Annihilation catastrophe: From formation to universal explosion

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I present a systematic theory of formation of the universal annihilation catastrophe which develops in an open system where species A and B diffuse from the bulk of restricted medium and die on its surface (desorb) by the reaction $A + B \rightarrow 0$. This phenomenon arises in the diffusion-controlled limit as a result of self-organizing explosive growth (drop) of the surface concentrations of, respectively, slow and fast particles (concentration explosion) and manifests itself in the form of an abrupt singular jump of the desorption flux relaxation rate. As striking results I find the dependences of time and amplitude of the catastrophe on the initial particle number, and answer the basic questions of when and how universality is achieved.

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I. INTRODUCTION

For the last decades it has been shown that in spite of the fundamental simplicity the reaction-diffusion system $A + B \rightarrow 0$ exhibits rich cooperative behavior [1]. One of the most impressive examples in the class of systems with bulk reaction is the phenomenon of Ovchinnikov-Zeldovich segregation (spontaneous growth of single species domains which leads to anomalous reaction deceleration). Here I focus on another wide class of systems where reaction proceeds on the catalytic surface of medium whereas diffusion proceeds in its bulk. In the work [2] it was first demonstrated that in this class of systems the interplay between reaction and diffusion acquires qualitatively new features and leads to a new type of self-organization. It has been found that once particles A and B diffuse at different mobilities from the bulk of restricted medium onto the surface and die on it (desorb) by the reaction $A + B \rightarrow 0$, there exists some threshold difference in the initial numbers of A and B particles, $\Delta$, above which the loop of positive feedback is "switched on" and the process of their death, instead of the usual deceleration, starts to accelerate autocatalytically. Recently, it has been discovered [3] that the deceleration-acceleration transition is a prelude to much more nontrivial dynamical effects: in the diffusion-controlled limit $\Delta \rightarrow \infty$ a new critical phenomenon develops - annihilation catastrophe, which arises as a result of self-organizing explosive growth (drop) of the surface concentrations of, respectively, slow and fast particles (concentration explosion) and manifests itself in the form of an abrupt singular jump of the desorption flux relaxation rate.

The key features of the annihilation catastrophe have been obtained on the assumption that the initial number of $A - B$ pairs is large, so that after a transient stage the annihilation dynamics crosses over to the independent of initial pair number universal regime [2], [3]. Until now, however, the principal questions remain open: When and how is the universal regime achieved? Moreover, the central question concerned with the time moment of the catastrophe as a function of the initial pair number remains open too. In this paper I present a systematic theory which gives the exhaustive answers to these questions.

II. MODEL

I consider a model, in which species A and B are supposed to be initially uniformly distributed in the bulk of an infinitely extended slab of thickness $2\ell$. Both species diffuse to the surface $X = \pm\ell$ ($X \in [-\ell, \ell]$) and irreversibly desorb as a result of surface reaction $A_{ads} + B_{ads} \rightarrow AB$ with the rate proportional to the product of surface concentrations $I = k c_A c_B$ (Fig. 1). Because of planar spatial homogeneity the system is effectively one dimensional. The boundary conditions are determined from the equality of diffusion $I^D$ and desorption $I$ flux densities at the surface $I^D|_s = I$, i.e., it is assumed that the surface layer capacity can be neglected. According to [2], [3] after introducing index "H" (heavy) for slower diffusing species and index "L" (light) for a faster one, the problem of species evolution in the dimensionless units reads (by symmetry I consider the interval $[0, \ell]$ only)

$$\frac{\partial h}{\partial \tau} = \nabla^2 h, \quad \frac{\partial l}{\partial \tau} = (1/p)\nabla^2 l,$$

$$\nabla h|_s = (1/p)\nabla l|_s = -h_l s,$$

with $\nabla(h, l) |_{x=0} = 0$ and initial conditions $h(x, 0) = h_0$ and $l(x, 0) = l_0$. Here $h(x, \tau) = c_H/c_s$ and $l(x, \tau) = c_L/c_s$ are the reduced concentrations, $\nabla \equiv \partial/\partial x$, $x = X/\ell \in [0, 1]$ is the dimensionless coordinate, $\tau = D_H t/\ell^2$ is the dimensionless time, $p = D_H/D_L \leq 1$ is the ratio of diffusivities, and $c_s = D_H k\tau$ is the characteristic concentration scale. According to (1b) particles disappear in pairs only, i.e.,

$$J = h_l s = -<\dot{h}> = -<\dot{l}>,$$

where $J = I/I_s$ is the reduced desorption flux density and $I_s = k c_s^2$ is its characteristic scale, therefore

$$<h> - <l> = \Delta = \text{const.},$$
i.e., the excess amount stays “inert” in the bulk (here \(< h > = \int_0^1 \text{d}x N_H/N_*\) and \(< l > = \int_0^1 \text{d}x N_L/N_*\) are the total reduced numbers of particles in the bulk per unit of surface and \(N_* = c_* \ell = D_H/\kappa\). This “inert” part of the majority species \(\Delta = \delta N/N_*\) acts as a control parameter, whereas its “active” part \(N = N_{pair}/N_*\) (equal to the total number of \(H - L\) pairs) acts as the only variable decaying from \(N_0\) to 0 as \(\tau \to \infty\). According to [2,3], the key features of nontrivial dynamics, developing in the system (1) in the diffusion-controlled limit \(N_0 = c_*(0)\kappa \ell / D_H \to \infty\), may be formulated as follows: When parameter \(\Delta\) achieves the threshold value

\[
\Delta_* = \sqrt{\omega_0/p \tan(\omega_0 p)}
\]  

(2)

(\(\omega_0 = \pi^2/4\) is the main eigenfrequency of the diffusion field relaxation), the system undergoes a transition to the state where after a transient stage the surface concentration of \(H\)-particles, \(h_s\), and as a result the rate of death of pairs start to grow with time autocatalytically (growth of \(h_s\) accelerates the drop of \(l_s\), the drop of \(l_s\) accelerates the growth of \(h_s\), and so on). With growing \(\Delta\) the autocatalytic stage becomes more and more pronounced so that far beyond the threshold self-acceleration acquires explosive character: at \(\Delta \to \infty\) the rates of growth \(\Omega_H = +d\ln h_s/d\tau\) and relaxation \(\Omega_L = -d\ln l_s/d\tau\) are synchronized singularly growing by the law

\[
\Omega_s = 1/|T|, \quad |T| = |\tau - \tau_\ast| \to 0,
\]

where the point of finite-time singularity \(\tau_\ast\) is achieved at the moment when the reduced number of pairs \(n(\tau) = N(\tau)/\Delta\) drops to some critical value \(n_\ast\). The most spectacular consequence of concentration explosion is singular behavior of the flux relaxation rate \(\tau^{-1}_j = -d\ln J/d\tau\) which is sustained constant up to the critical point \(\tau_\ast\) upon reaching which \(\tau^{-1}_j\) blows up abruptly to \(\infty\): at \(K = p^{3/2} \Delta/\Delta_* \to \infty\) the width of the jump is contracted and its amplitude grows by the laws

\[
|T|_{cat} \propto \Delta^{-2/5} \to 0, \quad \max \tau^{-1}_j \propto \Delta^{1/4} \to \infty.
\]

In the work [3] it has been shown that in the limit \(n_0 = N_0/\Delta \to \infty\) this catastrophic jump of \(\tau^{-1}_j\), called annihilation catastrophe, proceeds in the universal \((n_0 -\) independent) regime and the scaling theory of universal explosion has been given. However, the approach developed in [3] did not allow one to say anything neither about the dynamics of explosion formation, nor about how the universal regime is achieved, nor about how the point of catastrophe depends on the initial conditions. The goal of this paper is to give a closed theory of annihilation catastrophe formation and, based on it, (a) to reveal the catastrophe universalization regularities and (b) to find the dependence \(\tau_\ast(n_0)\) for arbitrary ratio of diffusivities. I show that this strongly nonlinear problem allows for strict and elegant analytical solution. I reveal its surprisingly rich “structure”, and demonstrate remarkable agreement with numerical calculation results.

III. THEORY OF UNIVERSAL ANNIHILATION CATASTROPHE FORMATION

I start with the exact formal solution of the problem (1) in the Laplace space \(\hat{f}(s) = \hat{\mathcal{L}}f(\tau)\)

\[
\hat{h}(x,s) = h_0/s + (\hat{h}_s - h_0/s) \cosh(x\sqrt{s})/\cosh(\sqrt{s}),
\]

\[
\hat{l}(x,s) = l_0/s + (\hat{l}_s - l_0/s) \cosh(x\sqrt{sp})/\cosh(\sqrt{sp}).
\]  

(3)

According to (3) the BC’s (1b) acquire the form

\[
\hat{f} = (h_0/s - \hat{h}_s)\sqrt{s}\tanh \sqrt{s} =
\]

\[
= (l_0/s - \hat{l}_s)\sqrt{sp}\tanh \sqrt{sp} = \hat{\mathcal{L}}(h_0l_0/s)
\]  

(4)

and in an implicit form completely define the behavior of surface concentrations \(h_s\) and \(l_s\) which in turn via Eqs.(3) define the evolution of spatial distribution. The strategy for solution of the nonlinear chain (4) is based on that in the \(H\)-diffusion-controlled regime the \(\Delta \to \infty\) ratio should rapidly drop with the time, therefore, according to (4) we can first (i) calculate \(J(\tau)\) and \(l_s(\tau)\) neglecting the \(h_s\) contribution, then (ii) derive \(h_s(\tau)\) from the condition \(h_s = J/l_s\), and finally (iii) calculate next-to-leading terms thereby defining the self-consistent picture of surface concentrations evolution.

A. Transient dynamics \(\tau \ll 1\).

At sufficiently small times the flux density is slightly changed so assuming \(J \approx J_0 = h_0l_0\) from (4) one obtains

\[
h_s = h_0(1 - v_h + \cdots), \quad l_s = l_0(1 - v_l + \cdots)
\]  

(5)

where \(v_i = 2\sqrt{\pi} \sqrt{\tau/\tau_i}, \quad \tau_h = 1/l_0^2\) and \(\tau_l = 1/ph_0^4\). According to (5) relative drop rate for \(l_s\) and \(h_s\) is governed by the value of the parameter

\[
R = v_l/v_h = r \sqrt{p}
\]

where \(r = h_0/l_0 = (1 + n_0)/n_0\). So, the necessary conditions for the \(H\)-diffusion-controlled annihilation regime are fulfillment of the requirements \(l_0 = N_0 \gg 1\) and \(R < R_c = 1\). Taking the both requirements fulfilled from (5) and (4) one concludes that at \(\tau_h \ll \tau \ll 1\) the flux should drop by the law

\[
J = h_0(1 - m)/\sqrt{\pi \tau} \approx J_0(\tau_h/\tau)^{1/2}/\sqrt{\pi}
\]  

(6)

with \(m = |\tau/\tau_h| \to 0\). In the region \(\tau_h \ll \tau \ll p\) where the both species diffuse in the semi-infinite medium regime, from (4) it follows \(l_s - h_s \sqrt{p} = l_0\epsilon\) where \(\epsilon = R_c - R\). Assuming \(\epsilon > 0\) to be not too small from (4) and (6) we find

\[
h_s = \frac{r}{\epsilon \sqrt{\pi \tau}}(1 - \phi + \cdots), \quad l_s = l_0\epsilon(1 + \phi + \cdots)
\]  

(7)

where \(\phi = (R/\sqrt{\pi \epsilon^2}) \sqrt{\tau_h/\tau}\). Using then (5) and (7) we self-consistently find \(m \sim (R/\epsilon^2)^2(\tau_h/\tau) \ll \phi\) to conclude
that asymptotics (7) is realized at the condition $\epsilon \gg \tau_h^{1/4} = 1/\sqrt{N_0}$. In the opposite limit $0 < \epsilon \ll \tau_h^{1/4}$ by the same procedure we come to the critical asymptotics

$$l_s(1 - g + \cdots) = \sqrt{\rho} h_s(1 + g + \cdots) = \frac{l_0}{\pi^{1/4}} \frac{(\tau_h)}{1/4} (1 - \phi_c + \cdots),$$

where $g \sim c(\tau/\tau_h)^{3/4}$ and $\phi_c = m_c/2 = c(\tau_h/\tau)^{3/4}$ with $c = \pi^{1/4}G(\frac{3}{2})/2G(\frac{3}{2})$. At sufficiently small $p$ and not too large $r$ (so that $R \ll R_c$) in the region $\tau_h, p \ll \tau \ll 1/\rho^2 < 1$ the $L$ particles distribution becomes uniform. In this regime from (4) and (6) we find

$$h_s = \frac{r}{\sqrt{\pi}} (1 - \rho + \cdots), \quad l_s = l_0 (1 - \sigma + \cdots), \quad (8)$$

where $\sigma = 2r\sqrt{\tau/\pi} + O(r\sqrt{\tau}/R\sqrt{p/\tau})$.

**B. Self-accelerating dynamics $\tau \gtrsim 1$.**

According to Eqs.(7), (8) at large $N_0 \to \infty$, $\epsilon \gg 1/\sqrt{N_0}$ and not too large $r$ (i.e. not too small $n_0$) by the moment $\tau \sim 1$ when the diffusion length of $H$ particles becomes comparable with the system’s size, the ratio $h_s/h_0 \propto r\sqrt{N_0} \to 0$. Neglecting the $h_s$ contribution, it can be shown (see below) that at $\tau > 1$ and large $n_0$ the $h_s$ value has to exponentially rapidly tend to a constant $C$. In view of this, according to (4) we write

$$\dot{J} = (h_0 - C) \tanh(\sqrt{s})/\sqrt{s},$$

whence it follows

$$J = A e^{-\omega_0 \tau} (1 + e^{-8\omega_0 \tau} + \cdots), \quad (9)$$

where $A = 2(h_0 - C) \approx 2h_0$. With the same accuracy from (4) we have

$$\dot{l}_s = l_0/s - [(h_0 - C)/s] \sqrt{\rho} \tanh(\sqrt{s}) \coth(\sqrt{s}\rho)$$

whence it follows

$$l_s = (A/\Delta_c) e^{-\omega_0 \tau} (1 - \Lambda), \quad (10)$$

where $\Delta_c$ is defined by Eq.(2) and the leading contribution to $\Lambda$ is governed by the sum of exponentially decaying, $\Lambda_-$, and exponentially growing, $\Lambda_+$, terms

$$\Lambda = \Lambda_- + \Lambda_+, \quad \Lambda_- = \delta_8 e^{-8\omega_0 \tau} + \delta_p e^{-\chi\omega_0 \tau}, \quad \Lambda_+ = \lambda e^{\omega_0 \tau} \quad (11)$$

with exponent $\chi = (4/p - 1)$ and amplitudes

$$\delta_8 = -\frac{(\Delta_c/3) \sqrt{p/\omega_0} \cot(3\sqrt{2\omega_0 p})}{\lambda \sqrt{p/\pi}}; \quad \delta_p = (\Delta_c \sqrt{p/\pi}) \tan(\pi/\sqrt{p}).$$

From the condition $h_s = J/l_s$ and Eqs.(9),(10) locking the chain we find

$$h_s = \Delta_c (1 + e^{-8\omega_0 \tau} + \cdots)/(1 - \Lambda). \quad (12)$$

According to (11),(12) in the limit of large $\Delta \to \infty$ the $h_s$ value at any $\Delta$ exponentially rapidly achieves universal asymptotics $h_s^* = \Delta_c$ whence it follows $\Lambda = \Delta_c$. Essentially that at $p < p_c = 4/9$ in $\Lambda_-$ the first term dominates, therefore the relaxation rate is independent of $p$, whereas at $p > p_c$ in $\Lambda_+$ the second term dominates, therefore the relaxation rate decays with growing $p$. In view of (7),(8), and (12) using the time convolution it is easy to check that the contribution of transient stage is reduced only to a relative shift of the amplitude

$$\delta A_{\text{tr}}/A |_{\tau_0 \to \infty} \sim (r/\epsilon h_0) \int_0^{O(1)} e^{\omega_0 \delta^2} d\theta \to 0$$
	herefore with an accuracy of vanishingly small terms we finally have

$$\lambda = \Delta_c (\Delta - \Delta_c)/2h_0.$$ 

Two important consequences immediately follow from Eqs. (11),(12): (i) at $\Delta = \Delta_c$ the amplitude $\lambda$ reverses its sign which is the first rigorous proof of the threshold arising of self-acceleration for arbitrary ratio of diffusivities $0 < p < 1$ (note that at the long-time tail of self-acceleration $\tau \to \infty$, $h_s \to \Delta$ a strict derivation of the threshold $\Delta_c$ has been given in the work [3]); (ii) for the time of self-acceleration start, $\tau_s$, and departure of the starting point $h_s^{\text{min}}$ from the critical asymptotics $h_s^*$, $\delta_s = (h_s^{\text{min}} - \Delta_c)/\Delta_c$, we find, respectively, $\tau_s = [1/\omega_0 (\alpha + 1)] \ln(\alpha \delta)/\lambda$ and

$$\delta_s = (\alpha + 1) \tilde{\delta}^{\frac{\alpha + 1}{\alpha}} (\lambda/\alpha)^{\frac{\alpha + 1}{\alpha}}, \quad (13)$$

where in the $p < p_c$ range $\alpha = 8, \tilde{\delta} = 1 + \delta_8$ whereas in the $p_c < p < 1$ range $\alpha = \chi, \tilde{\delta} = \delta_p$.

**C. Annihilation catastrophe.**

According to (4) and (12) the exponential growth $\delta h_s/h_s = \Delta_+$ leads to the exponentially growing contribution to the flux $\delta J/J = -\beta A_+^2$ where $\beta = \sqrt{\omega_0} \tanh(\sqrt{2\omega_0}/(\Delta - \Delta_c))$. Far beyond the threshold $\beta \propto \Delta^{-1}$ suggesting that in the limit $\Delta \to \infty$ at the initial stage of self-acceleration the contribution to the flux is vanishingly small. The remarkable fact to be proved below is that at $\Delta \to \infty$ the contribution to the flux remains vanishingly small up to the point of finite-time singularity $\Lambda(\tau_s) \to 1$ where $h_s/h_s \to \infty$. This means that Eqs.(9)-(12) give complete description of the explosion dynamics. Moreover, as at $\Delta \to \infty$ the parameter

$$\lambda = \Delta_c/2(1 + n_0)$$


becomes the unique function of \( n_0 = N_0/\Delta \), Eqs.(9)-(12) allow one to achieve two main goals: a) to find the time of the catastrophe \( \tau_*(n_0) \) and b) to obtain the description of explosion evolution with growing \( n_0 \). Taking \( \Lambda(\tau_*) = 1 \) and \( \lambda < 1 \) from Eqs.(11) we find

\[
\tau_* = \tau_*^u (1 + \delta_\tau),
\]

where

\[
\tau_*^u = \left(4/\pi^2\right) \ln \left|2(1 + n_0)/\Delta\right|
\]

and

\[
\delta_\tau(n_0) = -(g_8 \lambda^8 + g_p \lambda^\chi)/|\ln \lambda|.
\]

Introducing then a relative time \( T = \tau - \tau_* \) from Eq.(12) we find that at any \( p < 1 \) in the vicinity \( |T| \ll \omega_0^{-1} \) an explosive growth of \( h_s \) sets in by the law

\[
h_s = (1 + Q)/\mu|T|, \quad |T| \to 0,
\]

where \( \mu = \Delta c/\Delta_e \sim 1 - p \) and

\[
Q(n_0) = (1 + 9g_8)\lambda^8 + (1 + \chi)g_p\lambda^\chi.
\]

According to Eq.(9) in the course of explosion the flux is actually “frozen”

\[
J = J_s(1 + \omega_0(1 + w)|T| + \cdots)
\]

reaching at the point of singularity the value

\[
J_s = \Delta \Delta_e(1 + G), \quad |T| \to 0,
\]

where \( w(n_0) = 8\lambda^8 \) and

\[
G(n_0) = (1 + g_8)\lambda^8 + g_p\lambda^\chi.
\]

From Eqs.(15),(16) and the condition \( h_s l_s = J_s \) there immediately follows the synchronization of the growth, \( \Omega_{Hs} = \frac{d \ln h_s}{d\tau} \), and relaxation, \( \Omega_{Ls} = \frac{d \ln l_s}{d\tau} \), rates which singularly grow by the law

\[
\Omega_s = \Omega_{Hs} = \Omega_{Ls} = 1/|T|.
\]

Clearly the dominant contribution to the explosion-triggered “antiflux” \( J_{ex} \) occurs in the vicinity \( |T| \ll 1 \) where the diffusional response to the explosion forms in a narrow layer \( \sqrt{|T|} \ll 1 \). Thus, considering the medium to be a semi-infinite one and allowing for (15) we can write

\[
J_{ex} = - \int_{-\infty}^{T} dH_s \frac{d\theta}{\sqrt{\pi(T - \theta)}} \sim \frac{(1 + Q)}{\mu|T|^{3/2}}
\]

whence there follows smallness of \( |J_{ex}|/J_s \) down to \( |T| \propto \Delta^{-2/3} \to 0 \). Calculating then a singular contribution into the flux relaxation rate

\[
\tau_{j}^{-1} = - \frac{d \ln J}{d\tau} = \omega_0(1 + w) + [\tau_{j}^{-1}]
\]

we find

\[
[\tau_{j}^{-1}] = -\dot{J}_{ex}/J_s \sim \frac{(1 + Q - G)}{\Delta|T|^{5/2}}
\]

whence there follows the catastrophic jump of \( \tau_{j}^{-1} \) from \( \tau_{j}^{-1} \approx \omega_0 \) to \( \tau_{j}^{-1} \to \infty \) with the width

\[
|T|_{cat} \propto \Delta^{-2/3} \to 0.
\]

According to \( \mathbb{3} \), the culmination consequence of the explosion in the limit \( K \sim p^{3/2} \Delta/\Delta_e \to \infty \) is the exact scaling description of passing through the point of singularity based on two key conditions: a) requirement

\[
\sqrt{h_s} = \bar{l}_s
\]

providing for equality of diffusional responses \( J_{ex} = J_{ex}^{L} \) (here and in what follows \( \dot{J} \equiv d(J)/d\tau \) and b) self-consistent condition of passing through the singularity point at a "frozen" flux

\[
h_s l_s = J_s.
\]

It has to be mentioned, however, that the scaling behavior of \( \Omega_s \) was postulated in \( \mathbb{3} \) on a basis of indirect arguments and only later the postulated scaling function was analytically substantiated. Moreover, the space of \( \mathbb{3} \) being concise, an important chain of considerations remained beyond the analysis given there. Below, I shall give for the first time a systematic scaling theory of the annihilation catastrophe in the universal limit \( n_0 \to \infty \), and then, on its basis, a complete picture of catastrophe universalization with a growth of \( n_0 \) will be constructed.

### D. Scaling laws of concentration explosion and annihilation catastrophe.

For simplicity, I shall begin with inferring the scaling laws of concentration explosion and annihilation catastrophe in the universal limit \( n_0 \to \infty \). Taking \( \lambda, Q, G \to 0 \), according to (9) and (10) at the explosion stage \( \omega_0|T| \to 0 \) we have

\[
J^{(0)} = J_s(1 + \omega_0|T| + \cdots)
\]

and

\[
l_s^{(0)} = \mu J_s|T|(1 + \omega_0|T|)/2 + \cdots,
\]

whence it follows

\[
h_s^{\infty} = J^{(0)}/l_s^{(0)} = 1/\mu|T| + \cdots,
\]

where the index "(0)" marks the solutions which neglect the contribution of \( h_s = h_s^{\infty} \) \( (h_s^{(0)} = 0) \). As it has been mentioned above, an explosive growth of \( h_s^{\infty} \) ought to
trigger an explosive growth of "antiflux" \( J_{\text{ex}} \) in calculating which the medium can be regarded to be a semi-infinite one

\[
J_{\text{ex}} = -\int_{-\infty}^{T} \frac{dh_{\text{ex}}}{d\theta} \frac{d\theta}{\sqrt{\pi(T-\theta)}}. \tag{19}
\]

(apparently, to an accuracy of vanishingly small terms the lower limit of the integral can be directed to \(-\infty\)). Substituting here \( h_{\text{ex}} \), we find

\[
J_{\text{ex}} = -a_{f}/\sqrt{\pi}/2, \quad \text{where} \quad a_{f} = \sqrt{\pi/2}.
\]

So, for the total flux we have

\[
J = J^{(0)} + J_{\text{ex}} = J_{s} \left( 1 + \omega_{0}|T| - \frac{a_{f}}{\mu J_{s}|T|^{3/2}} + \cdots \right).
\]

As the diffusion fluxes of fast and slow particles must be equal \( J_{L}^{D}|_{s} = J_{H}^{D}|_{s} \approx J_{s} \), it is clear that against the background of dropping \( l_{s}^{(0)} \) there must arise an explosive growth of \( l_{s}^{\text{ex}} \) which must initiate exactly the same "antiflux" \( J_{s}^{\text{ex}} = J_{H}^{\text{ex}} = J_{\text{ex}} \). Assuming that at a developed explosion stage \( \Omega_{s}p \gg 1 \) the dominant contribution to \( J_{\text{ex}} \) occurs at times \( |T|/p \ll 1 \), when for \( L \) particles the medium can be regarded to be semi-infinite, by full analogy with Eq. (19) we can write

\[
J_{\text{ex}} = -\int_{-\infty}^{T} \frac{dl_{\text{ex}}}{d\theta} \frac{d\theta}{\sqrt{\pi(T-\theta)}}. \tag{20}
\]

Thus, by requiring the equality of (19) and (20) we have

\[
l_{s} = l_{s}^{(0)} + l_{s}^{\text{ex}} = \mu J_{s}|T| \left( 1 + \frac{\sqrt{p}}{\mu^{2} J_{s}^{2}} + \cdots \right) \tag{21}
\]

and finally from the condition \( h_{s} = J_{s}/l_{s} \) we find

\[
h_{s} = \frac{1}{\mu|T|} \left( 1 - \frac{\sqrt{p}}{\mu^{2} J_{s}^{2}}(1 + f_{f}) + \cdots \right), \tag{22}
\]

where \( f_{f} = a_{f}\mu\sqrt{|T|}/p \). From Eqs. (21) and (22) it follows that in the vicinity of some characteristic time \( T_{f} \sim p^{1/4}/\mu^{2} \), the explosion rate growth begins to drastically decelerate. Due to the requirement \( T_{f}/p \ll 1 \) necessary for the realization of the synchronous explosion regime (20), the explosion deceleration begins long before a noticeable flux departure from the critical one \( |J_{\text{ex}}(T_{f})|/J_{s} \ll 1 \). Introducing the parameter

\[
\mathcal{K} = \mu^{2}p^{3/2}J_{s}
\]

it can easily be seen that at any finite \( 0 < p < 1 \) with a growth of \( \Delta \) in the limit of large \( \mathcal{K} \sim p^{3/2}\Delta/\Delta_{c} \sim \infty \)

\[
|J_{\text{ex}}(T_{f})|/J_{s} \sim \sqrt{T_{f}/p} \sim 1/\mathcal{K}^{1/4} \to 0.
\]

and, therefore, down to \( T_{f} \to 0 \) the flux remains "frozen". One of the most important consequences of the drastic deceleration of the explosion rate growth is the drastic deceleration of the flux relaxation rate growth. As it will be shown in what follows, in the limit of large \( \mathcal{K} \to \infty \) as a result of such deceleration the flux remains "frozen" and, therefore, the explosion develops synchronously

\[
\Omega_{s} = \Omega_{H_{s}} = \Omega_{L_{s}} \tag{23}
\]

both before and after passing through the point of singularity where \( \Omega_{s} \) reaches a maximum. I shall now show that the condition (23) along with the following from (19) and (20) key condition

\[
\dot{i}_{s}^{\text{ex}} = \sqrt{\mathcal{K}_{s}^{\text{ex}}} \tag{24}
\]

lead to a remarkably complete scaling description of passing through the point of singularity. Taking \( l_{s} = l_{s}^{(0)} + l_{s}^{\text{ex}} \) we have

\[
\dot{l}_{s} = \dot{i}_{s} + C_{(0)}, \tag{25}
\]

whence it follows that the explosion rate goes through the maximum \( \Omega_{s}^{M} \) in the point where

\[
\dot{i}_{s}^{M}/h_{s}^{M} = \sqrt{\mathcal{K}}. \tag{26}
\]

Combining of (26) and (28) with the "frozen" flux condition

\[
h_{s}^{M} = h_{s}l_{s} = J_{s} \tag{29}
\]

enables one to lock the chain and to readily derive the scaling law of concentration explosion. Indeed, from (29) and (28) we find

\[
h_{s}^{M} = p^{-1/4}J_{s} \quad \text{and} \quad l_{s}^{M} = p^{1/4} \sqrt{J_{s}}. \tag{30}
\]

Introducing then the scaling function

\[
\zeta = h_{s}/h_{s}^{M} = l_{s}^{M}/l_{s}
\]

from (26) and (30) we obtain

\[
\Omega_{s} = \dot{\zeta} = \Omega_{s}^{M} F(\zeta), \quad F(\zeta) = \frac{2\zeta}{1 + \zeta^{2}}, \tag{31}
\]

where

\[
\Omega_{s}^{M} = C_{(0)}/l_{s}^{M} = (\mu/2)h_{s}^{M}. \tag{32}
\]
Integrating (31) with the proviso that $\zeta(T = 0) = 1$ we easily find

$$\zeta - 1/\zeta = 2\Omega_s^M T.$$  

(33)

From Eq. (33) it follows that the characteristic time scale of explosion is determined by the quantity $T_f = 1/\Omega_s^M$ therefore introducing the reduced time $T = T/T_f$, we finally obtain

$$\zeta(T) = T + \frac{1}{\sqrt{1 + T^2}}.$$  

(34)

whence it follows

$$\Omega_s = \Omega_s^M S(T), \quad S(T) = \frac{1}{\sqrt{1 + T^2}}.$$  

(35)

Two striking features of this result are symmetrical universalization $[T]^{-1} \leftrightarrow -T^{-1}$ of $\Omega_s$ beyond the scope of interval $[-T_f, T_f]$ and remarkable symmetry

$$T \leftrightarrow -T, \quad \zeta \leftrightarrow 1/\zeta.$$  

Substituting (34) into (19) and using (35) we come to the scaling law of growth of the explosion-triggered "antiflux" $J_{ex}$

$$J_{ex} = J_{ex}^M J(T)$$  

(36)

where the amplitude at the point of explosion maximum

$$J_{ex}^M = -a_M h_s^M \sqrt{\Omega_s^M}$$  

and the scaling function

$$J(T) = a_J \int_0^\infty d\theta \zeta(T - \theta)S(T - \theta)/\sqrt{\theta}.$$  

has the asymptotics

$$J(T) = (\pi a_J/4)|T|^{-3/2}, \quad -T \gg 1$$

$$J(T) = 4a_J T^{1/2}, \quad T \gg 1.$$  

The coefficients $a_M$ and $a_J$ are bound by the relation $a_M a_J = 1/\sqrt{\pi}$ therefore by satisfying $J(0) = 1$ we find $a_M = 2\Gamma^2(3/4)/\pi \approx 0.956$ and $a_J = \sqrt{\pi}/2\Gamma(3/4) \approx 0.590$.

Differentiating (36) we find the singular part of the flux relaxation rate in the form

$$[\tau_{ex}^{-1}] = -J_{ex}/J_s = [\tau_J^{-1}]_M W(T)$$  

(37)

where the amplitude at the point of explosion maximum

$$[\tau_{ex}^{-1}]_M = c_M h_s^M (\Omega_s^M)^{3/2}/J_s$$  

and the scaling function

$$W(T) = c_W \int_0^\infty d\theta/\sqrt{\theta}[1 + (T - \theta)^2]^{3/2}$$  

has the asymptotics

$$W(T) = (3\pi c_W/8)|T|^{-5/2}, \quad -T \gg 1$$

$$W(T) = 2c_W T^{-1/2}, \quad T \gg 1.$$  

The coefficients $c_M$ and $c_W$ are bound by the relation $c_M c_W = 1/\sqrt{\pi}$ therefore by satisfying $W(0) = 1$ we find $c_M = \Gamma^2(1/4)/4\pi \approx 1.046$ and $c_W = \frac{4\sqrt{\pi}}{\Gamma^2(1/4)} \approx 0.539$. The numerical analysis shows that at $T = 0.46205$ the scaling function $W(T)$ reaches the maximum

$$\max W(T) = 1.15627...$$  

whence for the amplitude of catastrophe at the point of maximum we find

$$\max [\tau_{ex}^{-1}] = (1.15627...) [\tau_{ex}^{-1}]_M.$$  

(38)

Eqs. (30), (32), (34) - (37) give a detailed picture of the concentration explosion and annihilation catastrophe in the asymptotic limit $K \rightarrow \infty$. Substituting into these expressions $J_s = \Delta \Delta_s$ and marking the asymptotic values of amplitudes with the index $(a)$ in full agreement with (36) we obtain

$$h_s^M(a) = p^{-1/4}\sqrt{\Delta \Delta_s}, \quad l_s^M(a) = p^{1/4}\sqrt{\Delta \Delta_s},$$  

(39)

$$\Omega_s^M(a) = (\mu/2)p^{-1/4}\sqrt{\Delta \Delta_s},$$  

(40)

$$[\tau_{ex}^{-1}]_M(a) = (1.43340)...p^{-5/8}\Delta \Delta_s^{-5/4}\Delta^{1/4},$$  

(41)

whence adopting (38)

$$\max [\tau_{ex}^{-1}]_M(a) = (1.65739...)p^{-5/8}\Delta \Delta_s^{-5/4}\Delta^{1/4}.$$  

From (17), (18), (37), and (41) it follows that the width of flux relaxation rate jump does not depend on $p$

$$|T|_{cat} \propto \Delta^{-2/5},$$  

whereas its amplitude

$$\max [\tau_{ex}^{-1}]_M \propto p^{-5/8}(1 - p)^{5/4}\Delta^{1/4}$$  

grows rapidly with diminishing $p$. So, the less is $p$, i.e. the less $L$-diffusion restrains the explosion development, the more brightly the effect is displayed.

According to (20), one of the necessary conditions for the scaling description of passing through the point of singularity is the requirement

$$\Omega_s p \gg 1$$  

which implies that for the medium to be considered as semi-infinite in the process of explosion, the explosion rate must be much beyond the characteristic rate of the $L$ particles diffusion. Combining this requirement with Eqs.
(34) and (35) and using the equality \( \Omega^M(a) = \sqrt{\mathcal{K}}/2p \)
onone can easily see that applicability limits of the scaling description are described by the inequalities

\[ \frac{1}{\sqrt{\mathcal{K}}} \ll \zeta \ll \sqrt{\mathcal{K}}, \quad |T| \ll \sqrt{\mathcal{K}}. \]

A more rigorous requirement to the quantity \( \mathcal{K} \) is imposed by the apparent chain of conditions

\[ \frac{\left| J^M_M \right|}{J_s} \sim \frac{\Omega^M_M - \Omega^M_s}{\Omega^M_{Hs}} \sim \frac{[\tau^{-1}_J]}{\Omega^M_s} \sim \mu/\mathcal{K}^{1/4} \ll 1, \]

whence it is to be expected that with a growth of \( \mathcal{K} \) the amplitudes (39) - (41) ought to be reached mainly by the law \( \mu/\mathcal{K}^{1/4} \). One of the remarkable analytical advantages of the above given approach is that it enables one not only to determine the exact asymptotic amplitudes (39) - (41) but, also, to answer the question of when and how they are reached. A systematic analysis of the crossover to the asymptotics (39)-(41) is given in the Appendix. Here I shall focus on the main results. The central conclusion of the presented analysis is that \( \Omega^M_{Hs} \) reaches the asymptotic limit \( \Omega^M(a) \) much faster than \( \Omega^M_s \), therefore the point of the explosion maximum is defined by precisely by the point of the \( \Omega_{Hs} \) maximum. According to (A7)

\[ \Omega^M_{Hs}/\Omega^M_s(a) = 1 - B_\zeta \mu/\mathcal{K}^{1/4} + O_\zeta(\mathcal{K}^{-1/2}), \]

where \( B_\zeta \approx 0.0318 \). With taking into account the equality \( \Omega^M_s = \Omega^M_M + \omega_0 + [\tau^{-1}_J] \) and Eq.(37) it yields

\[ \Omega^M_{Hs}/\Omega^M_s(a) = 1 + (c_M/\sqrt{\mathcal{K}} - B_\zeta)\mu/\mathcal{K}^{1/4} + \cdots. \]

According to (A8)

\[ [\tau^{-1}_J]_{M}/[\tau^{-1}_J]_{M}(a) = 1 + B_J\mu/\mathcal{K}^{1/4} + O_J(\mathcal{K}^{-1/2}) \]

where \( B_J \approx 0.776 \). From these expressions we conclude that \( \Omega^M_{Hs} \) always goes to its asymptotics from below whereas \( [\tau^{-1}_J] \) and \( \Omega^M_s \) always go to their asymptotics from above. Remarkably, the coefficient \( B_\zeta \) appears to be anomalously small so that the contribution of \( \mathcal{K}^{-1/4} \) term in the case of \( \Omega^M_{Hs} \) becomes less than 0.01 already at \( \mathcal{K} > 10^2 \). Below I shall present extensive numerical calculations in wide ranges of \( p, \Delta \) and \( \mathcal{K} \) which demonstrate excellent agreement between the numerical data and the analytical predictions.

**E. Universalization of annihilation catastrophe.**

Apparently the scaling theory of the annihilation catastrophe, developed in the previous section for the universal limit \( n_0 \to \infty \), holds in the general case of finite \( n_0 \) too. Indeed, according to (9) and (10) at finite \( n_0 \) and \( \lambda < 1 \) the chain (24)-(32) remains valid with the sole difference that now

\[ J_s(n_0) = \Delta \Delta_c[1 + G(n_0)] \]

and

\[ C_{(0)}(n_0) = \mu J_s(n_0)[1 - Q(n_0)] \]

become the functions of \( n_0 \). We thus have the complete scheme to lock the chain (5)-(18) and to answer the question of when and how the universality is reached. It remains for us to find the central characteristic of scaling, namely, the amplitude of explosion \( \Omega^M_s(n_0) \), and then from Eq.(37) to derive the amplitude of catastrophe \( [\tau^{-1}_J]_{M}(n_0) \).

Taking \( \zeta \ll 1 \) from Eq.(33) we have

\[ h_s = (h_s^M/2\Omega^M_s)/|T|. \]

Matching this result with Eq.(15) thereby locking the chain (5)-(18) we obtain

\[ \Omega^M_s = \frac{\mu}{2}(1 - Q)h_s^M = \frac{\mu}{2}(1 - Q)p^{-1/4}\sqrt{J_s}. \]

Using then Eq.(16) we conclude that at \( \lambda < 1 \) evolution of explosion with growing \( n_0 \) is completely defined by functions \( Q(n_0) \) and \( G(n_0) \), and find finally the laws of universalization of amplitudes of explosion

\[ \Omega^M_s(n_0) = \Omega^M_s(\infty)(1 + \delta_\zeta) \]

and catastrophe

\[ [\tau^{-1}_J]_{M}(n_0) = [\tau^{-1}_J]_{M}(\infty)(1 + \delta_J) \]

in the form

\[ \delta_\zeta = G/2 - Q, \quad \delta_J = G/4 - 3Q/2. \]

Leaving aside details here, I distinguish two main consequences of (42):

1) According to (15),(16) the drop of \( \delta_\zeta \) and \( \delta_J \) with growing \( n_0 \) is surprisingly rapid:

\[ Q, G \propto n_0^{-\chi}(p < p_c), \quad Q, G \propto n_0^{-\chi}(p > p_c), \]

where \( 3 < \chi(p) < 8 \). Comparing this with the relatively slow decrease of \( \delta_s[Eq.(13)] \)

\[ \delta_s(p < p_c) \propto n_0^{-\chi/9}, \quad \delta_s(p > p_c) \propto n_0^{-\chi/(x + 1)} \]

we conclude that universalization of explosion occurs long before \( h^\text{min}_s \) has reached \( h^\text{c} \);

2) According to (42) in the range \( p < p_c \) with decreasing \( p \) some critical values \( g^*_s, p^*_c \) are reached at which \( \delta_\zeta \) and \( \delta_J \) reverse their sign \((- \to +)\) so that contrary to an intuitive reasoning at \( p < p^*_\zeta \) and \( p < p^*_J \) the amplitudes \( \Omega^M_s \) and \( \text{max}[\tau^{-1}_J] \), respectively, drop with growing \( n_0 \). From (15),(16) and (42) we obtain

\[ g^* s, \Omega = -1/17, \quad p^*_c = 0.0609 \]

and

\[ g^* s, J = -5/53, \quad p^*_J = 0.0217. \]

Note, that this correlates with the behavior of the function \( \delta_s \) that pass through zero \((- \to +)\) at

\[ p^*_s = 1/9. \]
IV. NUMERICAL CALCULATIONS

To test analytical predictions I have carried out extensive numerical calculations of Eqs.(1). The numerical integration of Eqs.(1) was performed by means of the implicit discretization scheme of increased accuracy with an additional "fictitious" node at the surface [7], [8]. The scheme allowed performing the calculations in the system with strong difference in species diffusivities with an accuracy down to $10^{-3}$. The space and time steps were changed within the ranges $3 \times 10^{-4} \div 3 \times 10^{-6}$ and $10^{-4} \div 10^{-11}$, respectively, with the number of time steps being $10^5 \div 10^6$.

In Figs. 2 and 3 are shown the results for $\Delta = 10^5$ and $p = 0.25$, giving detailed picture of formation of the universal explosion with growing $n_0$. It is seen that in accord with Eqs.(42) already at small departures from $n_0^0 (R = R_c)$ the transient dynamics (7) terminates in explosion that remarkably rapidly becomes universal: further growth of $n_0$ leads to progressing shift of the critical point $\tau_s(n_0)$ (Figs. 2a and 3) without changing the explosive dynamics in its vicinity but gradually universalizing the entire self-acceleration trajectory (Fig. 2b). I distinguish two important points which characterize the universalization process:

i) In accord with Eqs. (35) and (37) a symmetrical "flash" of the explosion rate $\Omega_{Hs} (|T|^{-1} \leftrightarrow T^{-1})$ (Fig. 3a) and accompanying it sharply asymmetrical jump of the flux relaxation rate $\tau_{ij}^{-1} (|T|^{-5/2} \leftrightarrow T^{-1/2})$ (Fig. 3b) form long before the universalization of the corresponding amplitudes, shifting self-similarly with growing $n_0$.

ii) In accord with Eqs. (13) and (17) as $n_0$ grows, the starting point of catastrophe reaches the level $\omega_0$ (Fig. 3b) long before the starting point of self-acceleration, $\tau_{ij}^{\text{min}}$, reaches the level $\Delta_c$ (Fig. 2).

In the insets in Fig. 3 are shown the dependences $\Gamma_\Omega(n_0) = \Omega_{Hs}^M(n_0)/\Omega_{Hs}^M(\infty)$ and $\tau_s(n_0)$ plotted on the basis of the dependences $\Omega_{Hs}(\tau, n_0)$, represented on the main panel and the analogous dependences obtained in a wide $p$ range for $\Delta = 10^5$ (according to the Appendix, here and in what follows the critical point $\tau_s$ is defined to be the point of maximum of $\Omega_{Hs}$). The inset in Fig. 3a demonstrates that, in accord with (42), as $p$ decreases, the behavior of $\Omega_{Hs}^M(n_0)$ changes qualitatively: at $p > p_c^2$ the explosion amplitude $\Omega_{Hs}^M(n_0)$ grows monotonously with growing $n_0$, reaching $\Omega_{Hs}^M(\infty)$ from below whereas at $p < p_c^2$ the explosion amplitude first goes through a maximum and then drops with the growing $n_0$, reaching $\Omega_{Hs}^M(\infty)$ from above. The inset in Fig. 3b demonstrates that at all $p$ with the growing $n_0$ the numerically calculated $\tau_s$ values come to the function $\tau_s^u(p, n_0)$ calculated according to Eq. (14). Moreover, in full agreement with Eq. (14) at $p > p_c^2$ the numerical $\tau_s$ values come to $\tau_s^u$ from below whereas at $p < p_c^2$ the numerical $\tau_s$ values come to $\tau_s^u$ from above. Below I shall present the results of the detailed numerical study of the catastrophe universalization in a wide range of $p$ and $\Delta$ and compare them with the predictions of (13), (14), and (42) to plot on their basis the complete $n_0 - p$ diagram of universalization. Before discussing these results, my main goals will be:

1) To demonstrate numerically how with a growth of $\Delta$ in the vicinity of the critical point $\tau_s$ a singularity forms, and to show that with a growth of $\Delta$ and $n_0$ the time dependences $\Omega_{Hs}(T)$ and $[\tau_{ij}^{-1}](T)$ collapse to the predicted scaling functions $S(T)(35)$ and $W(T)(37)$.

2) Making use of Eqs. (42) for selecting the $n_0^0(p)$ region where the contribution of $n_0$ can be excluded with the required accuracy, to study numerically the behavior of the $\Omega_{Hs}^M$ and $[\tau_{ij}^{-1}]_M$ amplitudes in a wide range of $p$ and $\Delta$, and to demonstrate that with a growth of $K$ they reach their asymptotic values $\Omega_{Hs}^M(a)$ (40) and $[\tau_{ij}^{-1}]_M(a)$ (41) in accord with the predictions of (A7)-(A11).

In Fig. 4 are shown the numerically calculated dependences $\Omega_{Hs}(\tau)$ that demonstrate the formation of singularity with growing $\Delta$ at $n_0 = 4$ and $p = 0.25$. An analysis of the given data suggests that as $\Delta$ grows, the critical point of the explosion maximum $\tau_s(\Delta)$ rapidly ($\Delta \sim 1$) comes to the point of singularity $\tau_s(\infty)$, calculated according to Eq. (14), so that already at $\Delta > 10^4$ the ratio $\delta\tau_s(\Delta)/\tau_s(\infty)$ becomes less than 0.001. In the inset to Fig. 4 are compared the dependences $\Omega_{Hs}(\tau)$ and $\Omega_{Hs}(\tau)$ calculated numerically at $\Delta = 10^8$, $n_0 = 4$ and $p = 0.25$. In accord with Eq. (35), at large $\Omega$, the curves are seen to merge in "synchronous" explosion, asymptotically coming apart away from the critical point. In Fig. 5a are shown the data of Fig. 4 for $\Delta = 10^5, 10^6, 10^7, 10^8$, replotted in the coordinates $\Omega_{Hs} - T$ where $T = \tau - \tau_s$, $\tau_s$ being the point of the explosion maximum. Here are also represented the data of Fig. 3a for $n_0 = 1.8, 2, 4, 3.1$ ($\Delta = 10^5, p = 0.25$). It is seen that in full agreement with Eq. (35) i) the rate of explosion $\Omega_{Hs}(T)$ demonstrates the remarkable symmetry $-T \leftrightarrow T$ and ii) beyond the $[-T_f, T_f]$ region, unlimited contracting with a growth of $\Delta$, the explosion rate comes to the universal law $1/T$.

In the concluding Fig. 5b the data of Fig. 5a are represented in the scaling coordinates $\Omega_{Hs}/\Omega_{Hs}^M - T$ where $T = T/\tau_f = T\Omega_{Hs}^M$. It is seen that the numerically calculated dependences are perfectly collapse to the scaling function $S(T)(35)$.

Let us now turn to an analysis of the flux relaxation rate. Fig. 6a demonstrates the dependences $\tau_{ij}^{-1}(T)$ calculated numerically for the same parameters as in Fig. 5a (the data are shown only for $n_0 = 4$). The data analysis suggests that in accord with Eqs. (17), (18), and (37) with growing $\Delta$ in the vicinity of the critical point $\tau_s$ forms a singular jump of $\tau_s^{-1}$; the width of which contracts unlimitedly by the law $|T_c| \sim \Delta^{-2/5}$ and the amplitude of which grows unlimitedly by the law $\max\tau_s^{-1} \sim \Delta^{1/4}$ (see below). Note that in accord with Eq. (37), after the critical point has been passed ($T > T_f$), the relaxation rate drops by the $\Delta$ independent law $\sim 1/\sqrt{T_f}$, reaching at times $T \sim p/\omega_0^2$ the $L$-diffusion-controlled limit $\omega_0/p$ so that in the limit of small $p$ there arises a most dramatic consequence of the annihilation catastrophe: an abrupt, practically instantaneous (on the scale of
ω₀) disappearance of the flux [3]. Based on the data of Fig. 6a in accord with Eq. (17) the time dependences of the singular part of the flux relaxation rate were calculated \[ \tau^{-1}_f(T) = \gamma J^{-1}(T) - \omega_0(1 + w) \] which were then replotted in the scaling coordinates \[ \frac{\tau^{-1}_f(T)}{\omega_0} = \frac{\tau^{-1}_f(0)}{\tau^{-1}_f(0) - T}. \] The results are demonstrated in Fig. 6b. It is seen that in perfect agreement with Eq. (37) with growing \( \Delta \) the numerical results collapse to the scaling function \( W(T) \). For a more detailed illustration in Figs. 6c and 6d the ratio \[ \frac{\tau^{-1}_f}{\omega_0} \] is plotted in double logarithmic coordinates \[ \log_{10}(\tau^{-1}_f(0) - T) - \log_{10}(\omega_0) \] which demonstrate a collapse to the scaling function \( W(T) \) with growing \( \tau \). It is seen from Fig. 6c that at \( \Delta = 10^8 \) the range of the scaling growth regime of \( \tau^{-1}_f \) reaches six orders of magnitude. As in this case at the starting point of growth the ratio \( \frac{\tau^{-1}_f}{\omega_0} \sim 10^{-4} \), it implies that the accuracy of the numerical calculation of \( \tau^{-1}_f \) reaches \( 10^{-3}\% \). Extensive numerical calculations in a wide range \( 10^{-3} < p < 1 \), a part of which will be given below, have shown that at the investigated \( p \) values with a growth of \( \Delta \) (and therefore \( K \)) the obtained numerically normalized dependences \( \Omega_{Hs}(T) \) and \( \tau^{-1}_f(T) \) collapse, respectively, to the scaling functions \( S(T) \) and \( W(T) \). We thus conclude that the scaling theory of catastrophe perfectly agrees with the numerical results.

Let us now come to a numerical study of the behavior of the amplitudes \( \Omega_{Hs}(p, \Delta, n_0) \) and \( \tau^{-1}_f(M)(p, \Delta, n_0) \) which are the central characteristics of the scaling regime of catastrophe. Following the above stated program, I shall begin with the results derived in the universal limit \( n_0 \to \infty \). The numerical calculations were performed within \( \Delta = 10^4 \pm 10^6 \) for \( p = 0.01, 0.03, 0.1, 0.25, 0.5, 0.75 \). In order that the contribution of the initial conditions be excluded, the initial number of particles \( n_0 \) was depending on \( p \) selected from the range \( n_0 = 10 \div 200 \) so that in accord with Eqs. (42) this contribution may not exceed \( 10^{-3}\% \). In Fig. 7a are shown the numerically calculated dependences \( \gamma \Omega = \Omega_{Hs}^M/\Omega_{Hs}^a \) and \( \gamma_J = \tau^{-1}_f^M/\tau^{-1}_f^a \) as functions of \( K/\mu^4 \). It is seen that with growing \( K \) the numerically calculated amplitudes \( \Omega_{Hs}^M \) and \( \tau^{-1}_f^M \) come, respectively, to the asymptotic values \( \Omega_{Hs}^a \) and \( \tau^{-1}_f^a \) calculated analytically according to Eqs. (40), (41). Remarkably, in accord with the predictions of Eqs. (A7), (A8) \( \gamma \Omega \) comes to 1 from below whereas \( \gamma_J \) comes to 1 from above; ii) \( \gamma_0 \) comes to 1 much faster than \( \gamma_J \); iii) the law by which \( \gamma_J \) approaches 1 in a wide range of \( K/\mu^4 \) is described with excellent accuracy by the principal term of Eq. (A8). For a more detailed illustration of iii) in Fig. 7b in double logarithmic coordinates are presented the dependences \( \epsilon_J = \gamma_J - 1 \) vs. \( K/\mu^4 \). Ibid are shown the numerically calculated dependences \( \epsilon_s = (J_s - J_M)/J_s \) vs. \( K/\mu^4 \) which demonstrate the law by which \( J_M \) approaches \( J_s \) with growing \( K \). It is seen that the numerically calculated \( \epsilon_J \) and \( \epsilon_s \) values at \( p \) not too close to 1 perfectly fall on the analytic dependences \( B_{J\mu}/K^{1/4} \) [Eq. (A8)] and \( B_{s\mu}/K^{1/4} \) [Eq. (A4)], respectively, shown in thick lines (note that according to (A10) at \( p \to 1, \mu \sim 1 - p \to 0 \) the dominant term in \( \epsilon_J \) to \( K/\mu^4 \to \infty \) becomes \( \gamma \Omega \)). In accord with Eqs. (A7), (A9), (A11) owing to the anomalous smallness of the coefficient \( B_{J\mu} \) the value of \( \epsilon_J = 1 - \gamma_0 \) ought to decrease with growing \( K \) by the law \( \propto p/\sqrt{K} \) or (at small \( p \)) even faster down to very low values of \( \epsilon_J \sim 10^{-3} \). To illustrate these predictions in Fig. 7c are shown the dependences of \( \epsilon_J \) on \( \sqrt{K} \) in double logarithmic coordinates. At comparatively high \( p \) the numerically calculated \( \epsilon_J \) values are seen to fairly fall on the analytic dependences shown in dashed lines. As \( p \) decreases the effective “rate” of \( \epsilon_J \) drop grows only insignificantly, the \( \epsilon_J \) value itself becomes very small already at \( K \sim 10^2 - 10^3 \), therefore the analytical description of \( \epsilon_J \) in this region necessitates additional terms. Summarizing, we conclude that in the universal limit the represented theory gives an exhaustive picture of evolution of catastrophe and explosion amplitudes.

It only remains for me to complete this section by demonstrating the results of extensive numerical study of the regularities of catastrophe universalization with growing \( n_0 \). I have studied the behavior of the dependences \( \tau_s(n_0), \Omega_{Hs}(n_0), [\tau^{-1}_f(M)(n_0)] \) and \( h_{\epsilon_{\min}}(n_0) \) at “scanning” \( n_0 \) from \( n_0^* \) to \( 10^4 \) in wide ranges of \( \Delta = 10^5 \div 10^8 \) and \( p = 10^{-3} \div 0.97 \). Based on the obtained data for each of the studied \( p \) and \( \Delta \) values I calculated the dependences \( \epsilon_s(n_0) = \tau_s(n_0)/\tau_s^a - 1, \delta_0(n_0) = \Gamma_0(n_0) - 1, \epsilon_J(n_0) = [\tau^{-1}_f(M)(n_0)] \) and \( h_{\epsilon_{\min}}(n_0) \) at \( \Delta = 10^5 \) to \( 10^8 \) and \( n_0 \) from \( n_0^* \) to \( 10^4 \) for \( \Delta = 10^5 \) and \( n_0^* \) to \( 10^4 \) for \( \Delta = 10^8 \); \( \delta_0 = 0.1 \) result from a great number of numerical data (some of which are given in the inset) for \( \Delta = 10^5 \) (in the case \( i = J \) for \( \Delta = 10^5 \)) and calculated from (42), (14) and (12). Excellent agreement of the analytic and numerical results (not shifting with the further growing \( \Delta \)) needs no comments.

V. DISCUSSION AND CONCLUSION

Finite-time singularities - blowup solutions developing from a smooth initial conditions at a particular time - provide probably the most dramatic manifestation of strongly nonlinear effects that can occur in nature [10]. The formation of finite-time singularities is observable in a wide spectrum of nonlinear systems (Jang-Mills fields [11], black holes [12], self-gravitating Brownian particles [13], turbulent flows [14], jet eruption [15], chemotaxies [16], and earthquakes [17] to name only a few) therefore the description of scenarios of finite-time singularities development is a fundamental problem which attracts a
yield a complete dynamical picture at the both sides of the singularity development (based on properties of self-similarity) appears possible only to some narrow vicinity of the critical point beyond which the solution cannot as a rule be continued or is principally impossible. One of the main advantages of the here presented theory is the asymptotically exact scaling description of formation of finite-time singularity. I shall distinguish here two most bright features of annihilation catastrophe:

i) In the majority of the models which demonstrate the formation of finite-time singularities an analytical description of the singularity development (based on properties of self-similarity) appears possible only to some narrow vicinity of the critical point beyond which the solution cannot as a rule be continued or is principally impossible. One of the main advantages of the here presented theory is the asymptotically exact scaling description of passing through the point of singularity which yields a complete dynamical picture at the both sides of the critical point;

ii) Arising as a result of explosive growth of the "antitflux" $J_{c\xi}$ at the background of slow relaxation of the diffusion-controlled flux $J^{(0)}$, the annihilation catastrophe demonstrates a peculiar singular behavior at which two explosive processes ($\Omega^H_{s}$ and $\Omega^L_{s}$) are developing simultaneously, effectively "compensating" one another so that for an external observer of flux ($J$) the explosion dynamics goes unnoticed up to the critical point $\tau_s$ in the vicinity of which "decompensation" of explosions is manifested as a sudden singular jump of the flux relaxation rate. In the limit of small $p$ this brings about a most radical consequence - an abrupt disappearance of the flux.

Let us discuss in conclusion the conditions and possibilities of an experimental observation of the annihilation catastrophe. The irreversible bimolecular reaction $A + B \rightarrow 0$ is one of the most abundant reactions therefore it is to be expected that the predicted phenomena can, in principle, be observed in a wide class of physical, chemical and biological systems with a "catalytic" interface which, because of the high energetic barrier, does not let diffusing particles $A$ go from medium 1 to medium 2 and diffusing particles $B$ from medium 2 to medium 1 so that the reaction $A + B \rightarrow 0$ can occur only at the interface between the media $1$, $18$, $17$. Leaving aside here discussing systems of such type, I shall focus on the main object of the model in question, namely, adsorption - desorption systems (Fig. 1). Until now most of the theoretical studies on the $A_{ads} + B_{ads} \rightarrow 0$ catalytic reaction (the Langmuir-Hinshelwood process which is also often referred to as the monomer-monomer catalytic scheme) have been performed under the assumption that diffusion into the bulk can be neglected ($\Omega^0 - 26$ and references therein). Such an assumption is valid in low-temperature systems with high surface-bulk crossover barriers, i. e., in systems with the negligibly small bulk solubility of $A$ and $B$ particles. Here I address to the wide class of catalytic systems where the surface-bulk crossover barriers are not too high and, therefore, adsorption-desorption processes are always followed by a more or less intensive diffusion of $A$ and $B$ particles into or from the bulk where reaction between $A's$ and $B's$ is energetically forbidden $24$. This class of catalytic systems is not only of fundamental interest for surface science but also of considerable applied interest for describing the interaction kinetics of gases with metals at high temperatures ($24$ - 32 and references therein).

In the work $33$ the theory has been developed for the diffusion-controlled associative desorption of like particles, $A_{ads} + A_{ads} \rightarrow A_2\text{gas} \rightarrow 0$, from dissolved state into vacuum. Adopting this theory, a complete picture of diffusion-controlled thermodesorption of hydrogen and nitrogen has been constructed in good agreement with the available experimental data. The theory reported in this work gives a systematic description of the diffusion-controlled kinetics of associative desorption into vacuum of unlike particles

$$A_{ads} + B_{ads} \rightarrow AB_{\text{gas}} \rightarrow 0,$$

which are initially uniformly dissolved in the bulk. I shall focus here on discussing a possibility of observation of the predicted effects for one of the most important surface reactions of carbon monoxide $CO$ thermodesorption from metals into vacuum

$$C_{ads} + O_{ads} \rightarrow CO_{\text{gas}} \rightarrow 0.$$ 

It is to be mentioned first that the continual description (1) holds as long as the "diffusion length" of the explosion at the point of maximum remains much greater than the monolayer thickness $a$ $\delta_{xM} \sim 1/\sqrt{\Omega^M_{\text{ads}}} \gg a/\ell$, whence there follow the limitations

$$\Omega^M_{\text{ads}} \ll (\ell/a)^2, \quad K \ll p^2(\ell/a)^3.$$ 

Taking, for example, $\ell/a \sim 10^3$ and $p \sim 0.01$ we come to the requirements $\Omega^M_{\text{ads}} \ll 10^6$ and $K \ll 10^8$ to see that at
any value of the reaction rate constant $\kappa$ the specimens must have macroscopic sizes in order a considerable effect be observed. Based on the data of monograph \textsuperscript{31}, I shall make estimations for three refractory metals, i.e., niobium, tantalum, and molybdenum which at elevated temperatures dissolve carbon and oxygen in quite large amounts. According to \textsuperscript{31}, at temperatures of intensive thermodesorption of CO in the range from $T \sim 1600^\circ\mathrm{C}$ to melting point for coefficients of carbon and oxygen diffusion in these metals we find, respectively, $D_C \sim (10^{-7} \div 10^{-5}) \mathrm{cm}^2/\mathrm{s}$ and $D_O \sim (10^{-5} \div 10^{-4}) \mathrm{cm}^2/\mathrm{s}$, whence it follows $p = D_C/D_O \sim 10^{-2} \div 10^{-1}$. According to the data of \textsuperscript{31} - \textsuperscript{32} the desorption rate constant of CO in said temperature range alters within $\kappa \sim (10^{-23} \div 10^{-18}) \mathrm{cm}^3/\mathrm{s}$. Substituting these values into the expression

$$\Delta = \delta_C(0) \kappa \ell / D_C$$

and taking $\delta_C(0) = c_C(0) - c_O(0) \sim 10^{20} \mathrm{cm}^{-3}$ and $\ell \sim 0.1 \mathrm{cm}$ we find that in said range of temperatures the $\Delta$ parameter value changes within $\Delta \sim 10^{2} \div 10^{6}$. For the density of the diffusion-controlled desorption flux of CO at the critical point we find $I_s \sim D_C \delta_C(0)/\ell \sim 10^{14} \div 10^{16} \mathrm{particles/cm}^2 \mathrm{s}$. We thus conclude that in a study of isothermal desorption of CO at elevated temperatures under high vacuum the predicted \textit{sharp jump} of the flux relaxation rate can confidently be registered experimentally with a standard measuring technique.

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### APPENDIX A: CROSSOVER TO THE SCALING REGIME OF CATASTROPHE.

From (40) and (41) it follows that in the limit of large $K \rightarrow \infty$ the ratio

$$\frac{\Omega^M_{L_s} - \Omega^M_{H_s}}{\Omega^M_{H_s}} \sim \frac{[\dot{\tau}^{-1}_J]_M}{\Omega^M_s} \propto \mu/K^{1/4} \rightarrow 0.$$  

I shall show below that $\Omega^M_{H_s}$ reaches the asymptotic limit (40) much more rapidly than $\Omega^M_{L_s}$, therefore it is the point of maximum of $\Omega_{H_s}$ that defines the point of maximum of the explosion. With allowance for the fact that $\Omega_{L_s}/\Omega_{H_s} \rightarrow 1$ only asymptotically, at finite $K$ instead of (26) one has to write

$$\Omega_{H_s} \sqrt{h_s} + (\Omega_{L_s}/\Omega_{H_s}) l_s = C(0). \quad (A1)$$

whence at the point of explosion maximum $\Omega_{H_s} = 0$ we find

$$\sqrt{h_s^M} / l_s^M = \left( \frac{\Omega^M_{L_s}}{\Omega^M_{H_s}} \right)^2 \frac{[\dot{\tau}^{-1}_J]_M}{\Omega^M_s} \frac{C(0)}{l_s^M \Omega^M_{H_s}^2}, \quad (A2)$$

where for completeness the term with the derivative is held

$$\dot{C}(0) = -\dot{\tau}^{(0)}_s = -\omega_0 \mu J_*$$

and it is taken into account that from the condition $\Omega_{H_s} = 0$ it follows $\Omega_{L_s} = [\dot{\tau}^{-1}_J]$. Differentiating (37) and calculating the arising integral, we find the leading term in $[\dot{\tau}^{-1}_J]_M$ in the form

$$[\dot{\tau}^{-1}_J]_M = \gamma M h_s^M (\Omega^M_s)^{5/2}/J_*$$

where $\gamma M = 3\Gamma(3/4)^2/2\pi = (3/4) a_M \approx 0.717$. Substituting this result into Eq. (A2), using the equality $\Omega^M_{L_s} = \Omega^M_{H_s} + \omega_0 + [\dot{\tau}^{-1}_J]_M$, and taking $\Omega^M_{H_s} \approx \Omega^M_s$, after separating out the leading terms we find

$$\sqrt{h^M_s} / l_s^M = 1 + B_* \mu / K^{1/4} + O_\tau (K^{-1/2}) \quad (A3)$$

where

$$B_* = \frac{2c_M - \gamma M}{\sqrt{2}} \approx 0.972.$$  

At the point of the explosion maximum allowing for the contribution of $J_{cx}$ (36) instead of (29) one has to write

$$h^M_s / l_s^M = J_M = B_* (1 + J_{cx}^M / J_*).$$

Substituting (36) here we have

$$h^M_s / l_s^M = J_* [1 - B_* \mu / K^{1/4} + O_\tau (K^{-1/2})], \quad (A4)$$

where

$$B_* = a_M / \sqrt{2} \approx 0.676.$$  

Eqs.(A3) and (A4) immediately give

$$h^M_s / l_s^M(a) = 1 + B_h \mu / K^{1/4} + O_h (K^{-1/2}), \quad (A5)$$

where

$$h^M_s(a) = \rho^{-1/4} \sqrt{J_*}$$

and

$$B_h = \frac{(2c_M - a_M - \gamma M)}{2\sqrt{2}} \approx 0.148.$$  

and

$$l_s^M(a) = 1 - B_h \mu / K^{1/4} + O_l (K^{-1/2}), \quad (A6)$$

where

$$l_s^M(a) = \rho^{1/4} \sqrt{J_*}$$

and

$$B_l = \frac{2c_M + a_M - \gamma M}{2\sqrt{2}} \approx 0.824.$$
From (A5) and (A6) it follows that \( h_s^M \) always comes to its asymptotics \( h_s^M(a) \) from above whereas \( l_s^M \) always comes to its asymptotics \( l_s^M(a) \) from below. Essentially, the coefficient \( B_h \) is much smaller than \( B_l \) and, therefore, with growing \( K \) the asymptotics \( h_s^M(a) \) is reached much earlier than the asymptotics \( l_s^M(a) \). Substituting then (A3) into (A1) and using (A5), (A6) we obtain

\[
\Omega_{hs}^M/\Omega_h^M(a) = 1 - B_{hM}/K^{1/4} + O(K^{-1/2}), \quad (A7)
\]

where

\[
\Omega_s^M(a) = (\mu/2)p^{-1/4}\sqrt{J}.
\]

and

\[
B_{h} = \frac{c_M - a_M}{2\sqrt{2}} \approx 0.0318.
\]

From (A7) it follows that \( \Omega_{hs}^M \) always comes to its asymptotics \( \Omega_s^M(a) \) from below. Remarkably, the coefficient \( B_{h} \) appears so small that already at \( K > 10^2 \) the contribution of the \( K^{-1/4} \) term becomes less than 0.01. Substituting now (A4), (A5), and (A7) into the expression

\[
[\tau_j^{-1}]_M = c_M h_s^M(\Omega_{hs}^M)^{3/2}/J_M
\]

for the amplitude of the catastrophe at the point of explosion maximum we find

\[
[\tau_j^{-1}]_M/[\tau_j^{-1}]_M(a) = 1 + B_J\mu/K^{1/4} + O(J(K^{-1/2})). \quad (A8)
\]

where

\[
[\tau_j^{-1}]_M(a) = (0.369834...\mu^{3/2}p^{-5/8}J_s^{1/4}
\]

and

\[
B_J = \frac{a_M + (1/8)(2c_M - a_M)}{\sqrt{2}} \approx 0.776
\]

From (A8) it follows that \( [\tau_j^{-1}]_M \) always comes to its asymptotics \( [\tau_j^{-1}]_M(a) \) from above and, due to the comparatively high \( B_J \) value, reaches its asymptotics much slower than \( \Omega_{hs}^M \).

The expressions (A5), (A6), (A7), and (A8) completely define the principal picture of the crossover to the scaling catastrophe and explosion regime in the limit of large \( K \rightarrow \infty \). To be complete, I shall calculate now the corrections \( O(K^{-1/2}) \) and \( O(J(K^{-1/2}) \) which, as one can easily see, may be of two types \( O_p(p/\sqrt{K}) \) and \( O_p^p(\mu^2/\sqrt{K}) \). As \( \mu \sim 1-p \rightarrow 0 \) at \( p \rightarrow 1 \) the \( O_p^p \) corrections appear essential at \( p \) close to 1. The calculations give

\[
O_p^p = -\tau_{p}^2/4p/\sqrt{K} \approx -2.467p/\sqrt{K} \quad (A9)
\]

and

\[
O_p^p = (4\mu M/c - 3)a^2/8p/\sqrt{K} \approx +0.809p/\sqrt{K}. \quad (A10)
\]

Due to the anomalously low value of the coefficient \( B_{h} \) I shall also give the term \( O_p^p \). The calculations yield

\[
O_p^p = [B_3(3B_3/2 - B_3(8) - B^2/128]\mu^2/\sqrt{K} \quad (A11)
\]

whence after substituting the coefficients we find

\[
O_p^p \approx -0.00946\mu^2/\sqrt{K}.
\]

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[9] Acting in the spirit of Appendix it is easy to check that at large \( K \) and small \( \delta_{ij} \delta_{i0} \) the ratio \([\tau_j^{-1}]_M/[\Omega_x^M] \propto \epsilon_j(1 + \epsilon_j - \delta_j) \) so not too close to the critical points \( p_0^2 \) and \( p^2 \) at large \( \Delta \rightarrow \infty \) the relative deviations \([\delta - \delta_{\infty}] / \delta_{\infty} \) \( \propto \epsilon_j \rightarrow 0 \) (\( i = \Omega, J \)) must become vanishingly small.
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