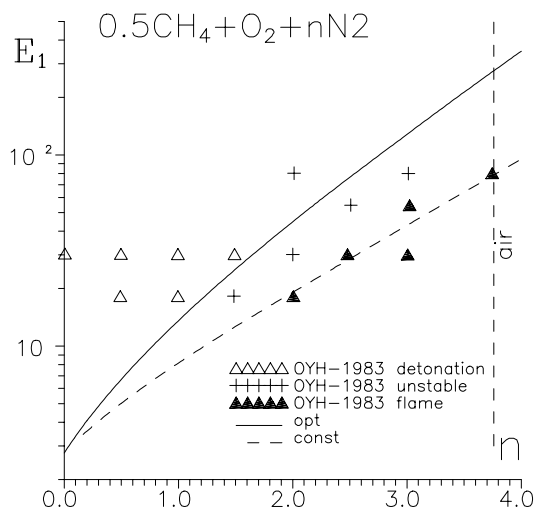


Fig. 6.

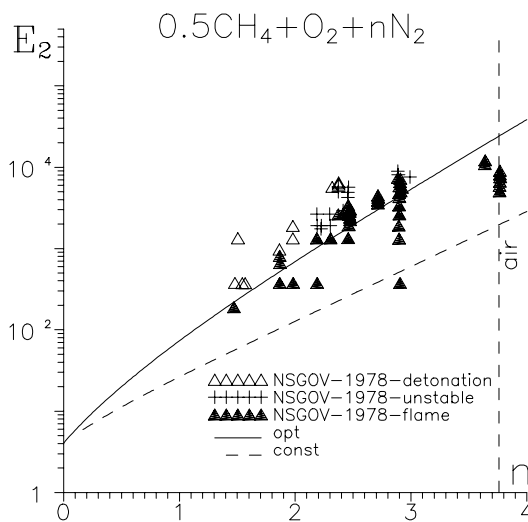


Fig. 7.

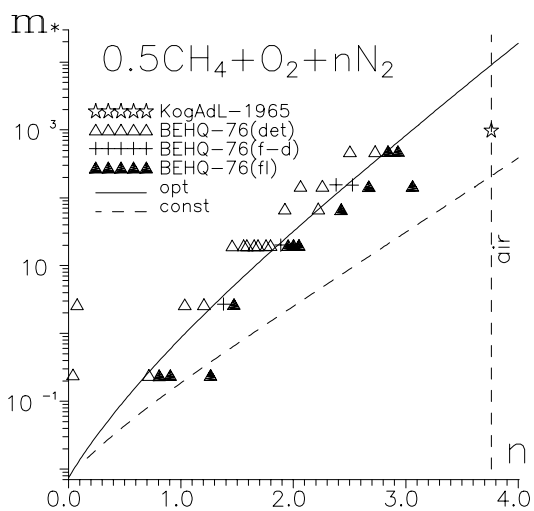


Fig. 8.

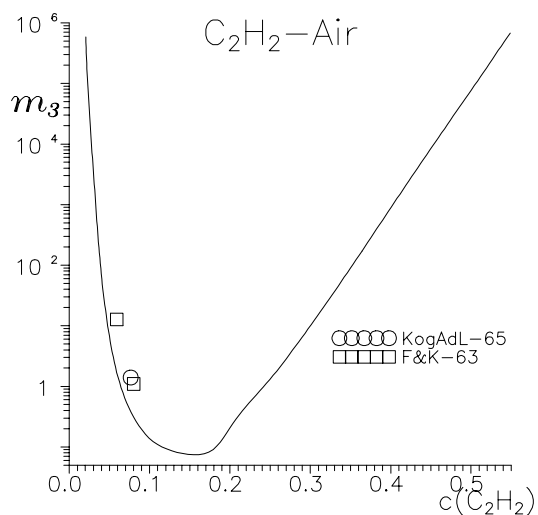


Fig. 9.

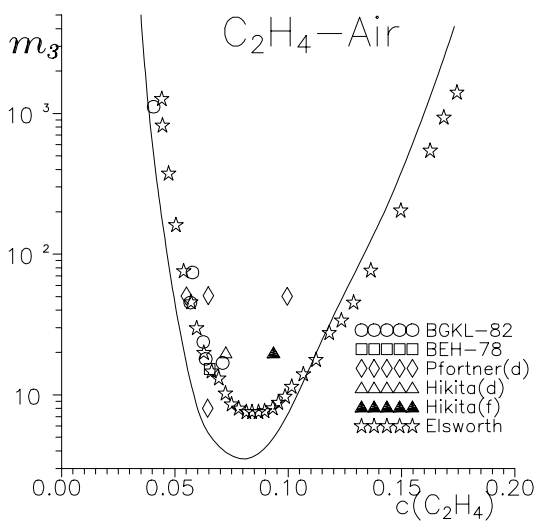


Fig. 10.

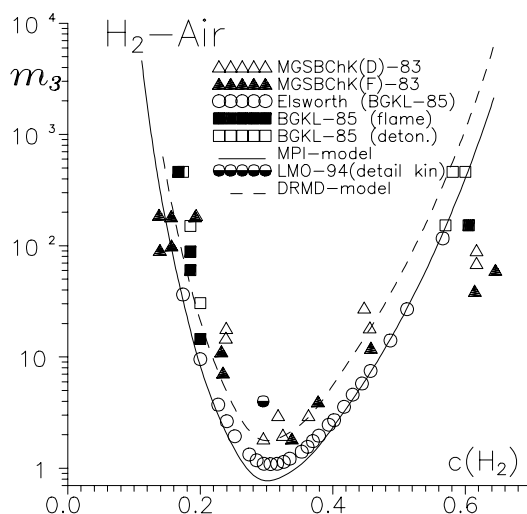


Fig. 11.

MPI-model may be used as the basic at determination of detonation safety of different gaseous fuels because it describes the experimental data the most adequately.

Some ways of optimization of DW–initiation can be proposed:

- 1) space distributions of energy–input;
- 2) initiation by a series of impulses;
- 3) initiation by the active particles;
- 4) initiation in mixture with gradients of parameters (density, temperature, composition,...);
- 5) initiation at focusing of shock waves;
- 6) initiation at reflection...

In first case two schema can produce the higher efficiency of DW–initiation:

a) spatial distribution of initiator (one or a few) with simultaneous triggering. At multi-charges schema it is possible to modify the charges quantity and its spatial distribution (ones another);

b) spatial distribution of initiators (two (as minimal) or more) with posttriggering – double-stroke mode (for example, schema with central and ring charges (of certain values of inner and outer radiuses), when at first the central charge is initiated and decaying blast wave is generated, then the ring charge is initiated with some optimal delay relatively the position of decaying wave).

Analogous idea is basic and for second case, when initiation is generated by pulse string. At this an amplitude and duration of individual impulse and off-duty factor of impulses have the certain optimal values for DW–initiation. Moreover, the efficiency of initiation can be increased at special configuration of electrodes system: instead of classical two–electrode schema with single initiator (type as spark-plug) the multi-electrodes schema with spatial distribution of individual electrodes can be used.

In third case the efficiency of DW–initiation can be increased by injection of hot or active substances, including ionized, into induction zone of decaying wave, generated by single initiator. Such particles play promoter role. The classical well-known schema for excitation of hard-initiated mixture is using of additional initiation section with high-active mixture. It must be emphasized that in any posttriggering schema the energy of first initiator is much lower the critical (analogously for another initiators). The DW–initiation in mixture with gradients of parameters is studied insufficiently, but this case is interested not only from scientific point of view, but of view its practical application in optimization tasks.

It is well-known now that reflection of shock wave from concave surface is more

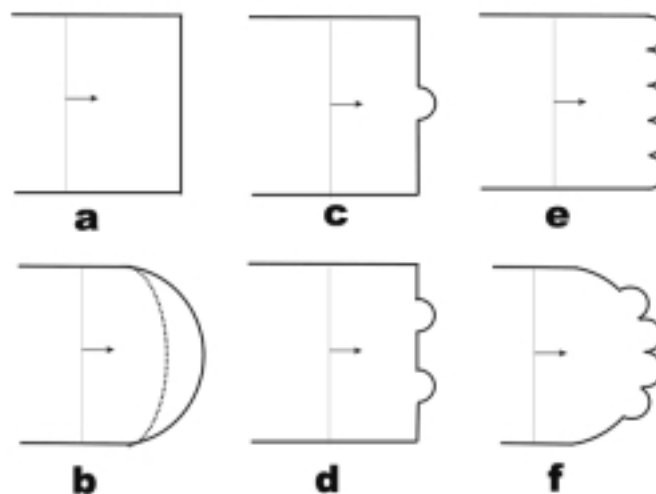


Fig.12.

effective for self-ignition processes in comparison with plane surface. The higher efficiency can be attained with schema of multi-focusing system (Fig.12,c-e) and especially at double focusing (Fig.12f). The experimental data demonstrates that the Mach number of SW for initiation of DW can be decreased visibly in case of multi-focusing system in compare with cases of reflection from plane surface or single concave reflector (Fig.13), left point corresponds to case of double focusing (Fig.12f).

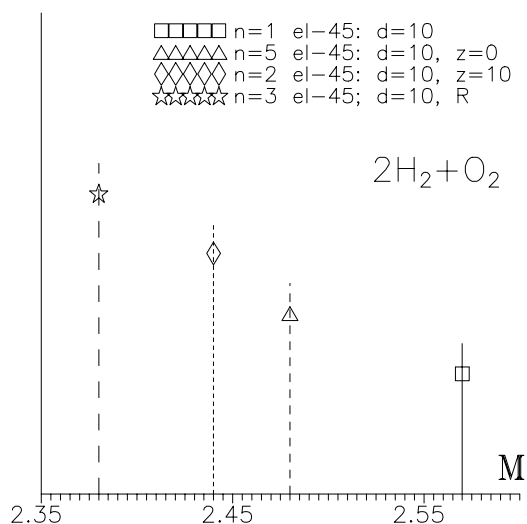


Fig.13.

It is possible to increase sharply temperature, pressure and density, if some part of a front of decaying wave will be reflected from obstacles. Such obstacles can be solid (permeable barrier with characteristic size which is smaller than channel size – an apertured disk in tube, for example) or perforated (metallic mesh, for example). At this the increasing of initiation efficiency was confirmed by experimental investigation and numerical modelling: the critical initiation energy can be decreased up to order at some optimal position of reflected “wall”.

The problem of optimal initiation of detonation wave is the most important at creating of Pulse Detonation Engine (PDE).

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(only devoted to MPI-model and some experimental data)

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