

REACTION-DIFFUSION WAVES: CLASSICAL THEORY AND RECENT DEVELOPMENTS

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Systematic studies of reaction-diffusion waves begin in the 1930s with the works by Zeldovich - Frank-Kamenetskii in combustion theory and by Fisher and Kolmogorov - Petrovskii - Piskunov in population dynamics. The theory of reaction-diffusion waves is now well developed and includes detailed analysis of the scalar reaction-diffusion equations and monotone systems, of flame stability and nonlinear dynamics, of waves in excitable media, of reaction-diffusion-convection waves, and so on. After a short review of the theory of reaction-diffusion waves, some recent developments in the theory of flame propagation will be presented. They concern some mathematical aspects of combustion waves with the Lewis number different from 1 and reaction-diffusion-convection waves. Models in population dynamics with intra-specific competition will be discussed. They provide a new mechanism of pattern formation in biology and can be used to describe the emergence of biological species in the process of evolution.

1. Scalar reaction-diffusion equations

Reaction-diffusion equations describe numerous phenomena in population dynamics, in chemical kinetics and combustion, in catalysis, and in many other applications. The pioneering works²³ and³⁶ on propagation of the dominant gene and⁶⁸ in combustion initiated the development of this area of research. The scalar reaction-diffusion equations in one space dimension were intensively studied till the 1980s (see, e.g., Refs. 22, 32, 34, 60 and the references therein). The existence, stability, and the speed of propagation of reaction-diffusion waves were well understood and formed the basis for further developments. In this section we will recall the main notions and results for the scalar reaction-diffusion equation. They can be found in particular in.⁶⁰

1.1. Existence of waves

Consider the reaction diffusion equation

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + F(u) \quad (1)$$

on the whole axis, $x \in \mathbb{R}$. Everywhere below we will assume that the function $F(u)$ is continuous together with its first derivative. Travelling wave solution of this equation is, by definition, the solution of the form

$$u(x, t) = w(x - ct),$$

where c is a constant, the wave speed. Then the function $w(x)$ satisfies the equation

$$w'' + cw' + F(w) = 0, \quad (2)$$

where prime denotes the derivative with respect to x . If we look for solutions of this equation with some limits at infinity,

$$\lim_{x \rightarrow \pm\infty} w(x) = w_{\pm}, \quad w_+ < w_-, \quad (3)$$

then it can be easily shown that

$$F(w_{\pm}) = 0.$$

The constant c is not given. We should find its values such that problem (2), (3) has a solution.

We will look for solutions $w(x)$ of problem (2), (3) such that $w_+ < w(x) < w_-$ for all $x \in \mathbb{R}$. In this case, if such solution exists, then it is monotonically decreasing. It appears that only such solutions are interesting from the point of view of applications. Non-monotone waves are unstable (see the next section).

It is also convenient to reduce equation (2) to the system of two first order equations

$$w' = p, \quad p' = -cp - F(w). \quad (4)$$

Solutions of problem (2), (3) correspond to trajectories connecting two stationary points of system (4), that are $(1, 0)$ and $(0, 0)$.

It is easy to verify that the points w_+ and w_- are stationary points of the equation

$$\frac{dw}{dt} = F(w). \quad (5)$$

If $F(w) \leq 0$ in a right-half neighborhood of the point w_+ , then this point is stable with respect to positive perturbations, that is the solution of equation (5) with the initial condition $w(0) > w_+$ and close to w_+ will remain in a neighborhood of this stationary point. If $F(w) < 0$ in a right-half neighborhood of w_+ , then this point is asymptotically stable, that is the solution will converge to it.

These observations justify the following terminology. We call problem (2), (3) *bistable* if $F(w) \leq 0$ in a right-half neighborhood of w_+ and $F(w) \geq 0$ in a left-half neighborhood of w_- . It is *monostable* if $F(w) > 0$ in a right-half neighborhood of w_+ and $F(w) \geq 0$ in a left-half neighborhood of w_- . Finally, it is *unstable* if $F(w) > 0$ in a right-half neighborhood of w_+ and $F(w) < 0$ in a left-half neighborhood of w_- .

The simplest example of the bistable case is given by the function $F(w)$ such that

$$F(w) < 0, w_+ < w < w_0, \quad F(w) > 0, w_0 < w < w_- \quad (6)$$

for some $w_0 \in (w_+, w_-)$.

We begin with the theorem on wave existence in the bistable case.

Theorem 1.1. *Let condition (6) be satisfied. Then there exists a unique value of c and a unique up to translation monotonically decreasing function $w(x)$ which satisfy problem (2), (3).*

This theorem can be proved by the analysis of system (4). We show the existence of a trajectory connecting the stationary points $(w_+, 0)$ and $(w_-, 0)$. Both of them are saddles. It appears that the trajectory going from the point $(w_+, 0)$ into the half-plane $p < 0$ and the trajectory which comes to the point $(w_-, 0)$ from this half-plane depend monotonically on c . They intersect and, consequently, coincide for a single value of c .

Theorem 1.1 can be generalized for other nonlinearities $F(w)$ in the bistable case. For some functions $F(w)$, solution of problem (2), (3) may not exist. In this case, we should introduce the notion of systems of waves which we do not discuss here (see⁶⁰).

Consider next the function $F(w)$ such that

$$F(w) > 0, w_+ < w < w_-. \quad (7)$$

It is the simplest example of the monostable case.

Theorem 1.2. *Let condition (7) be satisfied. Then there exists the minimal speed c_0 such that for all $c \geq c_0$ there exist monotonically decreasing solution $w(x)$ of (2), (3). Such solutions do not exist for $c < c_0$.*

The proof of this theorem can also be done studying trajectories of system (4). The stationary point $(w_-, 0)$ is a saddle as before. However, the point $(w_+, 0)$ is now a stable node. This is why the waves exist for all values of the velocity greater or equal to the minimal velocity.

For more general nonlinearities in the monostable case the waves may not exist. In this case, similar to the bistable case, systems of waves should be introduced. We finally note that in the unstable case solutions of problem (2), (3) do not exist.

1.2. Stability of waves

To define the notion of stability of travelling waves we consider the solution of equation (1) with some initial condition $u(x, 0) = u_0(x)$ supposed here to be a continuous function. If the initial condition is close to the wave, that is it can be represented in the form

$$u_0(x) = w(x) + v(x),$$

where $v(x)$ is a small perturbation, then the solution can approach the wave when time t goes to infinity. In this case the wave is stable. The perturbation can also grow in time, and in this case the wave is unstable. To be more precise, we should specify the class of perturbations and in what sense we understand the convergence.

We recall that the waves are invariant with respect to translation in space. This means that along with $w(x)$, all functions $w(x + h)$ for any $h \in \mathbb{R}$ satisfy equation (2). It appears that the solution with the initial condition close to the wave $w(x)$ can converge to a shifted wave $w(x + h)$. This is stability with shift.

Definition 1.1. If for some $\epsilon > 0$, the function $u_0(x)$ satisfies the estimate

$$\sup_x |u_0(x) - w(x)| \leq \epsilon,$$

and the solution of the equation (1) with the initial condition $u(x, 0) = u_0(x)$ converges to a wave $w(x + h)$ for some h ,

$$\sup_x |u(x, t) - w(x + h)| \rightarrow 0, \quad t \rightarrow \infty,$$

then the wave $w(x)$ is asymptotically stable with a shift.

The notion of asymptotic stability implies that the perturbation decays. If we impose a weaker condition that the perturbation remains bounded,

then stability of waves for the scalar equations follows directly from the comparison principle: if the initial condition satisfies the inequality

$$w(x) \leq u_0(x) \leq w(x-h), \quad x \in \mathbb{R}$$

for some positive h , then the same inequality holds for the solution:

$$w(x) \leq u(x, t) \leq w(x-h), \quad x \in \mathbb{R}, \quad t \geq 0.$$

This means that initially small perturbation remains small. The proof of the asymptotic stability is much more involved and requires the analysis of the spectrum of the linearized operators.

Consider the operator L linearized about the wave,

$$Lv = v'' + cv' + F'(w(x))v.$$

Theorem 1.3. *Suppose that $F'(w_{\pm}) < 0$ (bistable case). The principle eigenvalue of the operator L (that is the eigenvalue with the maximal real part) is real, simple, and the corresponding eigenfunction is positive up to a constant factor. There are no other eigenvalues with positive eigenfunctions.*

This result allows us to make some conclusions about the location of the spectrum of the operator L . Indeed, differentiating equation (2) with respect to x , we can easily verify that $v_0(x) = -w'(x)$ is a positive eigenfunction of the operator L corresponding to the zero eigenvalue. Hence, according to the last theorem, the zero eigenvalue is simple and all other spectrum lies in the left-half plane. This is exactly the situation which provides the asymptotic stability with a shift.

Theorem 1.4. *Suppose that $F'(w_{\pm}) < 0$ (bistable case). If for some $\epsilon > 0$,*

$$\sup_x |u_0(x) - w(x)| \leq \epsilon,$$

then the wave $w(x)$ is asymptotically stable with a shift, that is there exists a constant h such that the following estimate holds

$$\sup_x |u(x, t) - w(x+h)| \leq Me^{-\sigma t},$$

where M and σ are some positive constants.

Stability in the sense of Definition 1.1 is also called local stability or stability with respect to small perturbations. We can obtain a stronger result on global stability. We will assume for simplicity that the initial condition $u_0(x)$ is a monotonically decreasing function.

Theorem 1.5. *Suppose that $F'(w_{\pm}) < 0$ (bistable case) and*

$$F(u) < 0, w_+ < u < w_+ + a, \quad F(u) > 0, w_- - b < u < w_-,$$

where a and b are some positive constants. If the initial condition $u_0(x)$ is a monotonically decreasing function such that

$$w_+ < u_0(+\infty) < w_+ + a, \quad w_- - b < u_0(-\infty) < w_-,$$

then the solution of equation (1) exponentially converges to a wave, that is there exists a constant h such that the following estimate holds

$$\sup_x |u(x, t) - w(x + h)| \leq M e^{-\sigma t},$$

where M and σ are some positive constants.

We next introduce the notion of convergence in form and in speed. Consider the equation

$$u(x, t) = \frac{1}{2}(w_+ + w_-),$$

where $u(x, t)$ is a solution of equation (1). We will assume for simplicity that $u(x, t)$ is monotonically decreasing in x (this is the case if the initial condition is decreasing), with the limits w_{\pm} at $\pm\infty$. Then the last equation has a unique solution for all $t > 0$. Denote it by $m(t)$. Put

$$v(x, t) = u(x + m(t), t).$$

Then $v(x, t)$ is a solution of the equation

$$\frac{\partial v}{\partial t} = \frac{\partial^2 v}{\partial x^2} + m'(t) \frac{\partial v}{\partial x} + F(v) \quad (8)$$

and

$$v(x, 0) = \frac{1}{2}(w_+ + w_-).$$

Definition 1.2. If

$$\sup_x |v(x, t) - w(x)| \rightarrow 0, \quad t \rightarrow \infty,$$

then we will say that the solution $u(x, t)$ converges to the wave $w(x)$ in form. If $m'(t) \rightarrow c$, then it is the convergence in speed.

It can be verified that the uniform convergence discussed above implies the convergence in form and in speed but the converse is not generally true. The convergence in speed follows from the convergence in form.

Convergence in form can be proved for wider classes of nonlinearities than in the case of the uniform convergence. If we still consider the bistable case but the condition $F'(w_{\pm}) < 0$ is not satisfied, that is one of the derivatives equals zero, then the essential spectrum of the linearized operator passes through the origin (see Section 2) and the stability results presented above are not applicable. To simplify the formulation of the next theorem, we will restrict ourselves to monotone initial conditions with the limits w_{\pm} at $\pm\infty$.

Theorem 1.6. *Suppose that the nonlinearity $F(u)$ satisfies the conditions of the bistable case and that there exists a monotonically decreasing solution $w(x)$ of problem (2), (3). Then for any monotonically decreasing initial condition $u_0(x)$ such that $u_0(\pm\infty) = w_{\pm}$, the solution $u(x, t)$ of equation (1) converges to the wave $w(x)$ in form and in speed.*

We will finish this section with some results on the convergence to waves in the monostable case. We assume, for simplicity of presentation, that the function $F(u)$ is positive in the interval (w_+, w_-) . In this case monotone waves exist for all $c \geq c_0$. They have exponential behavior at $+\infty$ with the exponent λ , where

$$\lambda = \frac{c}{2} - \sqrt{\frac{c^2}{4} - F'(w_+)} \quad \text{for } c > c_0, \quad \lambda = \frac{c}{2} + \sqrt{\frac{c^2}{4} - F'(w_+)} \quad \text{for } c = c_0.$$

Thus, the waves can be characterized by the parameter

$$\lambda = - \lim_{x \rightarrow +\infty} w'_c(x) / (w_c(x) - w_+). \quad (9)$$

Theorem 1.7. *Let $F(u) > 0$ for $u \in (w_+, w_-)$. Suppose that $u_0(x)$ is a decreasing function continuous with its first derivative. If there exists the limit*

$$\lambda = - \lim_{x \rightarrow +\infty} u'_0(x) / (u_0(x) - w_+)$$

and

$$\lambda < \frac{c_0}{2} - \sqrt{\frac{c_0^2}{4} - F'(w_+)},$$

then the solution of equation (1) with the initial condition $u(x, 0) = u_0(x)$ converges in form and in speed to the wave $w_c(x)$, for which the limit (9) has the same value of λ . If

$$\lambda > \frac{c_0}{2} - \sqrt{\frac{c_0^2}{4} - F'(w_+)},$$

then the solution converges in form and speed to the wave $w_{c_0}(x)$ with the minimal velocity.

We note that this theorem can be generalized for much wider classes of nonlinearities and initial conditions. We will only mention that if the initial condition is a Heaviside function, $u_0(x) = w_-$ for $x \leq 0$ and $u_0(x) = w_+$ for $x > 0$, then the solution converges to the wave with the minimal velocity. This is the main result of the work KPP.³⁶

1.3. Velocity of waves

We recall that if the wave exists in the bistable case then the corresponding value of the velocity is unique. In the monostable case, if the waves exist, then their speed fill some interval $[c_0, c_1)$, for some $c_1 \leq \infty$. There are various ways to compute or to estimate the wave velocity.

We begin with the bistable case. From (4) we have

$$c \equiv -\frac{dp}{dw} - \frac{F(w)}{p(w)}, \quad w \in (w_+, w_-).$$

If instead of the exact solution $p(w)$ we consider a smooth function $\rho(w)$ such that

$$\rho(w_+) = \rho(w_-) = 0, \quad \rho(w) < 0, \quad w_+ < w < w_-, \quad (10)$$

then it can be shown that

$$\min_w \left(-\rho'(w) - \frac{F(w)}{\rho(w)} \right) \leq c \leq \max_w \left(-\rho'(w) - \frac{F(w)}{\rho(w)} \right).$$

If the wave exists, then its velocity admits the minimax representation

$$c = \inf_{\rho} \max_w \left(-\rho'(w) - \frac{F(w)}{\rho(w)} \right) = \sup_{\rho} \min_w \left(-\rho'(w) - \frac{F(w)}{\rho(w)} \right), \quad (11)$$

where the infimum and supremum are taken with respect to all functions ρ satisfying conditions (10).

In the monostable case the left equality in (11) gives the values of the minimal velocity.

There are some particular cases where the minimal velocity in the monostable case can be found explicitly. If $F'(w) \leq F'(w_+)$ for $w \in (w_+, w_-)$, then $c_0 = 2\sqrt{F'(w_+)}$. If this condition is not satisfied, then it is possible that $c_0 > 2\sqrt{F'(w_+)}$.

2. Chemical kinetics and combustion

Reaction-diffusion systems describe numerous applications in chemical kinetics and combustion. A general chemical reaction can be written in the form

$$\sum_{j=1}^m \alpha_{ij} A_j \rightarrow \sum_{j=1}^m \beta_{ij} A_j, \quad i = 1, \dots, n.$$

There are n elementary reactions and m species A_1, \dots, A_m . The constants α_{ij}, β_{ij} are called the stoichiometric coefficients. The rate of the i -th reaction W_i , according to the mass action law can be written as

$$W_i = k_i(T) A_1^{\alpha_{i1}} \times \dots \times A_m^{\alpha_{im}}.$$

The corresponding reaction-diffusion system has the form

$$\frac{\partial T}{\partial t} = \kappa \frac{\partial^2 T}{\partial x^2} + \sum_{i=1}^n q_i W_i, \quad (12)$$

$$\frac{\partial A_j}{\partial t} = d_j \frac{\partial^2 A_j}{\partial x^2} + \sum_{i=1}^n \gamma_{ij} W_i, \quad j = 1, \dots, m, \quad (13)$$

where $\gamma_{ij} = \beta_{ij} - \alpha_{ij}$. In the case of equality of transport coefficients, that is if $d_1 = \dots = d_m = \kappa$, and under some additional conditions on the reaction scheme,⁶⁰ system (12), (13) can be reduced to so-called monotone systems characterized by the applicability of the maximum principle and of comparison theorems (Section 2.1). In this case, most of the results on wave existence and stability obtained for the scalar equation remain valid for systems of equations. If the transport coefficients differ from each other, as it is the case for condensed phase combustion, then propagation of flames can show some new features. In particular, it can be accompanied by various instabilities resulting in complex nonlinear dynamics (Section 2.2).

2.1. Monotone systems

Consider now the system of equations

$$\frac{\partial u}{\partial t} = d \frac{\partial^2 u}{\partial x^2} + F(u), \quad (14)$$

where $u = (u_1, \dots, u_m)$, $F = (F_1, \dots, F_m)$, d is a diagonal matrix with positive diagonal elements. We assume that the vector-valued function $F(u)$ satisfies the following condition

$$\frac{\partial F_i}{\partial u_j} > 0, \quad i, j = 1, \dots, m, \quad i \neq j. \quad (15)$$

Such systems satisfy the positiveness and comparison theorems. They are essentially used in the investigation of travelling waves. The following theorem gives the existence of waves in the bistable case.

Theorem 2.1. *Suppose that $F(w_+) = F(w_-) = 0$, where $w_+ < w_-$ (the inequality is component-wise) and the matrices $F'(w_\pm)$ have all eigenvalues in the left-half plane. If there exists a finite number of points $w^j \neq w_\pm$, $j = 1, \dots, k$ such that $w_+ \leq w^j \leq w_-$ and each matrix $F'(w^j)$ has at least one eigenvalue in the right-half plane, then there exists a unique monotonically decreasing travelling wave solution $u(x, t) = w(x - ct)$ of system (14) with the limits $w(\pm\infty) = w_\pm$. Its velocity admits the following minimax representation*

$$c = \inf_{\rho \in K} \sup_{x,i} \frac{\rho''_i + F_i(\rho)}{-\rho'} = \sup_{\rho \in K} \inf_{x,i} \frac{\rho''_i + F_i(\rho)}{-\rho'},$$

where K is the class of monotonically decreasing vector-functions ρ continuous with their second derivatives and having limits $\rho(\pm\infty) = w_\pm$ at infinity.

This theorem generalizes Theorem 1.1 for monotone systems. Its proof is based on the topological degree theory and on some special a priori estimates of solutions. Under some additional conditions, it remains valid if inequality (15) is not strict. Detailed presentation of this and of the following result for the monostable case is given in.⁶⁰

Theorem 2.2. *Suppose that $F(w_+) = F(w_-) = 0$, where $w_+ < w_-$, the matrix $F'(w_-)$ has all eigenvalues in the left-half plane and the matrix $F'(w_+)$ has at least one eigenvalue in the right-half plane. If there are no other zeros of the function $F(u)$ for $w_+ \leq u \leq w_-$, then for all $c \geq c_0$ there exists a monotonically decreasing travelling wave solution $u(x, t) = w(x - ct)$ with the limits $w(\pm\infty) = w_\pm$. For $c < c_0$ such solutions do not exist. The minimal value c_0 of the velocity is given by the equality*

$$c_0 = \inf_{\rho \in K} \sup_{x,i} \frac{\rho''_i + F_i(\rho)}{-\rho'},$$

where K is the same as in the previous theorem.

We finally remark that the monotone waves are asymptotically stable.⁶⁰ The results on wave existence, stability and velocity for monotone systems in cylinders for the monostable and for the bistable cases are given in.^{61,63,64}

2.2. Flame propagation

The classical model describing flame propagation consists of the two reaction-diffusion equations

$$\frac{\partial T}{\partial t} = \kappa \frac{\partial^2 T}{\partial x^2} + qk(T)\phi(\alpha), \quad (16)$$

$$\frac{\partial \alpha}{\partial t} = d \frac{\partial^2 \alpha}{\partial x^2} + k(T)\phi(\alpha), \quad (17)$$

where T is the temperature, α the depth of conversion, κ the coefficient of thermal diffusivity, d the coefficient of mass diffusion, q the adiabatic heat release,

$$k(T) = \begin{cases} k_0 e^{-E/RT}, & T > T^* \\ 0, & T \leq T^* \end{cases},$$

$\phi(\alpha)$ is the kinetic function usually considered in the form $\phi(\alpha) = (1 - \alpha)^n$, $n \geq 0$. For $T > T^*$ the function $k(T)$ has the form of the Arrhenius exponential, where E is the activation energy, R the gas constant, k_0 the pre-exponential factor. We employ here the well known in combustion theory “cut-off” procedure assuming that $k(T)$ equals zero for $T < T^*$. Without this assumption, system (16), (17) does not have travelling wave solutions and flames can be considered only as an intermediate asymptotics.⁶⁶ If the activation energy is sufficiently large, which is the case for combustion processes, then the choice of T^* is not essential. System (16), (17) should be completed by the conditions at infinity:

$$x = +\infty : T = T_i, \alpha = 0, \quad x = -\infty : T = T_b, \alpha = 1,$$

where $T_b = T_i + q$. These conditions imply that the wave propagates from $-\infty$ to $+\infty$.

The temperature distribution in combustion wave is shown schematically in Figure 1. The black region is the reaction zone where the reaction rate $W = K(T)\phi(\alpha)$ is essentially different from zero. Outside of the reaction zone, the reaction rate is close to zero. In front of it (with respect to the direction of wave propagation), the temperature decreases and the Arrhenius exponential in the case of large activation energies becomes small. Behind the reaction zone, the temperature is high, but the depth of conversion becomes close to 1, that is $\phi(\alpha)$ is small.

Thus, if the activation energy is large, then the reaction zone is narrow. This observation allowed Zeldovich and Frank-Kamenetskii to develop the method of narrow reaction zone⁶⁸ which remains the basic analytical

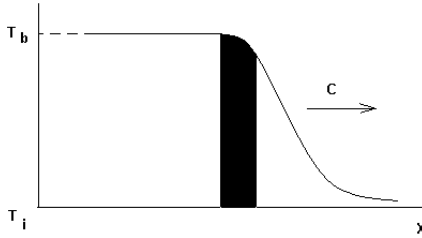


Fig. 1. Schematic representation of combustion wave. Black region corresponds to the reaction zone.

method to study combustion fronts. The idea of the method is to consider the limit where the width of the reaction zone tends to zero. In this limit, we obtain a free boundary problem with linear equations outside of the free boundary and with some jump conditions at the interface. In the case of $Le = 0$ and zero order reaction, the jump conditions have the form:

$$T(\xi + 0, t) = T(\xi - 0, t), \quad T'(\xi + 0, t) - T'(\xi - 0, t) = -\frac{q}{\kappa},$$

$$(T'(\xi + 0, t))^2 - (T'(\xi - 0, t))^2 = \frac{2q}{\kappa} \int_{T_i}^{T_b} k(T) dT,$$

where $\xi(t)$ is the position of the free boundary. The value of the temperature and of its derivatives at the interface can be explicitly found from the solution of linear equations outside of the reaction zone. This allows us to obtain the formula for the speed of propagation:

$$c^2 = \frac{2\kappa}{q} \int_{T_i}^{T_b} k(T) dT.$$

The method of narrow reaction zone is also used to study stability of combustion fronts. If $\kappa = d$, that is the Lewis number $Le = d/\kappa$ equals 1, then system (16), (17) can be reduced to the scalar reaction-diffusion equation considered in Section 1. In this case, the existence and stability of waves is discussed above. If $Le \neq 1$, then the wave existence is also known though its proof can be more involved. We will discuss here wave stability in more detail. Along with the Lewis number, we introduce another dimensionless parameter called Zeldovich number, $Z = qE/RT_b^2$. It is a large parameter (since the activation energy is large) inversely proportional to the width of the reaction zone.

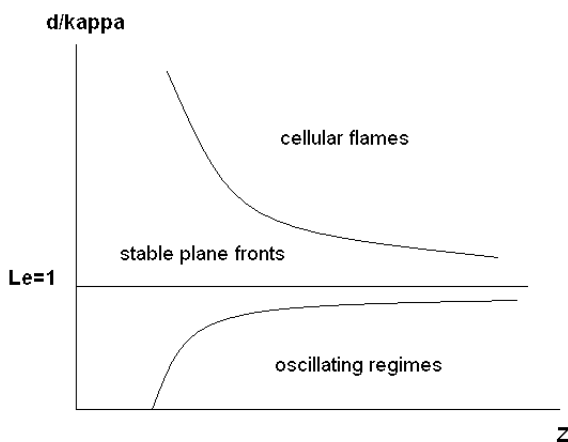


Fig. 2. Schematic representation of the stability and instability regions in the (Z, Le) -plane.

Schematic representation of stability regions in the (Z, Le) -plane is shown in Figure 2. As we indicated above, for $Le = 1$, the wave is stable for all values of Z . If $Le < 1$ and Z is sufficiently large, then the wave becomes unstable. When the parameter crosses the stability boundary, a Hopf-like bifurcation occurs. This means that a pair of complex conjugate eigenvalues of the corresponding linearized operator crosses the imaginary axis. We recall that this operator has also a zero eigenvalue related to the translation invariance of travelling wave solutions. Because of this, the bifurcation analysis and behavior of bifurcating solutions differs from the classical situation of Hopf bifurcation (see, e.g.,⁶⁰).

In the one-dimensional spatial case, with the Lewis number less than 1, the loss of stability of combustion front results in appearance of time oscillations. The speed of propagation is not constant any more, it becomes periodic in time. Further increase of the Zeldovich number leads to a period doubling bifurcations and to transition to chaos.

In the multi-dimensional case (the second derivatives in (16), (17) should be replaced by the Laplace operators), the loss of stability of plane fronts can result in a big variety of the propagating regimes, which depend on the geometry of the sample and on the values of parameters. The most well known among them are the so-called spinning modes of propagation where the high-temperature spots rotate along the cylindrical surface of the

sample. They are discovered experimentally first in the condensed phase combustion⁴⁷ and later in frontal polymerization.⁵⁷ There is a number of analytical and numerical studies devoted to spinning modes of gasless combustion (see^{39,42,52,60} and the references therein).

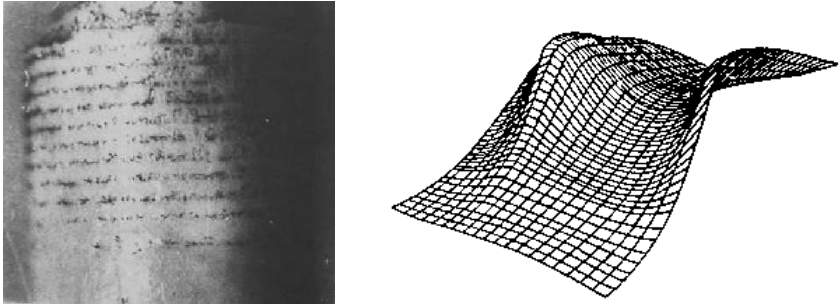


Fig. 3. Frontal polymerization sample after the spinning mode of propagation⁵⁷ (left). A snapshot of the temperature distribution in numerical simulations of spinning combustion⁵⁸ (right).

If the Lewis number is greater than 1 and the Zeldovich number is sufficiently large, then a bifurcation of change of stability occurs. A simple real eigenvalue of the linearized operator crosses the origin. The plane front loses its stability and a curved front appears. It propagates with a constant speed and a constant profile but it is essentially multi-dimensional. Such regimes are called in combustion theory cellular flames.⁵¹

2.3. *Mathematical theory of combustion waves with the Lewis number different from 1*

In the multi-dimensional case, travelling wave solution of the reaction-diffusion system describing flame propagation satisfies the elliptic system of equations

$$\Delta\theta + (c + \psi(y)) \frac{\partial\theta}{\partial x} + K(\theta, \alpha) = 0 \quad (18)$$

$$Le \Delta\alpha + (c + \psi(y)) \frac{\partial\psi}{\partial x} + K(\theta, \alpha) = 0. \quad (19)$$

Here θ is the dimensionless temperature, $K(\theta, \alpha)$ the reaction rate. We consider it in an unbounded cylinder

$$\Omega = \{(x, y), -\infty < x < +\infty, y \in G\},$$

where G is an open bounded subset of \mathbb{R}^m with $m = 1, 2$. The system is completed by the boundary conditions

$$\frac{\partial \theta}{\partial \nu} = \frac{\partial \alpha}{\partial \nu} = 0 \quad \text{on } \partial \Omega, \quad (20)$$

where ν is the outer normal vector, and by the following conditions at infinity

$$\theta(-\infty, y) = 1, \quad \alpha(-\infty, y) = 1; \quad \theta(+\infty, y) = 0, \quad \alpha(+\infty, y) = 0. \quad (21)$$

The function $\psi(y)$ describes the stationary gas velocity. It can be for example the Poiseuille profile.

The specific feature of system (18), (19) is that the nonlinearity is the same in both equations. In the general case where we have several reaction species and the system can contain more than two equations, the nonlinearities in these equations are linearly dependent. We restrict ourselves here to the case of two equations. If $\kappa = d$, that is $Le = 1$, then this system can be reduced to the single equation and $\theta(x, y) \equiv \alpha(x, y)$. However, if $Le \neq 1$, then this reduction cannot be done. We should consider both equations. It appears that linear dependence of the nonlinearities results in some ‘‘bad’’ properties of the corresponding elliptic operator. Namely, it does not satisfy the Fredholm property because the corresponding limiting operators are not invertible.^{19,21,65} This means that the usual solvability conditions of linear problems, which affirm that the problem is solvable if and only if the right-hand side is orthogonal to the solutions of the homogeneous adjoint problem, cannot be applied. However, the solvability conditions are used in many methods of linear and nonlinear analysis: asymptotic methods, methods of bifurcation theory, topological degree and so on. Thus, we cannot apply them to the problems under consideration or, which is often the case, can apply them only formally, without mathematical justification.

From the mathematical point of view, this is one of open questions in combustion theory. We describe here an approach which was recently developed in^{19–21} and which allows us to overcome this difficulty. It is based on the reduction of the reaction-diffusion system to some integro-differential problem in such a way that it satisfies the Fredholm property. We assume that $F(\theta) = K(\theta, \theta)$ is a C^2 function that satisfies the conditions:

$$F(0) = F(1) = 0, \quad F'(0) < 0, \quad F'(1) < 0. \quad (22)$$

They imply that the corresponding scalar equation is of the bistable type.

Let us describe the construction of the integro-differential operator. We

first introduce the function

$$H = \theta - \alpha. \quad (23)$$

Adding equations (18) and (19), we see that it satisfies the linear equation

$$\Delta H + (c + \psi(y)) \frac{\partial H}{\partial x} = (Le - 1)\Delta\alpha, \quad (24)$$

together with the boundary condition

$$\frac{\partial H}{\partial \nu} = 0 \text{ on } \partial\Omega, \quad H(\pm\infty, y) = 0. \quad (25)$$

It appears that the resolution of problem (24), (25) allows us to define H as a function of α and that the operator $H(\alpha)$ is bounded and differentiable in appropriate spaces. This allows the reduction of problem (18)-(21) to the integro-differential problem

$$Le \Delta\alpha + (c + \psi(y)) \frac{\partial \alpha}{\partial x} + K(H(\alpha) + \alpha, \alpha) = 0, \quad (26)$$

$$\frac{\partial \alpha}{\partial \nu} = 0 \text{ on } \partial\Omega. \quad (27)$$

The resolution of this problem will provide α while the unknown θ will be given by the equality $\theta = H(\alpha) + \alpha$. The analysis of the nonlinear problem is based on the properties of the corresponding linear operator

$$Lv = Le \Delta v + (c + \psi(y)) \frac{\partial v}{\partial x} + K'_\theta(\theta, \alpha)(H'(\alpha)v - v) + K'_\alpha(\theta, \alpha)v. \quad (28)$$

This new formulation of the problem allows us to obtain some existence results for problem (18)-(21) and to study bifurcations of solutions. We begin with the case where Le is close to 1 and where the system reduces to a scalar equation. The existence of multidimensional waves described by such scalar equations is studied in.^{8,9,24,28,33,56,64} Monotone systems of equations are considered in.^{59,63,64} Problem (18)-(21) with $\Lambda \neq 1$ and close to 1 is studied in^{17,18} with a completely different and less general method. The existence of solutions is first proved in a bounded rectangle. Next, a priori estimates independent of the rectangle allow the proof of the existence of solutions in the unbounded strip. Also, parabolic problems with the Lewis number different from one are studied in.^{35,37,40}

Theorem 2.3. *Suppose that for $Le = 1$ problem (18)-(21) has a solution $(\theta_0, \alpha_0 (= \theta_0), c_0)$ with $\int_G \psi(y) > 0$. Then for all Le sufficiently close to 1 it has a solution $(\theta_\Lambda, \psi_\Lambda, c_\Lambda)$.*

The proof of this theorem is based on the integro-differential formulation (26), (27). If $Le = 1$, then $H(\alpha) = H'(\alpha) \equiv 0$. In that particular case the operator L given by (28) is the usual differential operator with well known properties. These properties allow the application of the implicit function theorem and the proof of the theorem.

In the general case, the above perturbation argument requires to take into account properties of the operator H' . It is proved that the linearized operator L satisfies the Fredholm property.²¹ This result allows us to prove another existence theorem. If in the previous case we prove the existence of solutions close to a multi-dimensional solution with $Le = 1$, in this case we consider any Le and prove the existence of multi-dimensional solutions close to a one-dimensional solution under the assumption that the function $\psi(y)$ is close to a constant. This difference appears to be rather essential. In the first case, the linearized operator does not contain the operator H because it is identically zero for $Le = 1$. In the second case, the linearized operator contains H , and we need to prove its Fredholm property in order to obtain solvability conditions.

We finally note that this approach is also used to study bifurcations of solutions and the emergence of cellular flames.²¹

2.4. *Reaction-diffusion-convection waves*

Propagation of reaction fronts can be accompanied by a change of density due to the temperature and concentration variation. In a liquid or in a gaseous phase under the action of gravity, this can result in appearance of convection.

Figure 4 shows the propagation of a polymerization front in the vertical direction. The polymers below the front is solid, the monomer above it is liquid. The reaction is exothermic. It heats the liquid monomer from below and leads to convection. The convective instability appears if the frontal Rayleigh number is sufficiently large.^{25,26} The situation is different for horizontally propagating fronts (Figures 5). Convection appears here for any Raleigh numbers different from zero, and convective free solutions do not exist. Such problems can be modelled by reaction-diffusion system coupled with the Navier-Stokes equations:

$$\frac{\partial \theta}{\partial t} - \Delta \theta + \mathbf{v} \cdot \nabla \theta - K(\theta, \alpha) = 0, \quad (29)$$

$$\frac{\partial \alpha}{\partial t} - Le \Delta \alpha + \mathbf{v} \cdot \nabla \alpha - K(\theta, \alpha) = 0, \quad (30)$$

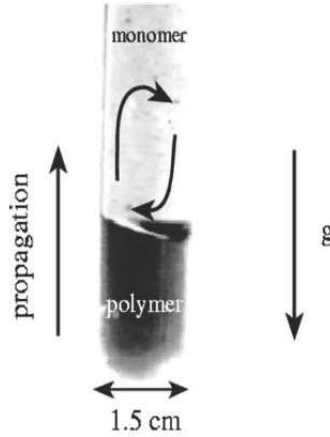


Fig. 4. Experimental results on propagation of a polymerization front with convection. The system consists of acrylamide dissolved in dymethyl sulfoxide. Adapted from¹⁰.

$$\frac{\partial \mathbf{v}}{\partial t} - P\Delta \mathbf{v} + (\mathbf{v} \cdot \nabla) \mathbf{v} + \nabla p - PR(\theta - \theta_0^*)\tau = 0, \quad (31)$$

$$\nabla \cdot \mathbf{v} = 0. \quad (32)$$

Here θ is the dimensionless temperature, α the depth of conversion, $\mathbf{v} = (v_1, v_2)$ the velocity of the medium, p the pressure. We consider here the case of two space dimensions. The equations (29), (30) describe the propagation of a premixed flame. The Navier-Stokes equations are written under the so-called Boussinesq approximation where the medium is considered as incompressible and the density is everywhere constant except for the buoyancy term, which describes the action of gravity. This term involves some characteristic temperature θ_0^* and $\tau = (\tau_1, \tau_2)$, a unit vector in \mathbb{R}^2 representing the orientation of the gravity force. Finally, the system depends on dimensionless parameters that are the Lewis number Le , the Prandtl number P and the Rayleigh number R .

System (29)-(32) is considered in an infinite strip Ω with the axis forming a given angle with the vertical direction. For convenience we will suppose that the domain is fixed,

$$\Omega = \{(x, y) \in \mathbb{R}^2, y \in (0, 1)\},$$

while the vector τ can be variable. Equations (29)-(32) are supplemented with the following boundary conditions for the temperature and for the

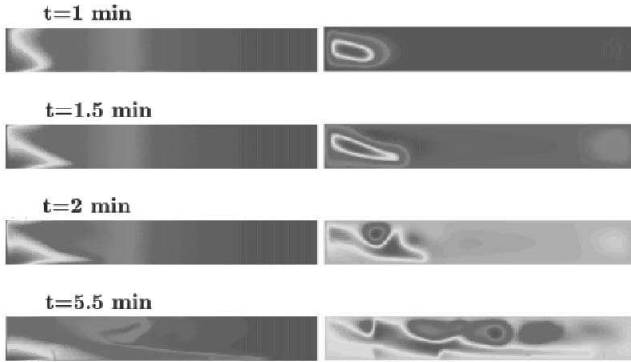


Fig. 5. Propagation of a horizontal front, concentration distribution (left), stream function (right). Numerical simulations. Adapted from⁶.

concentration

$$\frac{\partial \theta}{\partial y} = \frac{\partial \alpha}{\partial y} = 0 \text{ on } \partial\Omega, \quad (33)$$

and with the free surface boundary condition for the velocity

$$\frac{\partial v_1}{\partial y} = 0, \quad v_2 = 0 \text{ on } \partial\Omega. \quad (34)$$

In order to study this problem, it is convenient to rewrite the Navier-Stokes equations in the stream function-vorticity formulation. We introduce the stream function ψ defined by:

$$\mathbf{v} = \text{curl } \psi = \left(\frac{\partial \psi}{\partial y}, -\frac{\partial \psi}{\partial x} \right), \quad \psi = 0 \text{ on } \partial\Omega \quad (35)$$

and the vorticity

$$\omega = -\Delta\psi. \quad (36)$$

Then equations (31), (32) rewrite as

$$\frac{\partial \omega}{\partial t} - P\Delta\omega + \text{curl } \psi \cdot \nabla \omega - PR \text{curl } \theta \cdot \tau = 0, \quad (37)$$

$$\Delta\psi + \omega = 0, \quad (38)$$

while the boundary condition (34) provides

$$\omega = 0 \text{ on } \partial\Omega. \quad (39)$$

As already mentioned, the vector τ in (31) determines the orientation of the gravity force with respect to the strip. If $\tau = (1, 0)$, it is directed along the axis of the strip. If $\tau = (0, 1)$, it is oriented vertically and, consequently, perpendicular to the strip. These two cases appear to be essentially different. In the first case, the experimental results for polymerization fronts,^{10,46} formal asymptotic expansions,²⁵ and rigorous mathematical analysis for $Le = 1$ ^{54,55,62} show that for small Rayleigh numbers the vertically propagating reaction-diffusion wave is stable, and convection does not appear. For sufficiently large values of the Rayleigh number it loses its stability, and a reaction-diffusion-convection (RDC) wave appears due to a bifurcation of change of stability where a real eigenvalue of the linearized problem crosses the origin. For all other directions of the gravity force, including the case where it is perpendicular to the strip, propagation of waves is accompanied by convection even for small Rayleigh numbers. Existence of RDC waves in this case is proved in⁵ for $Le = 1$ and small R . Reaction-diffusion-convection waves in the case $Le \neq 1$ are studied in²⁰ by the method described in Section 2.3. Existence of waves for arbitrary Rayleigh numbers is studied in.^{13,38} The corresponding experimental results are described in.³ Existence of solutions of the evolution problem and some their properties are studied in,^{40,41} stability of RDC waves is discussed in.¹²

3. Population dynamics

3.1. *Classical models in population dynamics*

Beginning from the first works by Fisher²³ and KPP³⁶ on the propagation of dominant gene, reaction-diffusion equation are widely used in order to describe various phenomena in population dynamics. We can mention the logistic equation and the model of competition of species, prey-predator model, various models in epidemiology (see, e.g.,^{11,48} and the references therein).

We will briefly discuss here some classical models of growth and competition of populations. Let u denote a scaled density of the population. Then its evolution in space and in time can be described, under some simplifying assumptions, by the reaction-diffusion equation

$$\frac{\partial u}{\partial t} = d \frac{\partial^2 u}{\partial x^2} + ku(1 - u). \quad (40)$$

Here the diffusion term describes the displacement of the individuals in the population and the reaction term their reproduction which is proportional to the density of the population and to available resources $(1 - u)$. This is so-

called logistic equation. According to the terminology introduced in Section 1, this is the reaction-diffusion equation with a monostable nonlinearity. We recall that travelling waves exist in this case for all values of the speed $c \geq c_0 = 2\sqrt{k}$. These waves are stable with respect to small perturbations in the norm with a properly chosen exponential weight. Under some conditions on the initial functions, we can also prove the convergence of solutions of the Cauchy problem to the travelling waves in form and in speed.

If we take into account the bi-sexual reproduction, then the reproduction term will be proportional to u^2 :

$$\frac{\partial u}{\partial t} = d \frac{\partial^2 u}{\partial x^2} + ku^2(1 - u) - bu. \quad (41)$$

The last term in the right-hand side describes mortality of the population. In this case we have a bistable nonlinearity. We recall that the travelling wave is unique up to translation in space and it is globally asymptotically stable with shift.

If there are several populations, then they can compete with each other for resources. As it is well known (see, e.g.,⁴⁸), depending on the characteristics of the populations, they can co-exist or one of them can extinct while another one will expand. The simplest model of competition of two species is given by the reaction-diffusion system

$$\frac{\partial u}{\partial t} = d \frac{\partial^2 u}{\partial x^2} + k_1u(1 - a_1u - b_1v), \quad (42)$$

$$\frac{\partial v}{\partial t} = d \frac{\partial^2 v}{\partial x^2} + k_2v(1 - a_2u - b_2v). \quad (43)$$

There exist four stationary points of this system: $P_0 = (0, 0)$, $P_1 = (1/a_1, 0)$, $P_2 = (0, 1/b_2)$, and P_3 which can be found as a solution of the linear algebraic system

$$a_1u + b_1v = 1, \quad a_2u + b_2v = 1.$$

If $b_1 > b_2$ and $a_2 > a_1$, then P_3 is stable and the species co-exist. If the opposite inequalities hold, then P_1 and P_2 are stable. In this case, we can put the question about the existence of travelling waves connecting these two points. We note that system (42), (43) can be reduced to a monotone system by a change of variables. Hence, we can prove the wave existence and stability, and use the minimax representation of the wave speed. If its speed equals zero, then the two species co-exist occupying two different space regions. If the speed is different from zero, then one of the species will invade the whole space replacing the other species.

3.2. Intra-specific competition and nonlocal consumption of resources

The models presented in the previous section do not take into account intra-specific competition. Its importance for various questions in population dynamics is accepted already long time ago due to Darwin's famous book on the origin of species.¹⁴ One of the simplest models taking into account intra-specific competition is given by the integro-differential equation

$$\frac{\partial u}{\partial t} = d \frac{\partial^2 u}{\partial x^2} + ku \left(1 - \int_{-\infty}^{\infty} \varphi(x-y)u(y,t)dy \right). \quad (44)$$

Here u is the density of a population, the first term in the right-hand side describes displacement of the individuals either in the physical space or in the morphological space. In the latter case, x corresponds to some morphological characteristics, for example, the weight of some animals, their height, or some other metrical characteristics. The second term in the right-hand side describes the reproduction of the population which is proportional to its density and to available resources, the expression in the brackets. If $\varphi(y)$ is the Dirac δ -function, then the integral becomes equal $u(x,t)$, and we obtain equation (40). If $\varphi(y)$ has a finite support, then the integral describes the consumption of resources at the space point x by the individuals located at the space point y . Thus, we deal with nonlocal consumption of resources or, in the other words, with the intra-specific competition, that is the competition of individuals of the same species for resources.

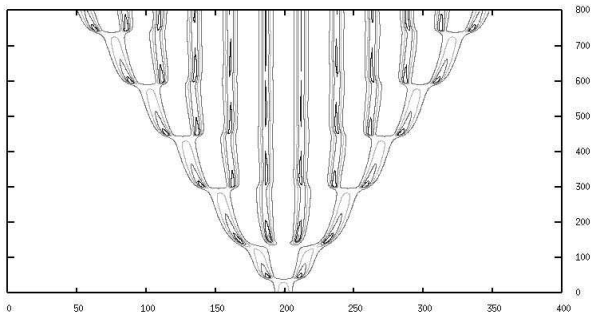


Fig. 6. Emergence of new species: level lines of the density in the bistable case.

Integro-differential equations in population dynamics can also arise in epidemiology and other applications. The review of early works can be

found in¹¹ (see 29,50 for more recent references).

The wave existence for equation (44) can be proved if the support of φ is sufficiently narrow. For the monostable case (44) it can be done by constructing some approximating sequences (see¹⁶ and the references therein). In the bistable case,

$$\frac{\partial u}{\partial t} = d \frac{\partial^2 u}{\partial x^2} + ku^2 \left(1 - \int_{-\infty}^{\infty} \varphi(x-y)u(y,t)dy \right) - bu, \quad (45)$$

which describes bisexual reproduction, it is proved in¹ by the implicit function theorem.

In both cases, monostable and bistable the waves have the limits $u = 0$ and $u = 1$ at infinity. If the support of φ becomes sufficiently large, then the homogeneous in space solution $u = 1$ loses its stability, and a periodic in space stationary solution emerges.²⁹⁻³¹ It is possible that the wave with the limit $u(-\infty) = 1$ still exists but becomes unstable. Numerical simulations show propagation of periodic waves. An example of such simulations is shown in Figure 6 (¹). It represents level lines of the solution $u(x,t)$ of equation (45). The horizontal axis is the x -variable, the vertical axis is time. The initial condition is localized in a narrow interval near $x = 200$. We see that a periodic in space structure emerges at the center of the interval and propagates to the left and to the right in the form of periodic travelling waves.

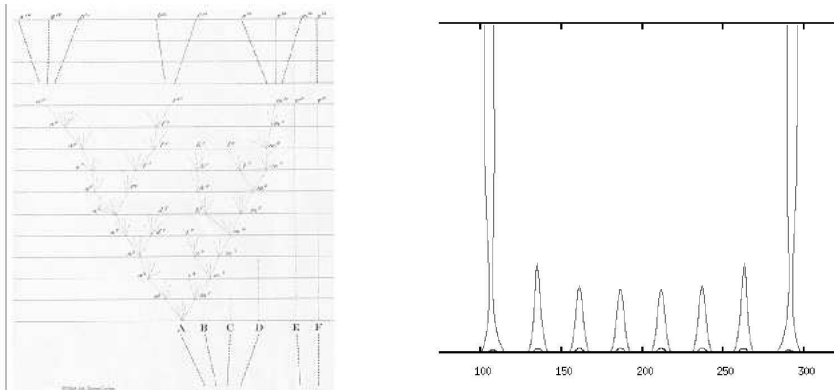


Fig. 7. Evolution of biological species: Darwin's diagram (left, adapted from¹⁴); numerical modelling of extinction (right).

There are various biological interpretations of these results. One of the most interesting is related to the evolution of biological species. If we con-

sider the space variable x as a morphological parameter, then the individuals that have approximately the same value of this parameter can be interpreted as a biological species, while two populations separated in the morphological space correspond to two different species. In the simulations shown in Figure 6, initially we have a unique species with approximately the same value of the morphological parameter. After some time, it splits into two subpopulations or two different species. Some time later, new species appear and so on until the whole morphological space is completely filled. These results correspond to Darwin's description of the emergence of biological species in the process of evolution (cf. Figure 7 (left)). In our modelling, it is based on three properties: random mutations (diffusion), intra-specific competition (integral), self-reproduction with the same phenotype (nonlinear term). It is interesting to note that the process of speciation can be modelled in a similar way for many other applications including the production of consumer goods or specialization in art and in science.

One of the differences between the modelling and Darwin's schematic diagram is that in the former, once a new species appears, it remains forever. In the diagram, some of the species disappear with time. One of possible explanations of this behavior can be related to variable environmental conditions. If we take them into account in the model through the values of parameters assuming that they can change with time, then we can describe the process of extinction (Figure 7 (right)).

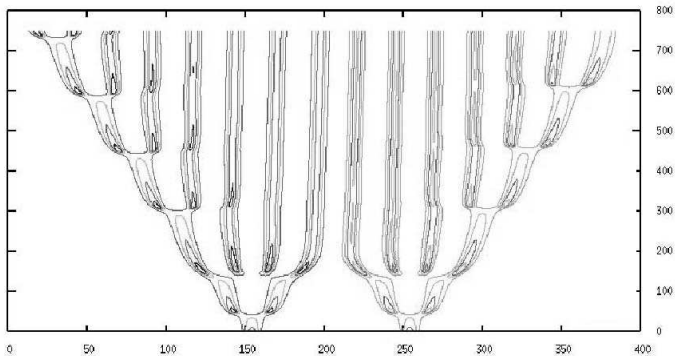


Fig. 8. Competition of species with intra-specific competition.

Thus, intra-specific competition can result in the emergence of new biological species. The new species continue to compete for resources in both

ways, intra-specifically and between the species. In order to model this phenomenon, we consider the integro-differential system of equations

$$\frac{\partial u}{\partial t} = d_1 \frac{\partial^2 u}{\partial x^2} + k_1 u^m \times \quad (46)$$

$$\left(1 - a_1 \int_{-\infty}^{\infty} \varphi(x-y)u(y,t)dy - b_1 \int_{-\infty}^{\infty} \varphi(x-y)v(y,t)dy \right) - p_1 u,$$

$$\frac{\partial v}{\partial t} = d_2 \frac{\partial^2 v}{\partial x^2} + k_2 v^m \times \quad (47)$$

$$\left(1 - a_2 \int_{-\infty}^{\infty} \varphi(x-y)u(y,t)dy - b_2 \int_{-\infty}^{\infty} \varphi(x-y)v(y,t)dy \right) - p_2 v.$$

If we replace ϕ by δ -function and put $m = 1$, $p_1 = p_2 = 0$, then we obtain system (42), (43).

An example of numerical simulations of system (46), (47) is shown in Figure 8. We take the initial conditions for functions u and v in such a way that they have finite supports and these support are separated. At the first stage, the corresponding populations develop independently of each other forming periodic structures (cf. Figure 6). After some time, they meet, and the function u gradually replaces the function v . From the mathematical point of view, this behavior corresponds to a periodic waves moving from the left to the right. It is interesting to note that its speed is less than in the case without the integral terms. This means that intra-specific competition helps weaker species to resist to the invasion of stronger species.

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In this survey I have used some results obtained in joint works with many co-authors. I would like to express them my profound gratitude. This review is necessarily incomplete, both from the point of view of the choice of topics and of the list of references. I hope that this does not touch the sensibility of the authors whose works remain out of the scope of this paper.

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