REACTION-DIFFUSION EQUATIONS IN COMBUSTION

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REACTION-DIFFUSION EQUATIONS IN COMBUSTION

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Abstract. Target patterns have been observed experimentally during combustion of premixed gases. To interpret these observations, we exploit a simple model, the Salnikov scheme involving two reaction steps with an Arrhenius temperature dependence. The mass and energy balance equations governing the temporal evolution of the intermediate species concentration and the reacting mixture temperature lead up to the reaction-diffusion system consisting of two partial differential equations whose dimensionless variant is the Scott-Wang-Showalter model. We used finite difference method and finite volume methods for the spatial discretization of the system. We approach the finite volume methods in cases where an advection term is included in the system. A time discretization is arranged by the semi-implicit time-stepping scheme. Target patterns and an influence of the advection were simulated. We will present numerical results of the several cases.

Key words. combustion, reaction-diffusion equations, advection, FVM, FDM

1. Scott-Wang-Showalter model of reaction and difussion. Combustion is chemical and physical phenomenon that is difficult to precisely describe by a mathematical model. It is suitable not to use purely chemical approach when developing mathematical model. That can be seen in [8] where the burning curves of coal particles are used thus a developing of the model is significantly simplified. Nevertheless, in this paper, we use the chemical approach because of relatively simple combustion of pre-mixed hydrocarbon gases.

1.1. Combustion of pre-mixed gases. Target patterns were experimentally observed during the combustion of pre-mixed gases. These patterns were created by the combustion of simple hydrocarbon gases and other elements; e.g., butane or octane mixed with oxygen and helium. A formation and a temporal evolution of the above mentioned patterns can be modelled by the Salnikov scheme [4]:

$$\begin{aligned} P &\longrightarrow A \\ A &\longrightarrow B + heat \ , \end{aligned}$$

where a rate of the first reaction is $k_1 p$ and a rate of the second reaction is $k_2 a$, where k_1, k_2 are rate constants and p, a denote concentrations of P, A species. The k_2 factor depends on temperature T and this dependence is of the Arrhenius type. Considering next assumption (see [4]), we can describe a concentration of the intermediate species A and temperature T by system of partial differential equations.

$$\begin{aligned} \frac{\partial a}{\partial \tau} &= k_1 p_0 - k_2(T)a + D_A \Delta a, \\ \frac{\partial T}{\partial \tau} &= \frac{Q}{C_p \sigma} k_2(T)a - \frac{T - T_a}{t_N} + D_T \Delta T, \end{aligned}$$

where meaning of symbols is as follows:

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- a is a concentration of the intermediate species A,
- p_0 is concentration of the initial species P,
- T is temperature,
- D_A is mass diffusivity of the species A,
- D_T is thermal diffusivity,
- $C_p\sigma$ gives the volumetric heat capacity (which is assumed to remain constant),
- t_N is the heat transfer timescale,
- T_a is the ambient temperature.

These equations can be transformed into the dimensionless form, so we obtain a below mentioned system of dimensionless equations

$$\begin{aligned}\frac{\partial \alpha}{\partial t} &= \mu - \alpha f(\Theta) + \Delta\alpha, \\ \frac{\partial \Theta}{\partial t} &= \frac{1}{\kappa}\left(\alpha f(\Theta) - \Theta\right) + Le\Delta\Theta,\end{aligned} \tag{1.1}$$

which is known as the Scott-Wang-Showalter model. Here, Le constant denotes the Lewis number, defined as $Le = \frac{D_T}{D_A}$. f function is defined as

$$f(\Theta) = \exp\left(\frac{\Theta}{1+\varepsilon\Theta}\right).$$

We achieved this dimensionless form using following formulas,

$$\Theta = \frac{E(T-T_a)}{RT_a^2}, \quad \alpha = \frac{a}{c_{ref}}, \quad t = \frac{\tau}{t_{chem}}, \quad x = \frac{\tilde{x}}{l_{ref}}, \quad y = \frac{\tilde{y}}{l_{ref}}, \tag{1.2}$$

where

$$t_{chem} = \frac{1}{k_{2,a}}, \quad c_{ref} = \frac{C_p\rho}{Q}\frac{RT_a^2}{E}\frac{t_{chem}}{t_N}, \quad l_{ref} = (D_A t_{chem})^{\frac{1}{2}}.$$

Finally, we rewrite the Arrhenius equation $k_2(T) = A\exp\left(-\frac{E}{RT}\right)$ as $k_2(T) = k_{2,a}f(\Theta)$, where $k_{2,a}$ is a value of function $k_2(T)$ in ambient temperature of T_a.

1.2. Scott-Wang-Showalter model. Let $\Omega \subset \mathbb{R}^2$ is bounded region where we study process over period $t \in (0,T)$. Then the evolution of the temperature and the concentration of intermediate species is described by system of equations

$$\begin{aligned}\frac{\partial \alpha}{\partial t} &= \Delta\alpha + \underbrace{\mu - \alpha f(\Theta)}_{g_1(\alpha,\Theta)}, \\ \frac{\partial \Theta}{\partial t} &= Le\Delta\Theta + \underbrace{\frac{1}{\kappa}\left(\alpha f(\Theta) - \Theta\right)}_{g_2(\alpha,\Theta)},\end{aligned}$$

defined on the set $(0,T)\times\Omega$.

We add initial condition to the system:

$$\alpha|_{t=0} = \alpha_{ini}, \qquad \Theta|_{t=0} = \Theta_{ini}.$$

Next, we define boundary conditions. The Dirichlet boundary conditions are defined as follows:

$$\alpha|_{\partial\Omega} = \frac{\mu}{\mathrm{e}^{\left(\frac{\mu}{1+\varepsilon\mu}\right)}}, \qquad \Theta|_{\partial\Omega} = \mu.$$

If we choose the Neumann boundary conditions we define them in the following way:

$$\left.\frac{\partial\alpha}{\partial n}\right|_{\partial\Omega} = 0, \qquad \left.\frac{\partial\Theta}{\partial n}\right|_{\partial\Omega} = 0,$$

where $\vec{n}$ is outer normal vector to the boundary of region Ω.

Reaction-diffusion equations with advection term. If advection of the medium is under way together with the combustion then the impact of this phenomenon on the course of the combustion is described by advection term which we add to equations

$$\begin{aligned} \frac{\partial\alpha}{\partial t} + \vec{v}\cdot\nabla\alpha &= \mu - \alpha f(\Theta) + \Delta\alpha, \\ \frac{\partial\Theta}{\partial t} + \vec{v}\cdot\nabla\Theta &= \frac{1}{\kappa}\left(\alpha f(\Theta) - \Theta\right) + Le\Delta\Theta, \end{aligned} \tag{1.3}$$

where $\vec{v} = (v_1, v_2)$ is a known vector of velocity of the medium advection.

We use following values of parameters (see [4])

parameter	values
Le	$[0.5, 5]$
κ	$1\cdot 10^{-4},\ 5\cdot 10^{-4}$
μ	$[0.7, 5]$
ε	$0.18,\ 0.165$

TABLE 1.1
Table of parameters.

2. Numerical methods. The system of evolution equations (1.2) can be solved by the method of lines as shown in [1], [7], [5]. In this paper, we focus on methods with semi-implicit time-stepping. We use finite difference method and finite volume methods for the spatial discretization of the system. We approach the finite volume methods in cases where an advection term is included in the system (see [2]). A time discretization is arranged by the semi-implicit time-stepping scheme.

2.1. Finite difference method. Let us consider an equidistant mesh on the set $(0\,,T)\times\Omega$, where Ω is squared region $(0,L)\times(0,L)$. we denote node points as a set $(t_k; x_i, y_j)$, where

$$t_k = k\tau, \quad k = 0,1,2,\ldots, \quad \tau > 0,$$
$$(x_i, y_j) = (ih, jh), \quad i,j = 0,1,...,m, \quad h = \frac{L}{m}.$$

We denote an approximation of solution as

$$\alpha^k_{i,j} \sim \alpha(t_k\,; x_i, y_j), \qquad \Theta^k_{i,j} \sim \Theta(t_k\,; x_i, y_j).$$

Differential terms in the system

$$\begin{aligned} \frac{\partial\alpha}{\partial t} &= \mu - \alpha f(\Theta) + \Delta\alpha, \\ \frac{\partial\Theta}{\partial t} &= \frac{1}{\kappa}\left(\alpha f(\Theta) - \Theta\right) + Le\Delta\Theta, \end{aligned}$$

are replaced by differences:

$$\frac{\partial \varphi}{\partial t} \mapsto \frac{\varphi_{i,j}^{k} - \varphi_{i,j}^{k-1}}{\tau},$$

$$\Delta\varphi = \frac{\partial^2 \varphi}{\partial x^2} + \frac{\partial^2 \varphi}{\partial y^2} \mapsto \frac{\varphi_{i-1,j}^{k} - 2\varphi_{i,j}^{k} + \varphi_{i+1,j}^{k}}{h^2} + \frac{\varphi_{i,j-1}^{k} - 2\varphi_{i,j}^{k} + \varphi_{i,j+1}^{k}}{h^2}.$$

We approximate non-linear terms g_1 and g_2 by their values calculated in a previous time step:

$$g_1(\alpha,\Theta) \mapsto {g_1}_{i,j}^{k-1} = g_1\left(\alpha_{i,j}^{k-1}, \Theta_{i,j}^{k-1}\right),$$
$$g_2(\alpha,\Theta) \mapsto {g_2}_{i,j}^{k-1} = g_2\left(\alpha_{i,j}^{k-1}, \Theta_{i,j}^{k-1}\right).$$

Thus we gain two system of linear equations in $(m-1)(m-1)$ unknowns

$$-\frac{\tau}{h^2}\left(\alpha_{i-1,j}^{k} + \alpha_{i,j-1}^{k}\right) + \left(1 + \frac{4\tau}{h^2}\right)\alpha_{i,j}^{k} - \frac{\tau}{h^2}\left(\alpha_{i+1,j}^{k} + \alpha_{i,j+1}^{k}\right)$$
$$= \alpha_{i,j}^{k-1} + \tau g_1\left(\alpha_{i,j}^{k-1}, \Theta_{i,j}^{k-1}\right),$$

$$-\frac{\tau Le}{h^2}\left(\Theta_{i-1,j}^{k} + \Theta_{i,j-1}^{k}\right) + \left(1 + \frac{4\tau Le}{h^2}\right)\Theta_{i,j}^{k} - \frac{\tau Le}{h^2}\left(\Theta_{i+1,j}^{k} + \Theta_{i,j+1}^{k}\right)$$
$$= \Theta_{i,j}^{k-1} + \tau g_2\left(\alpha_{i,j}^{k-1}, \Theta_{i,j}^{k-1}\right),$$

where $i, j = 1, 2, \ldots, m-1$.

2.2. Finite volume method. When advection predominates diffusion then it is suitable to apply finite volume method and use the upwind scheme to solve the system of equations (1.3).

Let us assume that we have the same equidistant orthogonal mesh as we use for the finite difference method in section 2.1. At first, we integrate the system (1.3) over the control volume K and we use the Green formula for the advection and diffusion terms so we obtain

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_K \alpha \,\mathrm{d}V + \int_{\partial K} \vec{v}\alpha\vec{n}\,\mathrm{d}S = \int_{\partial K} \nabla\alpha\,\vec{n}\,\mathrm{d}S + \int_K f_1(\alpha,\Theta)\,\mathrm{d}V,$$
$$\frac{\mathrm{d}}{\mathrm{d}t}\int_K \Theta \,\mathrm{d}V + \int_{\partial K} \vec{v}\Theta\vec{n}\,\mathrm{d}S = \int_{\partial K} Le\nabla\Theta\,\vec{n}\,\mathrm{d}S + \int_K f_2(\alpha,\Theta)\,\mathrm{d}V$$

and after discretization and applying the upwind scheme and the Euler time-stepping scheme we obtain

$$\frac{\alpha_K^{n+1} - \alpha_K^n}{\Delta t}|K| + \sum_{E\in\partial K} \alpha_{K,E}^{n+1}\vec{v}\cdot\vec{n}_{K,E}|E|$$
$$= \sum_{E\in\partial K} \frac{\alpha_{K'}^{n+1} - \alpha_K^{n+1}}{|KK'|}|E| + f_1(\alpha_K^n, \Theta_K^n)|K|,$$

$$\frac{\Theta_K^{n+1} - \Theta_K^n}{\Delta t}|K| + \sum_{E\in\partial K} \Theta_{K,E}^{n+1}\vec{v}\cdot\vec{n}_{K,E}|E|$$
$$= \sum_{E\in\partial K} Le\frac{\Theta_{K'}^{n+1} - \Theta_K^{n+1}}{|KK'|}|E| + f_2(\alpha_K^n, \Theta_K^n)|K|,$$

where K, K' are adjacent cells over edge E. Upwind values $\alpha^{n+1}_{K,E}, \Theta^{n+1}_{K,E}$ are chosen according to a following rule:

$$\phi^{n+1}_{K,E} = \begin{cases} \phi^{n+1}_{K} & \text{if } \vec{v}\cdot\vec{n}_{K,E} \geq 0, \\ \\ \phi^{n+1}_{K'} & \text{if } \vec{v}\cdot\vec{n}_{K,E} < 0. \end{cases}$$

After the discretization we also obtain the system of linear equations.

3. Numerical results. Those systems of linear equations were solved by Jacobi iterative method. This method were used, since it can be easily and efficiently parallelized. A setting of parameters is the same for all cases.

$$\mu = 1.8,\ Le = 1,\ \varepsilon = 0.18,\ \kappa = 0.0005. \tag{3.1}$$

Problem 1. Scott-Wang-Showalter model with Dirichlet boundary conditions:

$$\begin{aligned} \frac{\partial\alpha}{\partial t} &= \Delta\alpha + \mu - \alpha f(\Theta), \\ \frac{\partial\Theta}{\partial t} &= (Le)\Delta\Theta + \frac{1}{\kappa}\left(\alpha f(\Theta) - \Theta\right), \end{aligned}$$

Boundary conditions:

$$\alpha|_{\partial\Omega} = \frac{\mu}{\exp(\frac{\mu}{1+\varepsilon\mu})},\quad \Theta|_{\partial\Omega} = \mu.$$

Initial state:

$$\begin{aligned} \alpha|_{t=0} &= \frac{\mu}{\exp\left(\frac{\mu}{1+\varepsilon\mu}\right)}, \\ \Theta|_{t=0} &= \mu + \mathrm{e}^{\left(-50((x-5)^2+(y-6.5)^2)\right)} \qquad \text{for } y \geq x, \\ \Theta|_{t=0} &= \mu + \mathrm{e}^{\left(-50((x-5)^2+(y-3.5)^2)\right)} \qquad \text{for } y < x. \end{aligned}$$

Problem 2. Scott-Wang-Showalter model with advection:

$$\begin{aligned} \frac{\partial\alpha}{\partial t} + \vec{v}\cdot\nabla\alpha &= \mu - \alpha f(\Theta) + \Delta\alpha, \\ \frac{\partial\Theta}{\partial t} + \vec{v}\cdot\nabla\Theta &= \frac{1}{\kappa}\left(\alpha f(\Theta) - \Theta\right) + Le\Delta\Theta, \end{aligned}$$

Boundary conditions and the velocity vector field:

$$\alpha|_{\partial\Omega} = \frac{\mu}{\exp(\frac{\mu}{1+\varepsilon\mu})},\quad \Theta|_{\partial\Omega} = \mu,$$

$$\vec{v} = [80, 80]\,.$$

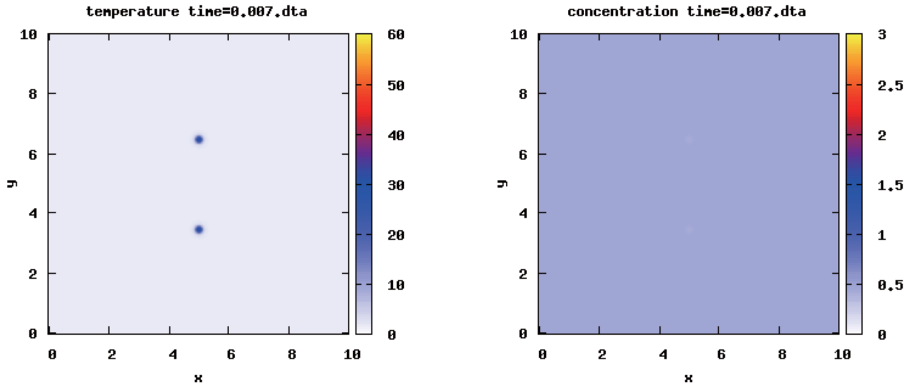

FIGURE 3.1. *A graphical representation of numerical result of the* ***Problem 1*** *solved on domain* 10×10 *with a spatial step* $h = \frac{1}{64}$ *and a time step* $\tau = 6,25 \cdot 10^{-5}$. *The solution is demonstrated in time* $t = 0.007$.

Initial state:

$$\alpha|_{t=0} = \frac{\mu}{\exp\left(\frac{\mu}{1+\varepsilon\mu}\right)},$$
$$\Theta|_{t=0} = \mu + \mathrm{e}^{\left(-50((x-3.5)^2+(y-4)^2)\right)} \quad \text{for } y \geq x,$$
$$\Theta|_{t=0} = \mu + \mathrm{e}^{\left(-50((x-4)^2+(y-3.5)^2)\right)} \quad \text{for } y < x.$$

Problem 3. Scott-Wang-Showalter model with advection:

$$\begin{aligned}\frac{\partial\alpha}{\partial t} + \vec{v}\cdot\nabla\alpha &= \mu - \alpha f(\Theta) + \Delta\alpha,\\ \frac{\partial\Theta}{\partial t} + \vec{v}\cdot\nabla\Theta &= \frac{1}{\kappa}\left(\alpha f(\Theta) - \Theta\right) + Le\Delta\Theta,\end{aligned}$$

Boundary conditions and the velocity vector field:

$$\alpha|_{\partial\Omega} = \frac{\mu}{\exp(\frac{\mu}{1+\varepsilon\mu})}, \quad \Theta|_{\partial\Omega} = \mu,$$
$$\vec{v} = \left[-50(y-5), 50(x-5)\right].$$

Initial state:

$$\alpha|_{t=0} = \frac{\mu}{\exp\left(\frac{\mu}{1+\varepsilon\mu}\right)},$$
$$\Theta|_{t=0} = \mu + \mathrm{e}^{\left(-50((x-3.5)^2+(y-4)^2)\right)} \quad \text{for } y \geq x,$$
$$\Theta|_{t=0} = \mu + \mathrm{e}^{\left(-50((x-4)^2+(y-3.5)^2)\right)} \quad \text{for } y < x.$$

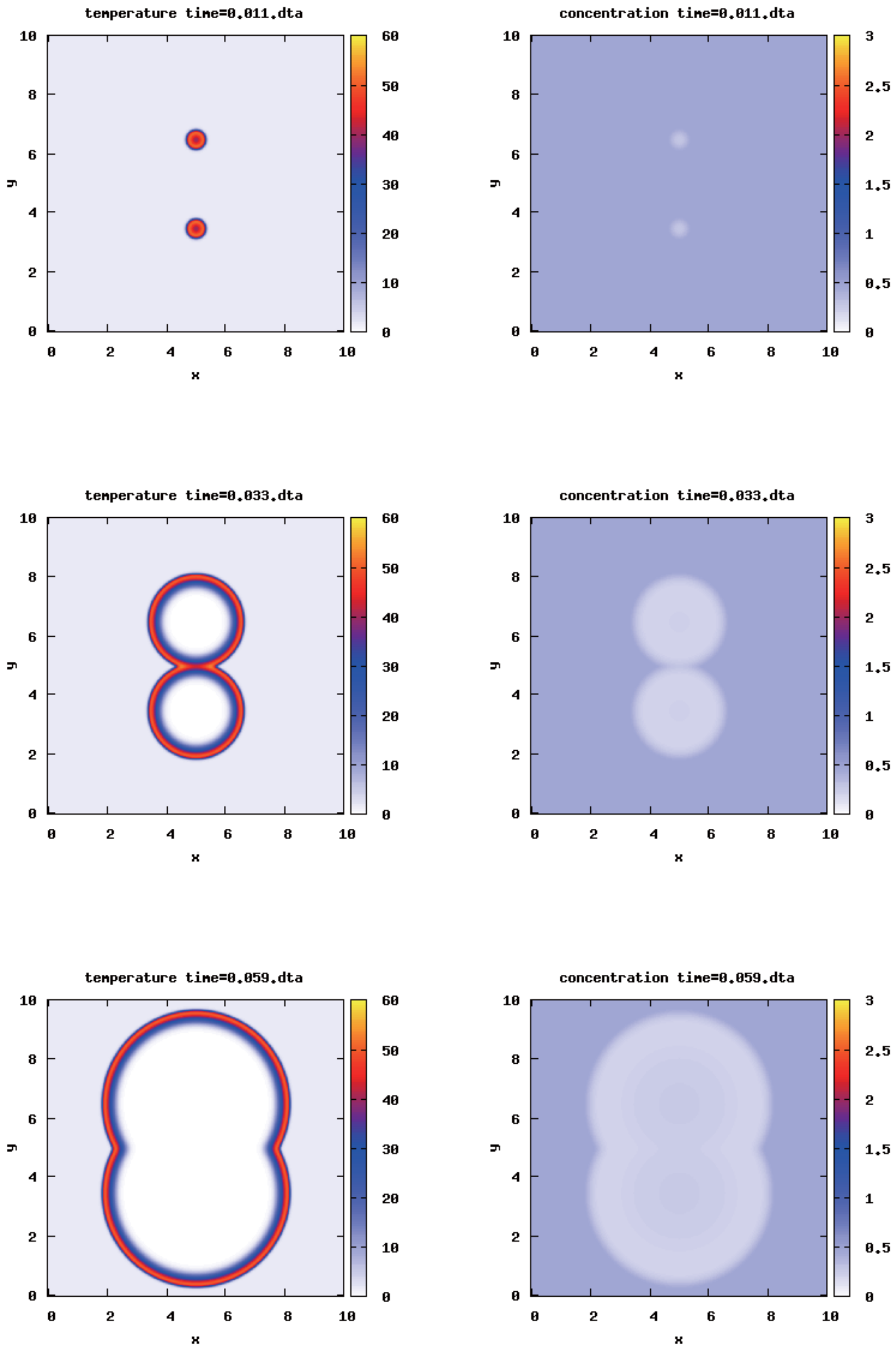

FIGURE 3.2. *A graphical representation of numerical result of the* ***Problem 1*** *solved on domain* 10×10 *with a spatial step* $h = \frac{1}{64}$ *and a time step* $\tau = 6,25 \cdot 10^{-5}$*. The solution is demonstrated in times* $t = 0.011$*,* $t = 0.033$ *and* $t = 0.059$*.*

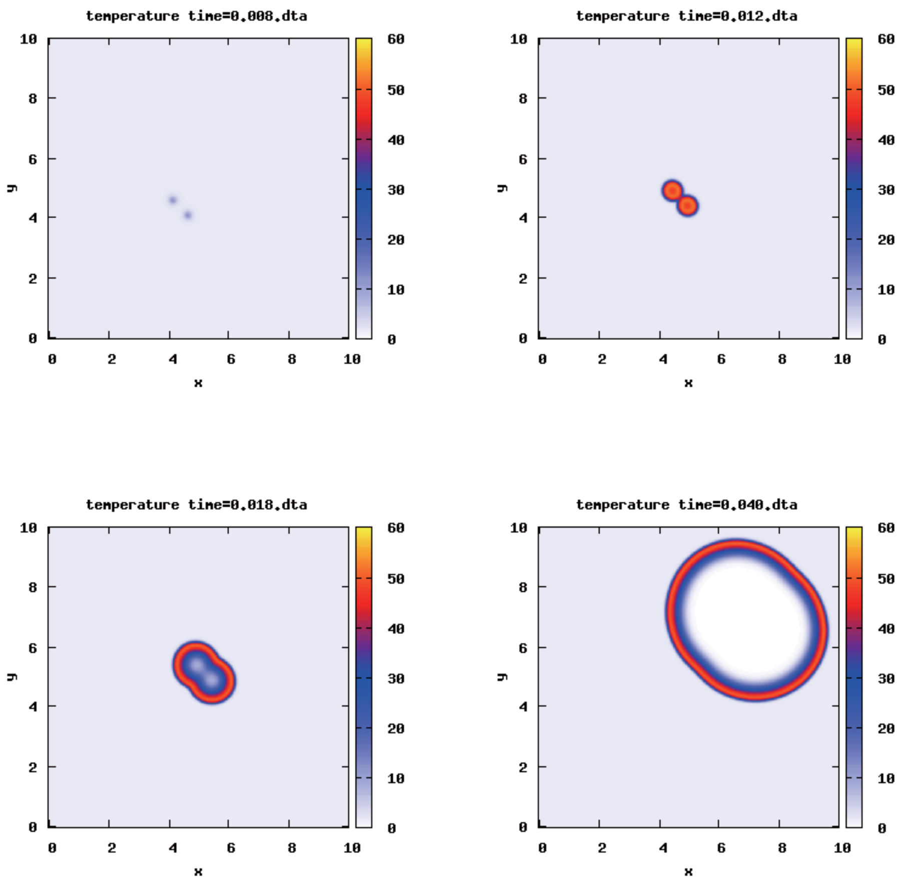

FIGURE 3.3. *A graphical representation of numerical result of the* ***Problem 2*** *solved on domain* 10×10 *with a spatial step* $h = \frac{1}{64}$ *and a time step* $\tau = 6,25 \cdot 10^{-5}$.

4. Conclusion. Numerical results show that we successfully simulated the experiment. We could see the target patterns during a simulation of the problem 1 which were experimentally observed. Next, we added advection to the origin model and studied its impact. We could see an influence of advection for the different velocity vector fields. Since we are not much interested in behavior of the model near boundaries we picked out results related to the Dirichlet boundary condition case for this paper. Neumann boundary condition case would have provided similar behavior in sufficient distance from boundaries.

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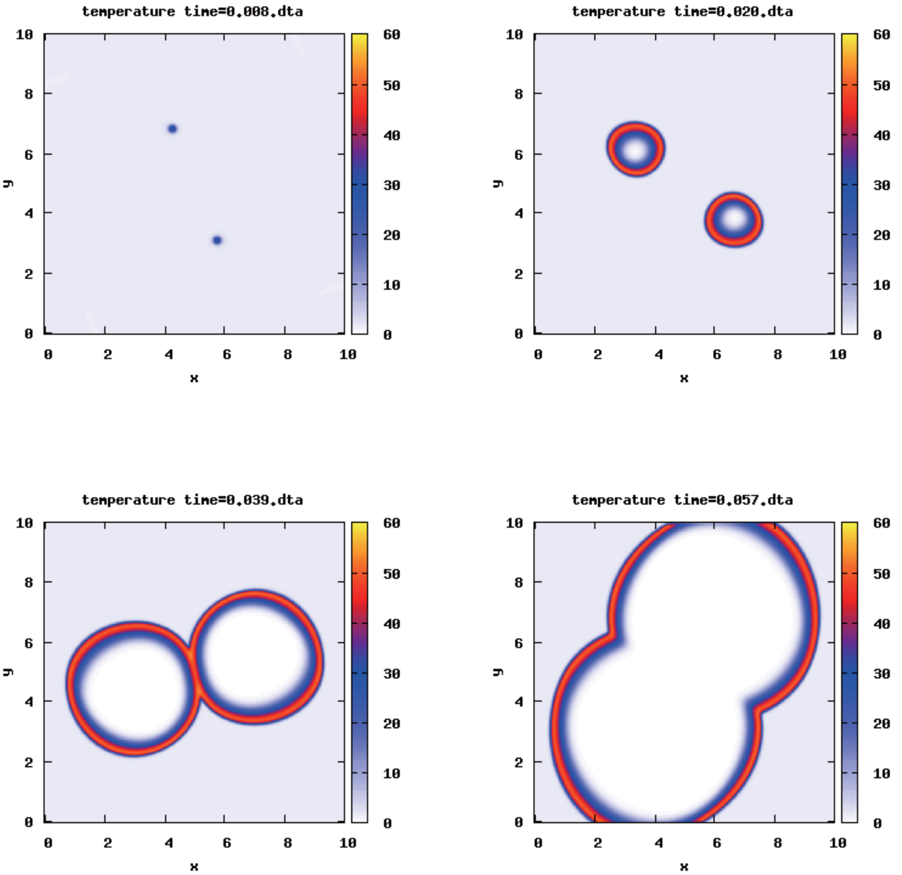

FIGURE 3.4. *A graphical representation of numerical result of the* ***Problem 3*** *solved on domain* 10×10 *with a spatial step* $h = \frac{1}{64}$ *and a time step* $\tau = 6,25 \cdot 10^{-5}$.

REFERENCES

[1] L. Eslerová. *Numerical analysis of dynamics of reaction-diffusion equations.* Diploma thesis, Department of mathematics FNSPE CTU, Prague 1996 (in Czech)

[2] W. Hundsdorfer and J. G. Verwer. *Numerical Solution of Time-Dependent Advection-Diffusion-Reaction Equations.* Springer, Berlin 2003

[3] Y. Ma and H. Pearlman. *Target and rotating spiral waves in premixed gas flames.* 31st International Symposium on Combustion, Heidelberg, Germany, 2006 poster.

[4] S. K. Scott and J. Wang and K. Showalter. *Modelling studies of spiral waves and target patterns in premixed flames.* `http://www.rsc.org/ej/FT/1997/a608474e.pdf`

[5] J. Šembera. *Numerical solution of reaction-diffusion equations Bruselator by the non-linear Galerkin method.* Diploma thesis, Department of mathematics FNSPE CTU, Prague 1997 (in Czech).

[6] M. Šenkýř. *Parallel algorithms for numerical solution of the Hamilton- Jacobi non-linear partial differential equations.* Diploma thesis, Department of mathematics FNSPE CTU, Prague 2004 (in Czech).

[7] R. Straka and Z. Čulík. *Numerical aspects of a bacteria growth model.* In ALGORITMY 2005, peer reviewed Proceedings of contributed papers and posters, pp. 175–184, Publ.

house of STU, 2005.

[8] R. Straka. *Mathematical Model of Pulverized Coal Fired Boiler.* Dissertation thesis, Department of mathematics FNSPE CTU, Prague 2010.

[9] V. Tomica. *Mathematical modelling of reaction processes in combustion.* Bachelor thesis, Department of mathematics FNSPE CTU, Prague 2008 (in Czech).

[10] E. Vitásek. *Numerical methods.* SNTL, Prague 1987 (in Czech).