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A POSTERIORI ERROR IDENTITIES FOR PARABOLIC CONVECTION–DIFFUSION PROBLEMS

Abstract. In the paper, we derive and discuss integral identities that hold for the difference between the exact solution of initial-boundary value problems generated by the reaction–convection–diffusion equation and any arbitrary function from admissible (energy) class. One side of the identity forms a natural measure of the distance between the exact solution and its approximation, while the other one is either directly computable or natural measure serves as a source of fully computable error bounds. A posteriori error identities and error estimates are derived in the most general form without using special features of a function compared with the exact solution. Therefore, they are valid for a wide spectrum of approximations constructed different numerical methods and can be also used for the evaluation of modelling errors.

§1. Introduction

Many mathematical models of evolutionary processes are based on the equation

$$u_t - \Delta u + a \cdot \nabla u + \rho^2 u = f \tag{1.1}$$

and its modifications (such as the Smoluchowski and Fokker–Planck equations). Usually u has the meaning of a concentration function, f is the source term, the term $\rho^2 u$ accounts local reactions, and a is the velocity field that u is moving with. The equation (1.1) describes effects generated by flow of mass or energy and has some features similar to equations used in the theory of viscous fluids. Two important special cases are the reaction-diffusion ($a = 0$) and convection-diffusion ($\rho = 0$) problems.

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Mathematical properties of initial boundary value problems based on (1.1) are well studied (e.g., see the monographs [5,6]). Numerous publications are devoted to qualitative analysis that includes existence and uniqueness of generalized solutions, regularity and local properties of solutions. However, with rare exceptions, exact solutions are unknown so that in the overwhelming majority of cases we are forced to consider a certain approximation v instead of the exact solution u. This fact generates two fundamental questions:

How to find a suitable v and how to verify that it is indeed close to u?

In the context of initial boundary values problems bases on the equation (1.1), the first question has been deeply studied by many authors (e.g.,see [10,21]). Consideration of the second question depends heavily on what one means by “verification”. A large number of works is devoted to error control methods where verification is understood in an asymptotic sense within the framework of a priori rate convergence estimates (e.g., see [1, 21]). A posteriori error estimation methods suggest a principally different approach. In this case, the accuracy of a particular numerical solution is analyzed. Typically, a posteriori estimates are derived for a concrete numerical method. They essentially use special properties of approximations (e.g., Galerkin orthogonality in the explicit residual method or the so called “saturation” in the hierarchically based methods) and/or extra regularity of exact solutions.

This paper, as well as a number of previous publications (e.g., see [14–17, 20]), follows a different concept, whose key point consists of studying deviations from exact solutions of differential equations in the most general form without using special properties of approximations associated with a particular numerical method. The purpose of this analysis is to obtain error identities and estimates that hold for *any* function from the admissible (energy) class. For elliptic boundary value problems and elliptic variational inequalities the corresponding results can be found in [13,14,18,20] and other papers cited therein. For evolutionary parabolic problems, first results of this kind were obtained in [15] and applications to various numerical approximations are studied in [4, 7–9]. The present work is concerned with the Cauchy problem based on (1.1). It should be considered as a continuation of the paper [17].

§2. Statement of the problem and basic notation

Let Ω be a bounded domain in $\mathbb{R}^d$, $d \geqslant 1$ with Lipshitz boundary Γ. We consider the Cauchy problem generated by the equation (1.1)

$$u_t - \operatorname{div} p^* + a \cdot \nabla u + \rho^2 u = f \quad \text{in} \ \ Q_T \, : \, \Omega \times (0,T), \tag{2.1}$$

$$u(x,t) = 0 \quad \text{on} \ \ S_T := \Gamma \times (0,T), \tag{2.2}$$

$$u(x,0) = \phi(x) \quad x \in \Omega, \tag{2.3}$$

$$p^* = A\nabla u \quad \text{in } Q_T. \tag{2.4}$$

It is assumed that the reaction and convection parameters satisfy the following conditions:

$$\mathrm{a} \in L^\infty(\Omega, \mathbb{R}^d), \ \operatorname{div} a \in L^\infty(\Omega), \tag{2.5}$$

$$\rho \in L^\infty(\Omega), \quad 0 \leqslant \rho \leqslant \rho_\oplus, \tag{2.6}$$

$$-\frac{1}{2}\operatorname{div}\mathrm{a} + \rho^2 := \sigma_a^2 \geqslant 0. \tag{2.7}$$

A is a symmetric matrix with bounded entries that do not depend on t. A satisfies the condition

$$c_1^2|\xi|^2 \leqslant A\xi \cdot \xi \leqslant c_2^2|\xi|^2 \qquad \forall \xi \in \mathbb{R}^d, \ c_1 > 0. \tag{2.8}$$

Throughout the paper we use standard notation for Lebesgue and Sobolev spaces ($L^p(\Omega)$ and $W_p^l(\Omega)$, respectively). A space is marked above by $\circ$ if the respective functions vanish on S_T, L^2 norms of the functions in Ω and Q_T are denoted by $\|\cdot\|_\Omega$ and $\|\cdot\|_{Q_T}$, respectively. Also, we define the norms

$$\|\nabla w\|_A^2 := \int\limits_\Omega A\nabla w \cdot \nabla w \, dx, \qquad \|y^*\|_{A^{-1}}^2 := \int\limits_\Omega A^{-1} y^* \cdot y^* \, dx,$$

$$\|\nabla w\|_{A,Q_T}^2 := \int\limits_0^T \|\nabla w\|_A^2 \, dt, \qquad \|y^*\|_{A^{-1},Q_T}^2 := \int\limits_0^T \|y^*\|_{A^{-1}}^2 \, dt.$$

Here, and later on the symbol := means “equals by definition”.

By $\{\!| g |\!\}_\omega$ we denote the mean value of g in $\omega \subset \Omega$ and use the notation

$$\Big[\!\Big[\, g(t) \, \Big]\!\Big]_0^T := g(T) - g(0).$$

In particular, if $v(x,t)$ is a function that has square summable traces for any t then $\Big[\!\Big[\, \|v\|_\Omega \, \Big]\!\Big]_0^T = \|v(x,T)\|_\Omega - \|v(x,0)\|_\Omega$. Derivatives of v with respect to x_i and t are denoted by $v_{,i}$ and v_t, respectively. Spatial gradient and divergence are denoted by ∇ and div, respectively.

We use standard notation for the Bochner spaces. For a separable Banach space X endowed with the norm $\|\cdot\|_X$, the space $L^2(0,T;X)$ contains functions with the norm $\|v\|^2_{L^2(0,T;X)} := \int\limits_0^T \|\nabla v\|^2_X\, dt < \infty$. In particular,

$$W_2^{1,0}(Q_T) := L^2(0,T;W_2^1(\Omega)), \quad \overset{\circ}{W}{}_2^{1,0}(Q_T) := L^2(0,T;\overset{\circ}{W}{}_2^1(\Omega)),$$

and

$$\overset{\circ}{W}{}_2^{1,1}(Q_T) := \Big\{ w \in \overset{\circ}{W}{}_2^{1,0}(Q_T), \|w\|_{1,1,Q_T} := \int\limits_{Q_T} (w^2 + w_t^2 + \mid \nabla w \mid^2)\, dx\, dt < +\infty \Big\}.$$

For the latter space we also use the abridged notation V_0 and by $V_0+\phi$ denote the subspace of V_0 that contains the functions satisfying the condition $v(x,0) = \phi(x)$.

Also, we use functional spaces associated with vector valued functions (fluxes). They are $Y^*(Q_T) := L^2(Q_T, \mathbb{R}^d)$, the space

$$Y^*_{\rm div}(Q_T) := \{ y^* \in Y^*(Q_T) \mid {\rm div} y^* \in L^2(Q_T)\}$$

supplied with the norm $\|y^*\|_{{\rm div},Q_T} := \big(\|y^*\|^2_{Q_T} + \|{\rm div} y^*\|^2_{Q_T}\big)^{1/2}$, and the product space

$$\mathcal{H}(Q_T) := V_0 \times Y^*_{\rm div}(Q_T).$$

We assume that

$$f \in L^2(Q_T), \qquad \phi \in \overset{\circ}{W}{}_2^1(\Omega), \tag{2.9}$$

and define the generalized solution of (2.1)–(2.4) as the function $u \in V_0+\phi$ satisfying the integral identity

$$\int\limits_{Q_T} \Big(A\nabla u \cdot \nabla w + ({\rm a} \cdot \nabla u) w + \rho^2 u w \Big)\, dx\, dt - \int\limits_{Q_T} u w_t\, dx\, dt + \int\limits_{\Omega} (u(x,T)w(x,T) - u(x,0)w(x,0))\, dx = \int\limits_{Q_T} f w\, dx\, dt \quad \forall w \in V_0. \tag{2.10}$$

In view of (2.1), the corresponding flux belongs to $Y^*_{\rm div}$, so that

$$(u, p^*) \in \mathcal{H}_0(Q_T).$$

Certainly, (2.10) defines a generalized solution for a much wider set of data including those cases where A, a, and ρ in (2.5), (2.6), (2.7), and (2.8) are bounded functions of t and the function ϕ in (2.9) is lesser regular. This paper is aimed to present the principle scheme of deriving a posteriori error identities. Therefore, for the sake of simplicity we exclude these extensions and only note that the derivation method discussed below remains valid for time dependent data provided that $u_t \in L^2(Q_T)$ (the exception is Section 4.2, where it is essentially used that ρ and A do not depend on t).

§3. The main error identity

In this section, we deduce the main error identity for the functions

$$e := v - u \quad \text{and} \quad e^* := y^* - p^*,$$

which are the deviations from u and p^* generated by the function $v(x,t) \in V_0$ and the vector valued function $y^*(x,t) \in Y^*_{\rm div}(Q_T)$. If these functions have been obtained in a numerical experiment, then e and e^* present *approximation errors*. In other cases, v and y^* may represent solutions of some close mathematical model. Then, the identity can be used to analyze *modeling errors*.

Computable functions

$$\mathrm{R}_f(v, y^*) := f - v_t + {\rm div} y^* - a \cdot \nabla v - \rho^2 v \quad \text{and} \quad \mathrm{R}_A(v, y^*) := A\nabla v - y^*$$

can be considered as residuals of the main relations (2.1) and (2.4). Recalling (2.1) and (2.4), we see that $\mathrm{R}_f(u, p^*) = \mathrm{R}_A(u, p^*) = 0$. Also, we introduce the quantity

$$\boldsymbol{\mu}_1(e, e^*) := \Big(\|\nabla e\|^2_{A,Q_T} + \|e^*\|^2_{A^{-1},Q_T} + 2\|\sigma_a e\|^2_{Q_T} \Big)^{1/2},$$

which is a measure that controls deviations from u and p^*. This measure satisfies the conditions natural for numerical methods that generate approximations converging in the corresponding energy spaces. It is easy to see that $\boldsymbol{\mu}_1(v_k - u, y^*_k - p^*)$ tends to zero for sequences of approximations $\{v_k\}$ and $y^*_k\}$ such that

$$v_k \to u \text{ in } \overset{\circ}{W}{}^{1,0}_2(Q_T) \quad \text{and } y^*_k \to p^* \text{ in } Y^*(Q_T). \tag{3.1}$$

Theorem 1. *For any* $(v, y^*) \in \mathcal{H}(Q_T)$*, it holds*

$$\boldsymbol{\mu}_1^2(e, e^*) + \Big[\!\Big[\ \|e\|_\Omega^2\ \Big]\!\Big]_0^T = \|\mathrm{R}_A(v, y^*)\|^2_{A^{-1},Q_T} - 2\int\limits_{Q_T} \mathrm{R}_f(v, y^*) e\, dx\, dt. \quad (3.2)$$

Proof. We rewrite (2.10) in the form

$$\int\limits_{Q_T} (A\nabla(u-v)\cdot\nabla w + (a\cdot\nabla(u-v))w + \rho^2(u-v)w)\, dx\, dt + \int\limits_{Q_T} (u_t - v_t) w\, dx\, dt$$
$$= \int\limits_{Q_T} \big(fw - A\nabla v\cdot\nabla w - (a\cdot\nabla v)w - \rho^2 vw - v_t w\big)\, dx\, dt \quad (3.3)$$

and set $w = u - v$. Now the identity reads

$$\|\nabla e\|^2_{A,Q_T} + \int\limits_{Q_T} (a\cdot\nabla e)e\, dx\, dt + \|\rho e\|^2_{Q_T} + \frac{1}{2}\Big[\!\Big[\ \|e\|_\Omega^2\ \Big]\!\Big]_0^T$$
$$= \int\limits_{Q_T} (A\nabla v\cdot\nabla e + (a\cdot\nabla v)e + \rho^2 ve + v_t e - fe)\, dx\, dt.$$

Using the relations

$$2\int\limits_\Omega (a\cdot\nabla e)e\, dx = \int\limits_\Omega a\cdot\nabla(e^2)\, dx = -\int\limits_\Omega (\mathrm{div} a)e^2\, dx, \quad (3.4)$$
$$\int\limits_\Omega \mathrm{div}(y^*\, e)\, dx = 0, \quad (3.5)$$

we modify it as follows:

$$\|\nabla e\|^2_{A,Q_T} + \|\sigma_a e\|^2_{Q_T} + \frac{1}{2}\Big[\!\Big[\ \|e\|_\Omega^2\ \Big]\!\Big]_0^T$$
$$= \int\limits_{Q_T} (A\nabla v\cdot\nabla e + \rho^2 ve + (a\cdot\nabla v)e + v_t e - fe)\, dx\, dt$$
$$= \int\limits_{Q_T} (A\nabla v - y^*)\cdot\nabla e\, dx\, dt - \int\limits_{Q_T} \mathrm{R}_f(v, y^*)e\, dx\, dt. \quad (3.6)$$

Notice that

$$\frac{1}{2}\|e^*\|^2_{A^{-1},Q_T}=\frac{1}{2}\|y^*-A\nabla u\|^2_{A^{-1},Q_T}=\frac{1}{2}\|y^*-A\nabla v+A\nabla e\|^2_{A^{-1},Q_T}$$
$$=\frac{1}{2}\|\nabla e\|^2_{A,Q_T}+\int\limits_{Q_T}\nabla e\cdot(y^*-A\nabla v)\,dx\,dt+\frac{1}{2}\|y^*-A\nabla v\|^2_{A^{-1},Q_T}. \tag{3.7}$$

Summation of (3.6) and (3.7) yields (3.2). □

It is worth adding several comments to the identity (3.2).

1. By setting $v=0$ and $y^*=0$, we use (2.4) and represent the left hand side of (3.2) in the form

$$\|\nabla u\|^2_{A,Q_T}+2\|\sigma_a u\|^2_{Q_T}+\|p^*\|^2_{A^{-1},Q_T}+\Big[\!\!\Big[\,\|u\|^2_\Omega\,\Big]\!\!\Big]_0^T$$
$$=2\|\nabla u\|^2_{A,Q_T}+2\int\limits_{Q_T}(\rho^2-\frac{1}{2}\mathrm{div}a)u^2\,dx\,dt+\Big[\!\!\Big[\,\|u\|^2_\Omega\,\Big]\!\!\Big]_0^T$$
$$=2\|\nabla u\|^2_{A,Q_T}+2\int\limits_{Q_T}(\rho^2u^2+(a\cdot\nabla u)u)\,dx\,dt+\Big[\!\!\Big[\,\|u\|^2_\Omega\,\Big]\!\!\Big]_0^T.$$

Since in this case the right hand side of (3.2) is equal to $2\int\limits_{Q_T} fu\,dx\,dt$, we divide both parts of the identity by 2 and arrive at that the well known energy balance relation written in terms of the exact solution u (e.g., see §3 of Ch. 3 in [6]). Hence the balance relation is a particular form of the identity (3.2). The latter identity establishes a more general form of balance. It shows that for any pair of functions $(v,y^*)\in\mathcal{H}(Q_T)$ a properly selected measure of deviations e and e^* is equal to a certain combination of space–time integrals formed by the residual functions $\mathrm{R}_f(v,y^*)$ and $\mathrm{R}_A(v,y^*)$.

2. The identity (3.2) holds for any $(v,y^*)\in\mathcal{H}(Q_T)$. Let the functions v and y^* belong to a narrower set $\mathcal{H}_0(Q_T)\subset\mathcal{H}(Q_T)$ that contains v and y^* such that

$$\int\limits_{Q_T}(y^*\cdot\nabla w-fw+(a\cdot\nabla v)w+\rho^2w+v_tw)\,dx\,dt=0\quad\forall\,w\in V_0. \tag{3.8}$$

Then the last integral in (3.2) vanishes and we arrive at the identity

$$\boldsymbol{\mu}_1^2(e,e^*)+\Big[\!\!\Big[\,\|e\|^2_\Omega\,\Big]\!\!\Big]_0^T=\|\mathrm{R}_A(v,y^*)\|^2_{A^{-1},Q_T}\quad\forall\,(v,y^*)\in\mathcal{H}_0(Q_T) \tag{3.9}$$

with fully computable right hand side. Notice that (3.8) amounts a differential condition $\mathrm{div} y^* + f - a \cdot \nabla v - \rho^2 v - v_t = 0$ imposed on v and y^* so that these functions cannot be independent and should always be properly coordinated. Hence this simplified (hypercircle type) error identity may be inconvenient from the practical point of view.

3. Take infimum of both parts of (3.2) with respect to $y^* \in Y^*_{\mathrm{div}}$. We find that

$$\|\nabla e\|^2_{A,Q_T} + 2\|\sigma_a e\|^2_{Q_T} + \Big[\!\Big[\, \|e\|^2_\Omega \, \Big]\!\Big]_0^T \\ = \inf_{y^* \in Y^*_{\mathrm{div}}} \left\{ \left\| \mathrm{R}_A(v, y^*) \right\|^2_{A^{-1},Q_T} - 2 \int\limits_{Q_T} \mathrm{R}_f(v, y^*) e \, dx \, dt \right\}. \quad (3.10)$$

Taking infimum with respect to $v \in V_0 + \phi$ we see that the left hand side is reduced to $\|e^*\|^2_{A^{-1},Q_T}$. Hence (3.2) yields

$$\|e^*\|^2_{A^{-1},Q_T} = \inf_{v \in V_0 + \phi} \left\{ \left\| \mathrm{R}_A(v, y^*) \right\|^2_{A^{-1},Q_T} - 2 \int\limits_{Q_T} \mathrm{R}_f(v, y^*) e \, dx \, dt \right\}. \quad (3.11)$$

The identities (3.11) and (3.10) show that the parts of $\boldsymbol{\mu}_1$ associated with e and e^* can be evaluated separately.

4. The identity (3.2) opens a way to compare exact solutions of (2.1)–(2.4) generated by different data. For elliptic boundary value problems this question is studied in detail in [20], where a posteriori error identities are used to evaluate errors generated by data simplification or dimension reduction. The identity (3.2) (and other identities derived below) can be used for similar analysis in the context of parabolic problems.

For example, assume that the functions $\widetilde{u}$ and $\widetilde{p^*}$ solve the problem (2.1), (2.2), and (2.4) with the initial condition that differs from (2.3), i.e.,

$$\widetilde{u}(x, 0) = \widetilde{\phi}(x) \neq \phi(x).$$

Then,

$$\widetilde{p^*} = A \nabla \widetilde{u} \quad \text{and} \quad \mathrm{div} \widetilde{p^*} + f - \widetilde{u}_t - \rho^2 \widetilde{u} - a \cdot \nabla \widetilde{u} = 0.$$

In this case, $\mathrm{R}_A(\widetilde{u}, \widetilde{p^*}) = \mathrm{R}_f(\widetilde{u}, \widetilde{p^*}) = 0$ and (3.2) reads

$$\|\nabla(u - \widetilde{u})\|^2_{A,Q_T} + \|p^* - \widetilde{p^*}\|^2_{A^{-1},Q_T} + 2\|\sigma_a(u - \widetilde{u})\|^2_{Q_T} \\ + \|(\widetilde{u} - u)(\cdot, T)\|^2_\Omega = \|\widetilde{\phi} - \phi\|^2_\Omega. \quad (3.12)$$

Since the first three norms in the left hand side monotonically grow as T grows and the right hand side does not depend on T, we conclude that $\widetilde{u}(x,T)$ tends to $u(x,T)$ as $T \to +\infty$. Hence (3.12) implies the well known stabilization property (e.g., see [2,3]).

Also, we can compare u and p^* with solutions $\widetilde{u}$ and $\widetilde{p^*}$ generated by the diffusion matrix $\widetilde{A}$, which differs from A. For example, $\widetilde{A}$ may be a simplification of the original matrix A. In this case, (3.2) yields the identity, which controls modeling errors caused by simplification.

We have $\widetilde{p^*} = \widetilde{A}\nabla\widetilde{u}$, $\mathrm{R}_f(\widetilde{u},\widetilde{p^*}) = 0$, and

$$\|\mathrm{R}_A(\widetilde{u},\widetilde{p^*})\|^2_{A^{-1},Q_T} = \int\limits_{Q_T} \left(A\nabla\widetilde{u}\cdot\nabla\widetilde{u} + A^{-1}\widetilde{p^*}\cdot p^* - 2\nabla\widetilde{u}\cdot\widetilde{p^*}\right)\,dx\,dt$$
$$= \int\limits_{Q_T} (\widetilde{A}A^{-1}\widetilde{A} + A - 2\widetilde{A})\nabla\widetilde{u}\cdot\nabla\widetilde{u}\,dx\,dt = \int\limits_{Q_T} D\nabla\widetilde{u}\cdot\nabla\widetilde{u}\,dx\,dt,$$

where

$$D := (A-\widetilde{A})A^{-1}(A-\widetilde{A})$$

is the deflection matrix. Notice that D is a positive matrix and $D \equiv 0$ if $\widetilde{A} = A$. In view of (3.2), the error between two solutions generated by the same initial data satisfies the relation

$$\|\nabla(u-\widetilde{u})\|^2_{A,Q_T} + \|p^* - \widetilde{p^*}\|^2_{A^{-1},Q_T} + 2\|\sigma_a(u-\widetilde{u})\|^2_{Q_T} + \|(\widetilde{u}-u)(\cdot,T)\|^2_\Omega = \int\limits_{Q_T} D\nabla\widetilde{u}\cdot\nabla\widetilde{u}\,dx\,dt. \quad (3.13)$$

The identity (3.13) shows that the difference between two solutions is controlled by the norm $\|\nabla\widetilde{u}\|_D$. It generalises a similar identity obtained for elliptic problems in Chapter 4 of [20].

§4. Special cases

4.1. Strictly positive reaction function.

Theorem 2. *Let $\rho(x) \geqslant \rho_0 > 0$ and $\rho_a^2 := \rho^2 - \mathrm{div}a \geqslant 0$. Then for any $(v,y^*) \in \mathcal{H}(Q_T)$ it holds the identity*

$$\boldsymbol{\mu}_2^2(e,e^*) + \left[\!\left[\, \|e\|^2_\Omega \,\right]\!\right]_0^T = \|\mathrm{R}_A(v,y^*)\|^2_{A^{-1},Q_T} + \|\frac{1}{\rho}\mathrm{R}_f(v,y^*)\|^2_{Q_T}, \quad (4.1)$$

where

$$\boldsymbol{\mu}_2(e,e^*):=\Big(\|\nabla e\|^2_{A,Q_T}+\|e^*\|^2_{A^{-1},Q_T}+\|\tfrac{1}{\rho}(\mathrm{div}e^*-a\cdot\nabla e-e_t)\|^2_{Q_T}+\|\rho_a e\|^2_{Q_T}\Big)^{1/2}.$$

Proof. First, we notice that

$$\begin{aligned}&\big\|\tfrac{1}{\rho}(\mathrm{div}y^*+f-v_t-a\cdot\nabla v-\rho^2 v)\big\|^2_{Q_T}=\big\|\frac{1}{\rho}(\mathrm{div}e^*-e_t-a\cdot\nabla e)-\rho e\big\|^2_{Q_T}\\ &=\big\|\tfrac{1}{\rho}(\mathrm{div}e^*-e_t-a\nabla e)\big\|^2_{Q_T}+\|\rho e\|^2_{Q_T}-2\int\limits_{Q_T}(\mathrm{div}e^*-e_t-a\cdot\nabla e)e\,dx\,dt.\end{aligned}\tag{4.2}$$

Next, we use (3.4) and the relations

$$\int\limits_{Q_T}(\mathrm{div}e^*)e\,dx\,dt=-\int\limits_{Q_T}e^*\cdot\nabla e\,dx\,dt$$

and

$$\int\limits_{Q_T}e_t e\,dt\,dx=\frac{1}{2}\Big[\!\!\Big[\,\|e\|^2_\Omega\,\Big]\!\!\Big]^T_0$$

to modify (4.2) as follows:

$$\begin{aligned}&\|\tfrac{1}{\rho}(\mathrm{div}y^*+f-v_t-a\cdot\nabla v-\rho^2 v)\|^2_{Q_T}\\ &=\|\tfrac{1}{\rho}(\mathrm{div}e^*-e_t-a\cdot\nabla e)\|^2_{Q_T}+\|\rho e\|^2_{Q_T}+\Big[\!\!\Big[\,\|e\|^2_\Omega\,\Big]\!\!\Big]^T_0\\ &+2\int\limits_{Q_T}e^*\cdot\nabla e\,dx\,dt-\int\limits_{Q_T}\mathrm{div}a e^2\,dx\,dt.\end{aligned}\tag{4.3}$$

It is easy to see that

$$\|\mathrm{R}_A(v,y^*)\|^2_{A^{-1},Q_T}=\|\nabla e\|^2_{A,Q_T}+\|e^*\|^2_{A^{-1},Q_T}-2\int\limits_{Q_T}e^*\cdot\nabla e\,dx\,dt.\tag{4.4}$$

Summation of (4.3) and (4.4) yields the identity

$$\begin{aligned}&\|\nabla e\|^2_{Q_T}+\|e^*\|^2_{A^{-1},Q_T}+\|\frac{1}{\rho}(\mathrm{div}e^*-e_t-a\cdot\nabla e)\|^2_{Q_T}\\ &+\int\limits_{Q_T}(\rho^2-\mathrm{div}a)|e|^2\,dx\,dt+\Big[\!\!\Big[\,\|e\|^2_\Omega\,\Big]\!\!\Big]^T_0\\ &=\|\mathrm{R}_A(v,y^*)\|^2_{A^{-1},Q_T}+\|\frac{1}{\rho}(\mathrm{div}y^*+f-v_t-a\cdot\nabla v-\rho^2 v)\|^2_{Q_T},\end{aligned}$$

which coincides with (4.1). □

Notice that the right hand side of (4.1) is fully computable. The left hand side contains a collection of nonnegative terms that form an error measure $\boldsymbol{\mu}_2(e, e^*)$. It differs from the measure $\boldsymbol{\mu}_1(e, e^*)$. The identity (4.1) allows us to directly control the quality of approximate solutions, but it contains integrals with weights $1/\rho$. Therefore, for very small ρ the corresponding terms strongly dominate and the identity may become uninformative.

4.2. The case $a = 0$. In [17], it was shown how to deduce error identities in terms of stronger measures provided that the exact solution and its approximations possess additional differentiability in time. Here we extend this method to the reaction-diffusion equation.

Theorem 3. *Let*

$$u, v \in \overset{\circ}{W}{}_2^{1,1+}(Q_T) := \{w \in \overset{\circ}{W}{}_2^{1,1}(Q_T) \mid w_{,it} \in L^2(\Omega) \quad i = 1, 2, \ldots, d\}.$$

and $p^*, y^* \in Y^{*+}_{\rm div} := \{y^* \in Y^*_{\rm div} \mid y^*_t \in L^2(Q_T, \mathbb{R}^d)\}$. *Then*

$$\begin{aligned} &\boldsymbol{\mu}_3^2(e, e^*) + \Big[\!\Big[\, \|e\|^2_\Omega \, \Big]\!\Big]_0^T + \Big[\!\Big[\int\limits_\Omega (1 + \rho^2) \, e^2 \, dx \Big]\!\Big]_0^T + \Big[\!\Big[\, \|e^*\|^2_{A^{-1},\Omega} \, \Big]\!\Big]_0^T \\ &= \|\mathrm{R}_A(v, y^*)\|^2_{A^{-1},\Omega} + \Big[\!\Big[\, \|\mathrm{R}_A(v, y^*)\|^2_{A^{-1},\Omega} \, \Big]\!\Big]_0^T - 2\mathcal{R}(v, y^*; e, e_t), \end{aligned} \tag{4.5}$$

where

$$\mathcal{R}(v, y^*; e, e_t) := \int\limits_{Q_T} \Big((\mathrm{R}_A(v, y^*))_t \cdot \nabla e + \mathrm{R}_f(v, y^*)(e + e_t) \Big) \, dx \, dt$$

and

$$\boldsymbol{\mu}_3^2(e, e^*) := \|\nabla e\|^2_{A,Q_T} + \|e^*\|^2_{A^{-1},Q_T} + 2\|\rho e\|^2_{Q_T} + 2\|e_t\|^2_{Q_T}.$$

Proof. Set in (3.3) $w = -e_t = u_t - v_t$. We obtain the identity

$$\int\limits_{Q_T} (A\nabla e \cdot \nabla e_t + \rho^2 e e_t + e_t^2) \, dx \, dt = \int\limits_{Q_T} \big((\rho^2 v + v_t - f) e_t + A\nabla v \cdot \nabla e_t \big) \, dx \, dt. \tag{4.6}$$

Since $e_t = 0$ on S_T, for any $y^* \in Y^{*+}_{\rm div}$ it holds

$$\int\limits_{Q_T} (e_t \mathrm{div} y^* + y^* \cdot \nabla e_t) \, dx \, dt = \int\limits_0^T \int\limits_\Gamma (y^* \cdot n) e_t \, dx \, dt = 0. \tag{4.7}$$

From (4.6) and (4.7), we obtain

$$\int_{Q_T} \Big(A\nabla e \cdot \nabla e_t + \rho^2 e e_t + e_t^2\Big)\,dx\,dt = \int_{Q_T} (A\nabla v - y^*)\cdot\nabla e_t\,dx\,dt - \int_{Q_T} \mathrm{R}_f(v,y^*)e_t\,dx\,dt. \quad (4.8)$$

Consider the first term in the right hand side of (4.8). We use the relation $p_t^* = A\nabla u_t$ and transform it as follows:

$$\begin{aligned}
&\int_{Q_T} (A\nabla v - y^*)\cdot\nabla e_t\,dx\,dt = \int_{Q_T} (A\nabla v - y^*)\cdot\nabla(v_t - u_t)\,dx\,dt \\
&= \int_{Q_T} (A\nabla v\cdot\nabla v_t + A^{-1}y^*\cdot y_t^* - \nabla v_t\cdot y^* - \nabla v\cdot y_t^*)\,dx\,dt \\
&+ \int_{Q_T} (A\nabla v - y^*)\cdot(A^{-1}(y_t^* - p_t^*)) \\
&= \int_{Q_T} (\frac{1}{2}A\nabla v\cdot\nabla v + \frac{1}{2}A^{-1}y^*\cdot y^* - \nabla v\cdot y^*)_t\,dx\,dt \\
&+ \int_{Q_T} (A\nabla v - A\nabla u + p^* - y^*)\cdot(A^{-1}(y_t^* - p_t^*)) \\
&= \frac{1}{2}\Big[\!\Big[\, \|\mathrm{R}_A(v,y^*)\|^2_{A^{-1},\Omega} \Big]\!\Big]_0^T + \int_{Q_T} \nabla(v-u)\cdot(y_t^* - p_t^*)\,dx\,dt \\
&- \int_{Q_T} A^{-1}(y_t^* - p_t^*)\cdot(y^* - p^*)\,dx\,dt.
\end{aligned} \quad (4.9)$$

Notice that

$$\int_{Q_T} \nabla(v-u)\cdot(y_t^* - p_t^*)\,dx\,dt = \int_{Q_T} A\nabla e_t\cdot\nabla e\,dx\,dt + \int_{Q_T} \nabla e\cdot(y^* - A\nabla v)_t\,dx\,dt \quad (4.10)$$

and

$$\int_{Q_T} A^{-1}(y_t^* - p_t^*)\cdot(y^* - p^*)\,dx\,dt = \frac{1}{2}\int_0^T \frac{d}{dt}(\|e^*\|_{A^{-1},\Omega})^2\,dt = \frac{1}{2}\Big[\!\!\Big[\ \|e^*\|^2_{A^{-1},\Omega}\Big]\!\!\Big]_0^T.$$

Hence

$$\begin{aligned}\int_{Q_T} (A\nabla v - y^*)\cdot\nabla e_t\,dx\,dt &= \frac{1}{2}\Big[\!\!\Big[\ \|\mathrm{R}_A(v,y^*)\|^2_{A^{-1},\Omega}\Big]\!\!\Big]_0^T \\ &+ \int_{Q_T} A\nabla e_t\cdot\nabla e\,dx\,dt - \int_{Q_T}(\mathrm{R}_A(v,y^*))_t\cdot\nabla e\,dx\,dt - \frac{1}{2}\Big[\!\!\Big[\|e^*\|^2_{A^{-1},\Omega}\Big]\!\!\Big]_0^T\end{aligned} \tag{4.11}$$

Let us consider now the second term in left hand side of (4.8). We have

$$\int_{Q_T} \rho^2 e e_t\,dx\,dt = \int_\Omega \rho^2 \int_0^T e e_t\,dx\,dt = \frac{1}{2}\Big[\!\!\Big[\ \|\rho\, e\,dx\|^2_\Omega\Big]\!\!\Big]_0^T. \tag{4.12}$$

We multiply both sides of (4.9) by two, use (4.11) and (4.12), and obtain the identity

$$\begin{aligned}&2\|e_t\|^2_{Q_T} + \Big[\!\!\Big[\ \|\rho\, e\,dx\|^2_\Omega\Big]\!\!\Big]_0^T + \Big[\!\!\Big[\ \|e^*\|^2_{A^{-1},\Omega}\Big]\!\!\Big]_0^T \\ &= \Big[\!\!\Big[\|\mathrm{R}_A(v,y^*)\|^2_{A^{-1},\Omega}\Big]\!\!\Big]_0^T - 2\int_{Q_T}\Big((\mathrm{R}_A(v,y^*))_t\cdot\nabla e + \mathrm{R}_f(v,y^*)e_t\Big)\,dx\,dt.\end{aligned} \tag{4.13}$$

Summation of (3.2) and (4.13) yields the identity (4.5). □

Remark 1. It is clear that the measure $\boldsymbol{\mu}_3(e,e^*)$ is stronger than $\boldsymbol{\mu}_1(e,e^*)$ used in (3.2). If v meets the initial condition, i.e., $v(x,0) = \phi(x)$ and $y^*(x,0) = A\nabla v(x,0)$, then (4.5) has the form

$$\begin{aligned}&\boldsymbol{\mu}_3^2(e,e^*) + \int_\Omega (1+\rho^2)|e(x,T)|^2\,dx + \|e^*(x,T)\|^2_{A^{-1},\Omega} \\ &= \|\mathrm{R}_A(v,y^*)\|^2_{A^{-1},\Omega} + \|\mathrm{R}_A(v(x,T),y^*(x,T))\|^2_{A^{-1},\Omega} - 2\mathcal{R}(v,y^*;e,e_t).\end{aligned} \tag{4.14}$$

§5. Estimates of deviations from u and p^*

Right hand sides of (3.2) and (4.5) contain the unknown function e and, therefore, cannot be directly computed. However, these identities provide a basis for the derivation of fully computable estimates.

5.1. First, we consider implications of the main identity (3.2). The simplest way to obtain a fully computable error majorant is to apply the Young's inequality and estimate the last integral as follows

$$
\begin{aligned}
2\left|\int\limits_{Q_T} \mathrm{R}_f(v,y^*)e\,dx\right| &\leqslant 2\int\limits_0^T \frac{C(\Omega)}{c_1}\|\mathrm{R}_f(v,y^*)\|_\Omega \|\nabla e\|_{A,\Omega}\,dt \\
&\leqslant \int\limits_0^T \beta(t)\|\nabla e\|^2_{A,\Omega}\,dt + \int\limits_0^T \frac{C^2(\Omega)}{c_1^2\beta(t)}\|\mathrm{R}_f(v,y^*)\|^2_\Omega\,dt,
\end{aligned}
\tag{5.1}
$$

where β is a function of t such that

$$\beta \in L^\infty_{[\beta_0,1]}(0,T) := \{\beta \in L^\infty(0,T) \mid 0 < \beta_0 \leqslant \beta(t) \leqslant 1 \ \forall t \in [0,T]\}$$

and $C(\Omega)$ is a constant in the inequality

$$\|w\|_\Omega \leqslant C(\Omega)\|\nabla w\|_\Omega \qquad \forall\ w \in \overset{\circ}{W}{}^1_2(\Omega). \tag{5.2}$$

We apply (5.1) to (3.2) and obtain the following two–sided estimates:

$$\int\limits_0^T (1-\beta)\|\nabla e\|^2_{A,\Omega}\,dt + \|e^*\|^2_{Q_T} + 2\|\sigma_a e\|^2_{A^{-1},Q_T} + \|e(\cdot,T)\|^2_\Omega \leqslant \mathrm{M}^+_1(v,y^*,\beta,T) \tag{5.3}$$

and

$$\int\limits_0^T (1+\beta)\|\nabla e\|^2_{A,\Omega}\,dt + \|e^*\|^2_{A^{-1},Q_T} + 2\|\sigma_a e\|^2_{A^{-1},Q_T} + \|e(\cdot,T)\|^2_\Omega \geqslant \mathrm{M}^-_1(v,y^*,\beta,T). \tag{5.4}$$

Here

$$\mathrm{M}^+_1(v,y^*,\beta,T) := \|v(\cdot,0)-\phi\|^2_\Omega + \|\mathrm{R}_A(v,y^*)\|^2_{A^{-1},Q_T} + \frac{C^2(\Omega)}{c_1^2}\int\limits_0^T \frac{1}{\beta}\|\mathrm{R}_f(v,y^*)\|^2_\Omega\,dt$$

is a fully computable majorant and

$$\mathbb{M}_1^-(v, y^*, \beta, T) := \|v(\cdot,0) - \phi\|_\Omega^2 + \|\mathrm{R}_A(v, y^*)\|^2_{A^{-1},Q_T} - \frac{C^2(\Omega)}{c_1^2} \int\limits_0^T \frac{1}{\beta} \|\mathrm{R}_f(v, y^*)\|^2_\Omega \, dt$$

is a minorant.

The estimates (5.3) and (5.4) hold for any $v \in V_0$ and $y^* \in Y^*_{\mathrm{div}}(Q_T)$. It is clear that $\mathbb{M}_1^+(v, y^*, \beta, T) = 0$ if and only if $v(x, 0) = \phi(x)$ and for $t \in (0, T)$ it holds

$$y^* = A\nabla v \quad \text{and} \quad v_t - \mathrm{div} y^* + a \cdot \nabla v + \rho^2 v - f = 0.$$

Hence $\mathbb{M}_1^+(v, y^*, \beta, T)$ vanishes if and only if $v = u$ and $y^* = p^*$.

Since $\mathbb{M}_1^+(v, y^*, \beta, T)$ is increasing monotonically with respect to T, (5.3) implies the estimate

$$\max_{t \in [0,T]} \|e(\cdot, t)\|^2_\Omega \leqslant \mathbb{M}_1^+(v, y^*, 1, T). \tag{5.5}$$

Also, (5.3) implies computable upper bounds for error measures related to e and e^* separately. Indeed, for a given function $\beta(t)$ we have

$$\int\limits_0^T (1-\beta)\|\nabla e\|^2_{A,\Omega} \, dt + 2\|\sigma_a e\|^2_{Q_T} + \|e(\cdot, T)\|^2_\Omega \leqslant \inf_{y^* \in Y^*_{\mathrm{div}}} \mathbb{M}_1^+(v, y^*, \beta, T). \tag{5.6}$$

Minimizing both sides of (5.3) with respect to v, we obtain an analogous estimate for another part of the error measure:

$$\|e^*\|^2_{A^{-1},Q_T} \leqslant \inf_{v \in V_0} \mathbb{M}_1^+(v, y^*, 1, T). \tag{5.7}$$

5.2. There are several ways get estimates sharper than (5.3) and (5.4). It is a large topic, which cannot be discussed in detail here so that we briefly describe only two possible methods. They have been earlier applied to elliptic problems (see [16, 20] and the literature cited therein).

One way is to modify the last term in (3.2) using a "correction function" $\tau^* \in Y^*_{\rm div}$ as follows:

$$\int\limits_{Q_T} \mathrm{R}(y^*, v)(v-u)\,dx\,dt$$
$$= \int\limits_{Q_T} (\mathrm{div}(y^*+\tau^*)+f-a\cdot\nabla v-\rho^2 v-v_t)(v-u)\,dx\,dt - \int\limits_{Q_T} \tau^*\cdot\nabla(v-u)\,dx\,dt.$$

Let β and γ be functions in $L^\infty_{[\beta_0,1]}(0,T)$ such that $\beta(t)+\gamma(t) \leqslant 1$ for $t \in [0,T]$. Since

$$2\left|\int\limits_0^T \int\limits_{Q_T} \tau^*\cdot\nabla e\,dx\,dt\right| \leqslant \int\limits_0^T \gamma\|\nabla e\|^2_{A,\Omega}\,dt + \int\limits_0^T \frac{1}{\gamma}\|\tau^*\|^2_{A^{-1},\Omega}\,dt$$

we obtain the estimate

$$\int\limits_0^T (1-\beta-\gamma)\|\nabla e\|^2_{A,\Omega}\,dt + 2\|\sigma_a e\|^2_{Q_T}$$
$$+ \|e^*\|^2_{A^{-1},Q_T} + \|e(\cdot,T)\|^2_\Omega \leqslant \mathbb{M}^+_1(v,y^*,\tau^*,\beta,\gamma,T), \quad (5.8)$$

where

$$\mathbb{M}^+_1(v,y^*,\tau^*,\beta,\gamma,T) := \|v(\cdot,0)-\phi\|^2_\Omega + \|\mathrm{R}_A(v,y^*)\|^2_{A^{-1},Q_T}$$
$$+ \frac{1}{\beta}C^2(\Omega)\|\mathrm{R}_f(v,y^*)+\mathrm{div}\tau^*\|^2_{Q_T} + \int\limits_0^T \frac{1}{\gamma}\|\tau^*\|^2_{A^{-1},\Omega}\,dt.$$

The right side of (5.8) can be minimized with respect to $\tau^*(x,t)$ by choosing an appropriate representation for this vector valued function. This procedure will give an upper bound smaller than in (5.3).

Another way is based on the idea of domain decomposition (which is often used in numerical methods for the considered class of initial boundary value problems, e.g., see [11,22]). Here we use Poincare type estimates associated with subdomains instead of the estimate (5.2). Let Ω be decomposed into a collection of nonintersecting Lipschitz subdomains Ω_m, $m = 1,2,\ldots,M$ such that $\overline{\Omega} = \cup_{k=1}^N \overline{\Omega}_m$. Assume that the approximations

v and y^* are integrally balanced and satisfy the conditions

$$\int\limits_{\Omega_m} \mathrm{R}_f(v,y^*)\,dx\,dt = 0 \qquad \forall\, m = 1,2,\ldots,M. \tag{5.9}$$

Then

$$\left|\int\limits_{\Omega_m} \mathrm{R}_f(v,y^*)\,e\,dx\,dt\right| \leqslant\; C_P(\Omega_m)\|\mathrm{R}_f(v,y^*)\|_{\Omega_m}\|\nabla e\|_{\Omega_m}.$$

Here $C_P(\Omega_m)$ is a constant in the Poincare inequality

$$\|w\|_{\Omega_m} \leqslant C_P(\Omega_m)\|\nabla w\|_{\Omega_m}, \tag{5.10}$$

which holds for any $w \in \overset{\circ}{W}{}^1_2(\Omega_m)$ provided that $\{\!|\, w \,|\!\}_{\Omega_m} = 0$. If Ω_m is a convex domain, then a simple upper bound for the constant in (5.10) $C_P(\Omega_m) \leqslant \frac{1}{\pi} \sup\limits_{x_1,x_2\in\Omega} |x_1 - x_2|$ was found in [12]. Certainly, the condition (5.9) imposes additional restrictions on v and y^*. However, these restrictions are much weaker than in (3.8) and for the values of M commonly used in practice, can be satisfied fairly easily.

Instead of (5.1), we use the estimate

$$2\left|\int\limits_{Q_T} \mathrm{R}_f(v,y^*)e\,dx\,dt\right| \leqslant 2\int\limits_0^T \sum_{i=1}^N \frac{C_P(\Omega_i)}{c_1}\|\mathrm{R}_f(v,y^*)\|_{\Omega}\|\nabla e\|_{A,\Omega_i}\,dt$$

$$\leqslant 2\int\limits_0^T S_f^N(v,y^*)\|\nabla e\|_A \leqslant \int\limits_0^T \beta(t)\|\nabla e\|^2_{A,\Omega}\,dt + \int\limits_0^T \frac{1}{\beta(t)}(S_f^N(v,y^*))^2\,dt,$$

where $\beta \in L^\infty_{[\beta_0,1]}$ and

$$S_f^N(v,y^*) := \left(\sum_{i=1}^N \frac{C_P^2(\Omega_i)}{c_1^2}\|\mathrm{R}_f(v,y^*)\|^2_{\Omega_i}\right)^{1/2}.$$

Then the estimates (5.3) and (5.4) hold if the majorant $\mathbb{M}_1^+(v,y^*,\beta,T)$ is replaced by

$$\widetilde{\mathbb{M}}_1^+(v,y^*,\beta,T) := \|v(\cdot,0)-\phi\|^2_\Omega + \|\mathrm{R}_A(v,y^*)\|^2_{A^{-1},Q_T} + \int\limits_0^T \frac{1}{\beta(t)}(S_f^N(v,y^*))^2\,dt.$$

Usually $C_P(\Omega_m)$ is much smaller than $C(\Omega)$ and, therefore, the corresponding estimates are sharper than (5.3) and (5.4).

5.3. Identity (4.1) implies a simple estimate

$$\|\nabla e\|^2_{Q_T} + \|e^*\|^2_{Q_T} + \|\rho_a e\|^2_{Q_T} + \|e(\cdot,T)\|^2_\Omega \leqslant \|e(\cdot,0)\|^2_\Omega + \|\mathrm{R}_A(v,y^*)\|^2_{A^{-1},Q_T} + \|\frac{1}{\rho}\mathrm{R}_f(v,y^*)\|^2_{Q_T}. \quad (5.11)$$

If ρ is not small then (4.1) and (5.11) provide direct control of errors e and e^* in terns of the measure $\boldsymbol{\mu}_2(e,e^*)$. Also (5.11) implies bounds for the errors e and e^* separately. Indeed, by taking infimum in both sides of (5.11) with respect to y^* and v we obtain the estimates

$$\|\nabla e\|^2_{Q_T} + \|\rho_a e\|^2_{Q_T} + \|e(\cdot,T)\|^2_\Omega \leqslant \|e(\cdot,0)\|^2_\Omega + \inf_{y^*\in Y^*_{\mathrm{div}}} \left\{ \|\mathrm{R}_A(v,y^*)\|^2_{A^{-1},Q_T} + \|\frac{1}{\rho}\mathrm{R}_f(v,y^*)\|^2_{Q_T} \right\}$$

and

$$\|e^*\|^2_{Q_T} \leqslant \inf_{v\in V_0} \left\{ \|v(x,0)-\phi(x)\|^2_\Omega + \|\mathrm{R}_A(v,y^*)\|^2_{A^{-1},Q_T} + \|\frac{1}{\rho}\mathrm{R}_f(v,y^*)\|^2_{Q_T} \right\}.$$

However, for small ρ the identity (4.1) and the estimate (5.11) is not convenient because these relations contain terms with large weights. This fact can significantly reduce their practical value, unless the function $\mathrm{R}_f(v,y^*)$ is not small enough.

We can deduce another majorant, which is applicable for $\rho \leqslant 1$ and robust for small values of ρ. First, we notice that

$$\begin{aligned} \frac{1}{\rho}\left(\mathrm{div}e^* - e_t - a\cdot\nabla e\right) &= \frac{1}{\rho}\left(\mathrm{div}y^* - v_t - \mathrm{div}p^* + u_t - a\cdot\nabla(v-u)\right) \\ &= \frac{1}{\rho}\left(\mathrm{div}y^* - v_t - a\cdot\nabla v + f - \rho^2 u\right) = \frac{1}{\rho}\mathrm{R}_f(v,y^*) + \rho e. \end{aligned} \quad (5.12)$$

Using (5.12), the identity (4.1) can be represented in the form

$$\|\nabla e\|^2_{A,Q_T} + \|e^*\|^2_{A^{-1},Q_T} + \int\limits_{Q_T} 2\sigma_a^2|e\|^2\,dx\,dt + \Big[\!\Big[\, \|e\|^2_\Omega \,\Big]\!\Big]_0^T = \|\mathrm{R}_A(v,y^*)\|^2_{Q_T} - 2\int\limits_{Q_T} \mathrm{R}_f(v,y^*) e\,dx\,dt, \quad (5.13)$$

which does not contain $\frac{1}{\rho}$. It is easy to see that if $\rho \to 0$ then (5.13) transfers to the identity (3.2). The last term in (5.13) contains unknown function e. To get a fully computable error majorant, we decompose and estimate the last integral as follows. Let

$$\chi \in L^{\infty}_{[0,1]}(0,T) := \{0 \leqslant \chi(t) \leqslant 1 \quad \forall t \in [0,T]\}\,.$$

First, we split the integral

$$2\int\limits_{Q_T} \mathrm{R}_f(v,y^*)e\,dx\,dt = 2\int\limits_{Q_T}(1-\chi)\mathrm{R}_f(v,y^*)e\,dx\,dt + 2\int\limits_{Q_T}\chi\mathrm{R}_f(v,y^*)e\,dx\,dt \tag{5.14}$$

and estimate each of the two parts separately. We have

$$\begin{aligned} 2\Big|\int\limits_{Q_T}(1-\chi)\mathrm{R}_f(v,y^*)e\,dx\,dt\Big| &\leqslant 2\int\limits_{Q_T}|(1-\chi)\mathrm{R}_f(v,y^*)|\,|e|\,dx\,dt \\ &\leqslant \int\limits_{Q_T}\left(\frac{(1-\chi)^2}{\lambda}|\mathrm{R}_f(v,y^*)|^2 + \lambda|e|^2\right)dx\,dt \\ &\leqslant \int\limits_{Q_T}\frac{(1-\chi)^2}{\lambda}|\mathrm{R}_f(v,y^*)|^2\,dx\,dt + \int\limits_0^T \lambda\|e\|^2_{\Omega}\,dt \\ &\leqslant \int\limits_{Q_T}\frac{(1-\chi)^2}{\lambda}|\mathrm{R}_f(v,y^*)|^2 + \frac{C^2(\Omega)}{c_1^2}\int\limits_0^T \lambda\|\nabla e\|^2_{A,\Omega}\,dt \end{aligned} \tag{5.15}$$

and

$$2\Big|\int\limits_{Q_T}\chi\mathrm{R}_f(v,y^*)e\,dx\,dt\Big| \leqslant \int\limits_{Q_T}\left(\frac{\chi^2}{\mu}|\mathrm{R}_f(v,y^*)|^2 + \mu|e|^2\right)dx\,dt. \tag{5.16}$$

where $\lambda(t)$ and $\mu(x,t)$ are a positive functions such that $\lambda(t) \leqslant \frac{c_1^2}{C^2(\Omega)}$ and $\mu(x,t) \leqslant 2\sigma_a^2$. In view of (5.14), (5.15), and (5.16) the identity (5.13) implies the estimate

$$\int_0^T \left(1 - \lambda \frac{C^2(\Omega)}{c_1^2}\right) \|\nabla e\|^2_{A,\Omega}\, dt + \|e^*\|^2_{A^{-1},Q_T} + \int_{Q_T} (2\sigma_a^2 - \mu)|e|^2\, dx\, dt + \Big[\!\Big[\, \|e\|^2_\Omega \,\Big]\!\Big]_0^T \leqslant \|\mathrm{R}_A(v,y^*)\|^2_{Q_T} + \int_{Q_T} \left(\frac{(1-\chi)^2}{\lambda} + \frac{\chi^2}{\mu}\right) |\mathrm{R}_f(v,y^*)|^2\, dx\, dt.$$

Infimum of the last integral is attained at $\chi = \frac{\mu}{\lambda+\mu}$ and we obtain

$$\int_0^T \left(1 - \lambda \frac{C^2(\Omega)}{c_1^2}\right) \|\nabla e\|^2_{A,\Omega}\, dt + \|e^*\|^2_{A^{-1},Q_T} + \int_{Q_T} (2\sigma_a^2 - \mu)|e|^2\, dx\, dt + \|e(\cdot,T)\|^2_\Omega \leqslant \|v(x,0) - \phi(x)\|^2_\Omega + \|\mathrm{R}_A(v,y^*)\|^2_{Q_T} + \int_{Q_T} \frac{1}{\lambda+\mu} |\mathrm{R}_f(v,y^*)|^2\, dx\, dt, \tag{5.17}$$

which is applicable for arbitrary small ρ.

In particular, setting $\beta = \lambda \frac{C^2(\Omega)}{c_1^2}$ and tending μ to zero, we arrive at the estimate

$$\int_0^T (1-\beta)\, \|\nabla e\|^2_{A,\Omega}\, dt + \|e^*\|^2_{A^{-1},Q_T} + 2\|\sigma_a e\|^2_{Q_T} + \|e(\cdot,T)\|^2_\Omega \leqslant \|v(x,0) - \phi(x)\|^2_\Omega + \|\mathrm{R}_A(v,y^*)\|^2_{Q_T} + \int_{Q_T} \frac{C^2(\Omega)}{\beta c_1^2 + 2\rho^2 C^2(\Omega)} |\mathrm{R}_f(v,y^*)|^2\, dx\, dt. \tag{5.18}$$

If $\rho = 0$, then (5.14) coincides with (5.3).

Remark 2. The estimates (5.17) and (5.18) can be viewed as a generalisation of the estimate derived in [19] for the stationary reaction–diffusion problems with small values of the reaction function ρ.

5.4. The identity (4.5) also yields computable bounds of the errors e and e^*. If v and y^* satisfy the conditions of Theorem 3, then the following estimate holds:

$$\int_0^T (1-\beta(t)-\gamma(t))\|\nabla e\|_A^2\,dt+\int_0^T (2-\alpha(t))\|e_t\|^2\,dt+2\|\rho e\|_{Q_T}^2+\|e^*\|_{A^{-1},Q_T}^2$$
$$+\Big[\!\!\Big[\|e\|_\Omega^2\Big]\!\!\Big]_0^T+\Big[\!\!\Big[\|\rho\, e\,dx\|_\Omega^2\Big]\!\!\Big]_0^T+\Big[\!\!\Big[\|e^*\|_{A^{-1}}^2\Big]\!\!\Big]_0^T\leqslant \mathbb{M}_2^+(v,y^*,\alpha,\beta,\gamma). \quad (5.19)$$

Here

$$\mathbb{M}_2^+(v,y^*,\alpha,\beta,\gamma):=\|\mathrm{R}_A(v,y^*)\|_{A^{-1},Q_T}^2+\Big[\!\!\Big[\,\|\mathrm{R}_A(v,y^*)\|_{A^{-1},\Omega}^2\Big]\!\!\Big]_0^T$$
$$+\int_0^T\left[\left(\frac{1}{\alpha(t)}+\frac{C^2(\Omega)}{c_1^2\beta(t)}\right)\|\mathrm{R}_f(v,y^*)\|_\Omega^2+\frac{1}{\gamma(t)}\|(\mathrm{R}_A(v,y^*)_t\|_{A^{-1}}^2\,dt\right]dt,$$

and α,β, and γ are arbitrary positive functions in $L^\infty(0,T)$ such that $0<\beta+\gamma\leqslant 1$ and $\alpha\leqslant 2$.

To prove (5.19), we estimate the last integral of $\mathcal{R}(v,y^*;e,e_t)$ by the Cauchy and Young's inequalities:

$$\left|\int_{Q_T}\mathrm{R}_f(v,y^*)e\,dx\,dt\right|\leqslant\int_0^T\|\mathrm{R}_f(v,y^*)\|_\Omega\|e\|_\Omega\,dt$$
$$\leqslant\int_0^T\frac{C(\Omega)}{c_1}\|\mathrm{R}_f(v,y^*)\|_\Omega\|\nabla e\|_A\,dt$$
$$\leqslant\frac{C^2(\Omega)}{c_1^2}\int_0^T\frac{1}{2\beta(t)}\|\mathrm{R}_f(v,y^*)\|_\Omega^2\,dt+\int_0^T\frac{\beta(t)}{2}\|\nabla e\|_A^2\,dt.$$

Hence

$$2\left|\int\limits_{Q_T} \mathrm{R}_f(v,y^*)(e+e_t)\,dx\,dt\right| \leqslant \int\limits_0^T \left(\frac{1}{\alpha(t)} + \frac{C^2(\Omega)}{c_1^2\beta(t)}\right)\|\mathrm{R}_f(v,y^*)\|_\Omega^2\,dt + \int\limits_0^T \alpha(t)\|e_t\|_\Omega^2\,dt + \int\limits_0^T \beta(t)\|\nabla e\|_A^2\,dt. \quad (5.20)$$

Also, we have

$$\int\limits_{Q_T} \nabla e\cdot(y^* - A\nabla v)_t\,dx\,dt = \int\limits_{Q_T} A\nabla e\cdot(A^{-1}y^* - \nabla v)_t\,dx\,dt$$
$$\leqslant \int\limits_0^T \|\nabla e\|_A \left(\int\limits_\Omega A(A^{-1}y_t^* - \nabla v_t)\cdot(A^{-1}y_t^* - \nabla v_t)\,dx\right)^{1/2} dt$$
$$= \int\limits_0^T \|\nabla e\|_A \|y_t^* - A\nabla v_t\|_{A^{-1}}\,dt$$
$$\leqslant \int\limits_0^T \gamma(t)\|\nabla e\|_A^2\,dt + \int\limits_0^T \frac{1}{\gamma(t)}\|(\mathrm{R}_A(v,y^*)_t\|_{A^{-1}}^2\,dt. \quad (5.21)$$

By (5.20) and (5.21) we conclude that

$$2|\mathcal{R}(v,y^*;e,e_t)|$$
$$\leqslant \int\limits_0^T \left(\frac{1}{\alpha(t)} + \frac{C^2(\Omega)}{c_1^2\beta(t)}\right)\|\mathrm{R}_f(v,y^*)\|_\Omega^2\,dt + \int\limits_0^T \frac{1}{\gamma(t)}\|(\mathrm{R}_A(v,y^*)_t\|_{A^{-1}}^2\,dt + \int\limits_0^T \alpha(t)\|e_t\|_\Omega^2\,dt + \int\limits_0^T (\beta(t)+\gamma(t))\|\nabla e\|_A^2\,dt. \quad (5.22)$$

Applying (5.22) to (4.5), we obtain (5.19).

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