

# A UNIFIED A POSTERIORI ERROR ANALYSIS FOR DISCONTINUOUS GALERKIN APPROXIMATIONS OF REACTIVE TRANSPORT EQUATIONS <sup>\*1)</sup>

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Dedicated to the 70th birthday of Professor Lin Qun

## Abstract

Four primal discontinuous Galerkin methods are applied to solve reactive transport problems, namely, Oden-Babuška-Baumann DG (OBB-DG), non-symmetric interior penalty Galerkin (NIPG), symmetric interior penalty Galerkin (SIPG), and incomplete interior penalty Galerkin (IIPG). A unified a posteriori residual-type error estimation is derived explicitly for these methods. From the computed solution and given data, explicit estimators can be computed efficiently and directly, which can be used as error indicators for adaptation. Unlike in the reference [10], we obtain the error estimators in  $L^2(L^2)$  norm by using duality techniques instead of in  $L^2(H^1)$  norm.

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*Key words:* A posteriori error estimates, Duality techniques, Discontinuous Galerkin methods.

## 1. Introduction

Numerical modeling of reactive transport problems in porous media is widely used in many fields, such as petroleum engineering, groundwater hydrology, environmental engineering, soil mechanics, earth sciences, chemical engineering and biomedical engineering. But, real simulations for simultaneous transport and chemical reaction present significant computational challenges [1, 2].

The discontinuous Galerkin (DG) method was initially introduced by Reed and Hill in 1973 as a technique to solve neutron transport problems. Recently, the discontinuous Galerkin methods (DG) [3, 4, 5] have been popular for solving a wide variety of problems. DG has a lot of advantages over traditional finite element methods. Firstly, it is flexible which allows for general non-conforming meshes with variable degrees of approximation. secondly, it is locally mass conservative and the average of the trace of the fluxes along an element edge is continuous. Thirdly, it has less numerical diffusion and can deal with rough coefficient problems. Finally, it is easier for  $h$ - $p$  adaptivity. DG applications for flow and transport problems in porous media

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have been studied in [6, 7].

A posteriori error estimators do not involve the knowledge of the exact unknown solution and are computable. At the same time, a posteriori error estimators are useful for adaptivity because they signify where refinement in spatial quantities or polynomial degree may be adaptively modified.

A posteriori error estimators for DG methods have mainly focused on steady-state equations of elliptic and hyperbolic type [8, 9]. And there are very few papers that deal with a posteriori error estimation for DG methods applied to transient problems. Explicitly, a posteriori error estimates in the  $L^2(H^1)$  norm have been derived for four primal DG methods applied to reactive transport problems [10] without dual assumptions. Sun and Wheeler [11] derived an explicit  $L^2(L^2)$  estimates for a symmetric discretization of the diffusion operator using a duality argument. In [12],  $L^2(L^2)$  estimates of a non-symmetric interior penalty formulation and the related local discontinuous Galerkin formulation are explored. We remark that error indicators in the  $L^2(L^2)$  norm are preferred over the indicators in  $L^2(H^1)$  for problems concerning the concentration itself rather than the transport flux. In this paper, we will establish a unified a posteriori error estimation for four primal DG methods (i.e. OBB-DG, NIPG, SIPG, and IIPG) using duality techniques.

We consider a model reactive transport problem in a porous media

$$\phi \partial_t c + \nabla \cdot (\mathbf{u}c - \mathbf{D}\nabla c) = \phi f \quad \text{in } \Omega, \quad t \in (0, T], \quad (1.1)$$

$$(\mathbf{u}c - \mathbf{D}\nabla c) \cdot \mathbf{n} = (\mathbf{u}g) \cdot \mathbf{n} \quad \text{on } \Gamma_{in}, \quad t \in (0, T], \quad (1.2)$$

$$(-\mathbf{D}\nabla c) \cdot \mathbf{n} = 0 \quad \text{on } \Gamma_{out}, \quad t \in (0, T], \quad (1.3)$$

$$c(x, 0) = c_0(x) \quad \text{in } \Omega. \quad (1.4)$$

where  $\Omega$  is a polygonal and bounded domain in  $R^d$  ( $d = 1, 2$  or  $3$ ) with boundary  $\partial\Omega = \Gamma_{in} \cup \Gamma_{out}$ ,  $\Gamma_{in} = \{x \in \partial\Omega : \mathbf{u} \cdot \mathbf{n} < 0\}$  and  $\Gamma_{out} = \{x \in \partial\Omega : \mathbf{u} \cdot \mathbf{n} \geq 0\}$  are the inflow boundary and the outflow boundary,  $\mathbf{n}$  denotes the unit outward normal vector to  $\partial\Omega$ ;  $\mathbf{u}(x, t)$  represents the Darcy velocity and we assume that  $\mathbf{u}$  is given and satisfies  $\nabla \cdot \mathbf{u} = 0$ ;  $c(x, t)$  is the concentration of some chemical component,  $\phi(x)$  is the effective porosity of the medium and is bounded above and below by positive constants,  $\mathbf{D}(x, \mathbf{u}, t)$  denotes a diffusion or dispersion tensor and is uniformly positive definite, and  $f(x, t)$  is a source term.

The paper is organized as follows. In section 2, we introduce the DG schemes. In section 3, a posteriori error estimators in  $L^2(L^2)$  norm for the semi-discrete schemes are obtained using duality techniques explicitly. The numerical experiments are listed in section 4.

## 2. Discontinuous Galerkin Method

### 2.1. Notation

Let  $\varepsilon_h$  be a family of non-degenerate (or called regularity, which means that the element is convex and that there exists  $\lambda > 0$  such that if  $h_j$  is the diameter of  $E_j \in \varepsilon_h$ , then each of the sub-triangles (for  $d = 2$ ) or sub-tetrahedra (for  $d = 3$ ) of element  $E_j$  contains a ball of radius  $\lambda h_j$  in its interior), and possibly non-conforming finite element partitions of  $\Omega$  composed of triangles or quadrilaterals if  $d = 2$ , or tetrahedra, prisms or hexahedra if  $d = 3$ .

Let  $\Gamma_h$  be the set of all interior edges (for 2 dimensional domain) or faces (for 3 dimensional domain) for  $\varepsilon_h$ .  $\Gamma_{h,in}$  and  $\Gamma_{h,out}$  denote the set of all edges or faces on  $\Gamma_{in}$  and  $\Gamma_{out}$  for  $\varepsilon_h$ , respectively.  $\mathbf{n}_\gamma$  is the outward unit normal vector on each edge or face  $\gamma \in \Gamma_h \cup \Gamma_{h,in} \cup \Gamma_{h,out}$ .

The inner product in  $(L^2(\Omega))^d$  or  $L^2(\Omega)$  is indicated by  $(\cdot, \cdot)_\Omega$  and the inner product in the boundary function space  $L^2(\gamma)$  is indicated by  $(\cdot, \cdot)_\gamma$ .

For  $s \geq 0$ , we define

$$H^s(\varepsilon_h) = \{v \in L^2(\Omega) : v|_E \in H^s(E), E \in \varepsilon_h\}. \quad (2.1)$$

The average and the jump for  $v \in H^s(\varepsilon_h)$ ,  $s > 1/2$  are defined as follows. Let  $E_i \in \varepsilon_h$ ,  $E_j \in \varepsilon_h$  and  $\gamma = \partial E_i \cap \partial E_j \in \Gamma_h$  with  $\mathbf{n}$  exterior to  $E_i$ . Denote

$$\{v\} = \frac{1}{2}((v|_{E_i})|_\gamma + (v|_{E_j})|_\gamma), \quad (2.2)$$

$$[v] = (v|_{E_i})|_\gamma - (v|_{E_j})|_\gamma. \quad (2.3)$$

Define the upwind value of  $v$ :

$$v^*|_\gamma = \begin{cases} v|_{E_i} & \text{if } \mathbf{u} \cdot \mathbf{n} \geq 0, \\ v|_{E_j} & \text{if } \mathbf{u} \cdot \mathbf{n} < 0. \end{cases}$$

We set the discontinuous finite element space:

$$D_k(\varepsilon_h) \equiv \{v \in L^2(\Omega) : v|_E \in P_k(E), E \in \varepsilon_h\}, \quad (2.4)$$

where  $P_k(E)$  denotes the space of polynomials of total degree less than or equal to  $k$  on  $E$ .

## 2.2. Weak Formulation

First, we give the weak formulation of the reactive transport problem, which can be found in [13].

**Lemma 2.1.** *If  $c$  is the solution of (1.1)-(1.4) and  $c$  is essentially bounded, then  $c$  satisfies*

$$(\phi \partial_t c, w)_\Omega + B(c, w) = L(w), \quad \forall w \in H^s(\varepsilon_h), s > \frac{3}{2}, \forall t \in (0, T]. \quad (2.5)$$

where the bilinear form  $B(c, w)$  and the linear functional  $L(w)$  are defined as follows:

$$\begin{aligned} B(c, w) &= - \sum_{E \in \varepsilon_h} \int_E (\mathbf{u}c - \mathbf{D}\nabla c) \cdot \nabla w + \sum_{\gamma \in \Gamma_{h, out}} \int_\gamma \mathbf{c}u \cdot \mathbf{n}w \\ &\quad - \sum_{\gamma \in \Gamma_h} \int_\gamma \{\mathbf{D}\nabla c \cdot \mathbf{n}\}[w] - \theta \sum_{\gamma \in \Gamma_h} \int_\gamma \{\mathbf{D}\nabla w \cdot \mathbf{n}\}[c] \\ &\quad + \sum_{\gamma \in \Gamma_h} \int_\gamma \mathbf{u}c^* \cdot \mathbf{n}[w] + \sum_{\gamma \in \Gamma_h} \frac{\tau_\gamma^2 \sigma_\gamma}{h_\gamma} \int_\gamma [c][w], \\ L(w) &= \int_\Omega \phi f w - \sum_{\gamma \in \Gamma_{h, in}} \int_\gamma (\mathbf{u}g \cdot \mathbf{n})w. \end{aligned} \quad (2.6)$$

Here, the parameter  $\theta$  indicates the type of different DG schemes,  $\theta = -1$  for NIPG or OBB-DG (the non-symmetric formulation),  $\theta = 1$  for SIPG (the symmetric formulation) and  $\theta = 0$  for IIPG method. And  $\sigma_\gamma$  is a positive constant. In OBB-DG scheme,  $\sigma_\gamma \equiv 0$ . For SIPG, IIPG or NIPG,  $\sigma_\gamma > 0$  and  $\sigma_\gamma$  is bounded above and below by positive numbers.

Then, we get the continuous in time DG approximation  $c_h \in W^{1, \infty}(0, T; D_k(\varepsilon_h))$  of (1.1)-(1.4):

$$(\phi \partial_t c_h, w)_\Omega + B(c_h, w) = L(w), \quad \forall w \in D_k(\varepsilon_h), \quad t \in (0, T], \quad (2.7)$$

$$(\phi c_h, w)_\Omega = (\phi c_0, w)_\Omega, \quad \forall w \in D_k(\varepsilon_h), \quad t = 0. \quad (2.8)$$

Let  $e_c = c - c_h$  be the error in the solution. By subtracting (2.7) from (2.5), we easily get the Galerkin orthogonality

$$(\phi \partial_t e_c, w)_\Omega + B(e_c, w) = 0, \quad \forall w \in D_k(\varepsilon_h), \quad t \in (0, T]. \quad (2.9)$$

## 3. A Posteriori Error Estimates

Let  $\xi$  satisfy the duality problem

$$\phi \partial_t \xi + \nabla \cdot (\mathbf{u}\xi + \mathbf{D}^T \nabla \xi) = e_c \quad \text{in } \Omega, \quad t \in (0, T], \quad (3.1)$$

$$(\mathbf{u}\xi + \mathbf{D}^T \nabla \xi) \cdot \mathbf{n} = 0 \quad \text{on } \partial\Omega_{out}, \quad t \in (0, T], \quad (3.2)$$

$$(-\mathbf{D}^T \nabla \xi) \cdot \mathbf{n} = 0 \quad \text{on } \partial\Omega_{in}, \quad t \in (0, T], \quad (3.3)$$

$$\xi(x, T) = 0 \quad \text{in } \Omega. \quad (3.4)$$

Assume that the dual problem (3.1)-(3.4) satisfies the stability estimate

$$\max_{0 \leq t \leq T} \|\xi(\cdot, t)\|_{\Omega}^2 + \int_0^T \|\xi\|_{H^2(\Omega)}^2 dt \leq C \int_0^T \|e_c\|_{L^2(\Omega)}^2 dt \quad (3.5)$$

And we also assume that the following approximation properties hold (see [14]) for  $d = 2$  or  $3$ . For  $E_i \in \varepsilon_h$  and  $v \in H^s(\varepsilon_h)$ , there exists a constant  $C$  depending on  $s$  but independent of  $v$ ,  $k$ , the diameter  $h_i$  of element  $E_i$  and  $\tilde{v} \in P^k(E_i)$  (where  $P^k(E_i)$  denotes the polynomial of degree less than or equal to  $k$  on  $E_i$ ), such that for  $0 \leq q \leq s$  and for  $\mu = \min(k+1, s)$ ,

$$\|v - \tilde{v}\|_{H^q(E_i)} \leq C \frac{h_i^{\mu-q}}{k^{s-q}} \|v\|_{H^s(E_i)} \quad s \geq 0, \quad (3.6)$$

$$\|v - \tilde{v}\|_{H^r(\partial E_i)} \leq C \frac{h_i^{\mu-r-1/2}}{k^{s-r-1/2}} \|v\|_{H^s(E_i)} \quad s > \frac{1}{2} + \delta, \quad \delta = 0, 1. \quad (3.7)$$

Introduce the residuals

$$R_I = \phi f - \phi \partial_t c_h + \nabla \cdot (\mathbf{u} c_h - \mathbf{D} \nabla c_h), \quad (3.8)$$

$$R_{B0} = [c_h], \quad (3.9)$$

$$R_{B1} = \begin{cases} [\mathbf{D} \nabla c_h \cdot \mathbf{n}], & x \in \gamma, \quad \gamma \in \Gamma_h, \\ \mathbf{u} g \cdot \mathbf{n} - (\mathbf{u} c_h - \mathbf{D} \nabla c_h) \cdot \mathbf{n}, & x \in \Gamma_{h,in}, \\ -\mathbf{D} \nabla c_h \cdot \mathbf{n}, & x \in \Gamma_{h,out}, \end{cases} \quad (3.10)$$

$$R_{B2} = c_0 - c_{h,0}. \quad (3.11)$$

For convenience, we also introduce some notations which we shall use in the approximation estimates below.  $L^2(L^2(E)) := L^2(0, T; L^2(E))$ ,  $L^2(L^\infty(\Omega)) := L^2(0, T; L^\infty(\Omega))$ ,  $L^2(L^2(\Omega)) := L^2(0, T; L^2(\Omega))$ , and  $L^2(L^2(\gamma)) := L^2(0, T; L^2(\gamma))$ .

Next, we will derive a unified a posteriori error estimation for four primal DG methods.

**Theorem 3.1.** *Let  $c$  be the solution to (1.1)-(1.4) and  $\xi$  be the solution to (3.1)-(3.4). Assume that  $c \in L^2(0, T; H^s(\varepsilon_h))$ ,  $\partial_t c \in L^2(0, T; H^{s-1}(\varepsilon_h))$  and  $c_0 \in \mathbf{D}_k(\varepsilon_h)$ . Furthermore, we assume that  $c$ ,  $\mathbf{u}$  are essentially bounded and  $\mathbf{D}$  is continuous. Then*

$$\|e_c\|_{L^2(L^2(\Omega))}^2 \leq C \sum_{E \in \varepsilon_h} \eta_E^2, \quad (3.12)$$

where

$$\begin{aligned} \eta_E^2 &= \frac{h^4}{k^4} \|R_I\|_{L^2(L^2(E))}^2 + \frac{h^4}{k^4} \|R_{B2}\|_{L^2(E)}^2 + \\ &\quad \frac{h^3}{k^3} \sum_{\gamma \in \Gamma_{h,in} \cup \Gamma_{h,out}} \|R_{B1}\|_{L^2(L^2(\gamma))}^2 + \\ &\quad \frac{h^3}{k^3} \sum_{\gamma \in \Gamma_h} \|R_{B1} + \mathbf{u} \cdot R_{B0}\|_{L^2(L^2(\gamma))}^2 + \\ &\quad \sum_{\gamma \in \Gamma_h} \|R_{B0}\|_{L^2(L^2(\gamma))}^2 \cdot \left( \frac{h^2}{k^2} \|\mathbf{D}\|_{L^2(L^\infty(\Omega))}^2 + \|\mathbf{D}\|_{L^2(L^\infty(\Omega))}^2 \right) \end{aligned}$$

for  $h = \max_i h_i$  the maximal element diameter over all elements with the common edge or face  $\gamma = \partial E_i \cap \partial E_j \in \Gamma_h$  and  $C$  a constant independent of  $h_\gamma$ .

*Proof.* By using equations (3.1), (3.4), (3.11), and integration by parts, we get

$$\begin{aligned}
\|e_c\|_{L^2(L^2(\Omega))}^2 &= \int_0^T (e_c, e_c)_\Omega dt \\
&= \int_0^T (\phi \partial_t \xi + \nabla \cdot (\mathbf{u}\xi + \mathbf{D}^T \nabla \xi), e_c)_\Omega dt \\
&= - \int_0^T (\phi \partial_t e_c, \xi)_\Omega dt + (R_{B2}, \phi \xi(\cdot, 0))_\Omega \\
&\quad + \int_0^T (\nabla \cdot (\mathbf{u}\xi), e_c)_\Omega dt + \int_0^T (\nabla \cdot (\mathbf{D}^T \nabla \xi), e_c)_\Omega dt,
\end{aligned}$$

Integrate by parts to the last term and use (3.3) to obtain

$$\begin{aligned}
\int_0^T (\nabla \cdot (\mathbf{D}^T \nabla \xi), e_c)_\Omega dt &= \int_0^T \left( - \sum_{E \in \varepsilon_h} (\nabla \xi, \mathbf{D} \nabla e_c)_E + \sum_{\gamma \in \Gamma_h} (\mathbf{D}^T \nabla \xi \cdot \mathbf{n}, [e_c])_\gamma \right. \\
&\quad \left. + \sum_{\gamma \in \Gamma_{h,out}} (\mathbf{D}^T \nabla \xi \cdot \mathbf{n}, e_c)_\gamma \right. \\
&\quad \left. + \sum_{\gamma \in \Gamma_{h,in}} (\mathbf{D}^T \nabla \xi \cdot \mathbf{n}, e_c)_\gamma \right) dt \\
&= \int_0^T \left( - \sum_{E \in \varepsilon_h} (\nabla \xi, \mathbf{D} \nabla e_c)_E + \sum_{\gamma \in \Gamma_h} (\mathbf{D}^T \nabla \xi \cdot \mathbf{n}, [e_c])_\gamma \right. \\
&\quad \left. + \sum_{\gamma \in \Gamma_{h,out}} (\mathbf{D}^T \nabla \xi \cdot \mathbf{n}, e_c)_\gamma \right) dt
\end{aligned}$$

For  $\forall \tilde{\xi} \in D_k(\varepsilon_h) \cap C^0(\Omega)$ , we have  $[\tilde{\xi}] = 0$ . so, by using Galerkin orthogonality (2.9), we obtain

$$\begin{aligned}
&(\phi \partial_t e_c, \tilde{\xi})_\Omega + \left( - \sum_{E \in \varepsilon_h} (\mathbf{u} e_c - \mathbf{D} \nabla e_c, \nabla \tilde{\xi})_E + \sum_{\gamma \in \Gamma_{h,out}} (\mathbf{u} e_c \cdot \mathbf{n}, \tilde{\xi})_\gamma \right. \\
&\quad \left. + \sum_{\gamma \in \Gamma_h} (\mathbf{u} e_c^* \cdot \mathbf{n}, [\tilde{\xi}])_\gamma - \sum_{\gamma \in \Gamma_h} (\{\mathbf{D} \nabla e_c \cdot \mathbf{n}\}, [\tilde{\xi}])_\gamma - \theta \sum_{\gamma \in \Gamma_h} (\{\mathbf{D} \nabla \tilde{\xi} \cdot \mathbf{n}\}, [e_c])_\gamma \right. \\
&\quad \left. + \sum_{\gamma \in \Gamma_h} \left( \frac{r^2 \sigma_\gamma}{h_\gamma} [e_c], [\tilde{\xi}] \right)_\gamma \right) \\
&= (\phi \partial_t e_c, \tilde{\xi})_\Omega - \sum_{E \in \varepsilon_h} (\mathbf{u} e_c - \mathbf{D} \nabla e_c, \nabla \tilde{\xi})_E + \sum_{\gamma \in \Gamma_{h,out}} (\mathbf{u} e_c \cdot \mathbf{n}, \tilde{\xi})_\gamma \\
&\quad - \theta \sum_{\gamma \in \Gamma_h} (\{\mathbf{D} \nabla \tilde{\xi} \cdot \mathbf{n}\}, [e_c])_\gamma \\
&= 0.
\end{aligned}$$

Then,

$$\begin{aligned}
\int_0^T (e_c, e_c)_\Omega dt &= - \int_0^T (\phi \partial_t e_c, \xi - \tilde{\xi})_\Omega dt + (R_{B2}, \phi(\xi - \tilde{\xi})(\cdot, 0))_\Omega \\
&+ \int_0^T \sum_{E \in \varepsilon_h} (\mathbf{u}e_c - \mathbf{D}\nabla e_c, \nabla(\xi - \tilde{\xi}))_E dt \\
&+ \int_0^T \sum_{\gamma \in \Gamma_h} (\mathbf{D}^T \nabla \xi \cdot \mathbf{n}, [e_c])_\gamma dt + \int_0^T \sum_{\gamma \in \Gamma_{h,out}} (\mathbf{D}^T \nabla \xi \cdot \mathbf{n}, e_c)_\gamma dt \\
&+ \int_0^T -\theta \sum_{\gamma \in \Gamma_h} (\{\mathbf{D}\nabla \tilde{\xi} \cdot \mathbf{n}\}, [e_c])_\gamma dt + \int_0^T \sum_{\gamma \in \Gamma_{h,out}} (\mathbf{u}e_c \cdot \mathbf{n}, \tilde{\xi})_\gamma dt
\end{aligned}$$

Applying the integration by parts technique to the third term of the above equation, we get

$$\begin{aligned}
\sum_{E \in \varepsilon_h} (\mathbf{u}e_c - \mathbf{D}\nabla e_c, \nabla(\xi - \tilde{\xi}))_E &= - \sum_{E \in \varepsilon_h} (\nabla \cdot (\mathbf{u}e_c - \mathbf{D}\nabla e_c), \xi - \tilde{\xi})_E \\
&+ \sum_{\gamma \in \Gamma_h} ((\mathbf{u}e_c - \mathbf{D}\nabla e_c) \cdot \mathbf{n}, \xi - \tilde{\xi})_\gamma \\
&+ \sum_{\gamma \in \Gamma_{h,in} \cup \Gamma_{h,out}} ((\mathbf{u}e_c - \mathbf{D}\nabla e_c) \cdot \mathbf{n}, \xi - \tilde{\xi})_\gamma
\end{aligned}$$

Thus,

$$\begin{aligned}
\|e_c\|_{L^2(L^2(\Omega))}^2 &= - \int_0^T (R_I, \xi - \tilde{\xi})_\Omega dt + (R_{B2}, \phi(\xi - \tilde{\xi})(\cdot, 0))_\Omega \\
&+ \int_0^T \sum_{\gamma \in \Gamma_{h,in} \cup \Gamma_{h,out}} (R_{B1}, \xi - \tilde{\xi})_\gamma dt \\
&+ \int_0^T \sum_{\gamma \in \Gamma_h} (R_{B0}, (\mathbf{D}^T \nabla \xi - \theta \mathbf{D}\nabla \tilde{\xi}) \cdot \mathbf{n})_\gamma dt \\
&- \int_0^T \sum_{\gamma \in \Gamma_h} (R_{B1} - \mathbf{u}R_{B0}, \xi - \tilde{\xi})_\gamma dt
\end{aligned} \tag{3.13}$$

where (1.1) and (3.2) are used. To bound the items on the right side of the above equation, we proceed as follows.

By virtue of the equations (3.5), (3.6), (3.7), and the Cauchy-Schwartz inequality, we have

$$\begin{aligned}
- \int_0^T (R_I, \xi - \tilde{\xi})_\Omega dt &\leq C \left( \frac{h^4}{k^4} \sum_{E \in \Gamma_h} \|e_c\|_{L^2(L^2(E))}^2 \right)^{1/2} \cdot \left( \sum_{E \in \Gamma_h} \|R_I\|_{L^2(L^2(E))}^2 \right)^{1/2}, \\
(R_{B2}, \phi(\xi - \tilde{\xi})(\cdot, 0))_\Omega &\leq C \left( \sum_{E \in \Gamma_h} \frac{h^4}{k^4} \sum_{E \in \Gamma_h} \|e_c\|_{L^2(L^2(E))}^2 \right)^{1/2} \cdot \left( \sum_{E \in \Gamma_h} \|R_{B2}\|_{L^2(E)}^2 \right)^{1/2},
\end{aligned}$$

$$\begin{aligned}
\int_0^T \sum_{\gamma \in \Gamma_{h,in} \cup \Gamma_{h,out}} (R_{B1}, \xi - \tilde{\xi})_\gamma dt &\leq C \frac{h^{3/2}}{k^{3/2}} \|e_c\|_{L^2(L^2(\Omega))} \cdot \left( \sum_{\gamma \in \Gamma_{h,in} \cup \Gamma_{h,out}} \|R_{B1}\|_{L^2(L^2(\gamma))}^2 \right)^{1/2}, \\
- \int_0^T \sum_{\gamma \in \Gamma_h} (R_{B1} - \mathbf{u}R_{B0}, \xi - \tilde{\xi})_\gamma dt &\leq C \frac{h^{3/2}}{k^{3/2}} \|e_c\|_{L^2(L^2(\Omega))} \cdot \left( \sum_{\gamma \in \Gamma_h} \|R_{B1} + \mathbf{u} \cdot R_{B0}\|_{L^2(L^2(\gamma))}^2 \right)^{1/2}.
\end{aligned}$$

and

$$\begin{aligned}
& \int_0^T \sum_{\gamma \in \Gamma_h} (R_{B0}, (\mathbf{D}^T \nabla \xi - \theta \mathbf{D} \nabla \tilde{\xi}) \cdot \mathbf{n})_{\gamma} dt \\
&= \int_0^T \sum_{\gamma \in \Gamma_h} (R_{B0}, ((-\theta \mathbf{D} + \mathbf{D}^T) \nabla \xi + \theta \mathbf{D} \nabla (\xi - \tilde{\xi})) \cdot \mathbf{n})_{\gamma} dt \\
&= \int_0^T \sum_{\gamma \in \Gamma_h} (R_{B0}, (-\theta \mathbf{D} + \mathbf{D}^T) \nabla \xi \cdot \mathbf{n})_{\gamma} dt + \int_0^T \sum_{\gamma \in \Gamma_h} (R_{B0}, \theta \mathbf{D} \nabla (\xi - \tilde{\xi}) \cdot \mathbf{n})_{\gamma} dt \\
&\leq C \int_0^T \sum_{\gamma \in \Gamma_h} \left( \int_{\gamma} R_{B0}^2 d\gamma \right)^{1/2} \cdot \left( \int_{\gamma} ((-\theta \mathbf{D} + \mathbf{D}^T) \nabla \xi \cdot \mathbf{n})^2 d\gamma \right)^{1/2} \\
&\quad + C \int_0^T \sum_{\gamma \in \Gamma_h} \left( \int_{\gamma} R_{B0}^2 d\gamma \right)^{1/2} \cdot \left( \int_{\gamma} (\theta \mathbf{D} \nabla (\xi - \tilde{\xi}) \cdot \mathbf{n})^2 d\gamma \right)^{1/2} \\
&\leq C \sum_{\gamma \in \Gamma_h} \|R_{B0}\|_{L^2(L^2(\gamma))} \cdot \left( \frac{h}{k} \|\mathbf{D}\|_{L^2(L^\infty(\Omega))} + \|\mathbf{D}\|_{L^2(L^\infty(\Omega))} \right) \cdot \|e_c\|_{L^2(L^2(\Omega))}
\end{aligned}$$

Finally, the error estimate (3.12) is followed.

#### 4. Numerical Experiments

We consider a simplified problem in 1-D related to (1.1)-(1.4), posed over domain  $\Omega = (-4, 4)$  with initial value  $c_0(x) = \exp(-x^2)$ , source term  $f = 0$ ,  $\phi = 1$ , diffusion tensor  $\mathbf{D} = \mathbf{0}$ , advection velocity  $\mathbf{u} = \mathbf{I}$  and inflow data  $g(t) = -\sin(t)$ . The simulation time interval is  $(0, 0.5)$ .

To approximate the exact solution, OBB-DG scheme is employed because we do not need to choose a proper penalty parameter. A uniform mesh  $\{x_i\}$  and Legendre polynomial of degree  $p$  ( $0 \leq p \leq 3$ ) are used for spatial discretization. Time is discretized using an explicit Euler method with a uniform time step of  $2.5 \times 10^{-5}$ . The error of the DG solution is defined as the difference between the DG solution and the exact solution.

The following quantities are evaluated.

$$\begin{aligned}
T_1 &= \left( \sum_{x_i \in (-4,4)} [c_h(x_i)]^2 \right)^{1/2}, \\
T_2 &= \left( \sum_{x_i \in (-4,4)} [c'_h(x_i)]^2 \right)^{1/2}, \\
T_3 &= \left( \sum_{E \in (-4,4)} \|R_{B2}\|_{L^2(E)}^2 \right)^{1/2}
\end{aligned}$$

where  $x_i$  is the mesh vertices. We also give the convergence rates  $r$ , where  $r$  is defined as follows. Let  $e_p$  is the error with fixed  $h$  and variable  $p$ . Let  $e_h$  is the error with fixed  $p$  and variable  $h$ . Then,  $r = \log_2(\frac{e_p}{e_{p+1}})$  or  $r = \log_2(\frac{e_h}{e_{h/2}})$ . Results are presented in Figure 1–Figure 2 and Table 1–Table 2.

From these figures and tables, we can see that the error will decrease with the increasing of polynomial degree or condensing of the mesh. The convergence rates in practical computation coincide with the theoretical analysis, which confirms that Theorem 3.1 is right.

**Remark.** In this paper, we only consider the semi-discretization of discontinuous Galerkin finite element methods. The analysis for the full-discretization of DG is more challenged. It is our next work to investigate the error estimates for the full-discretization of DG schemes.

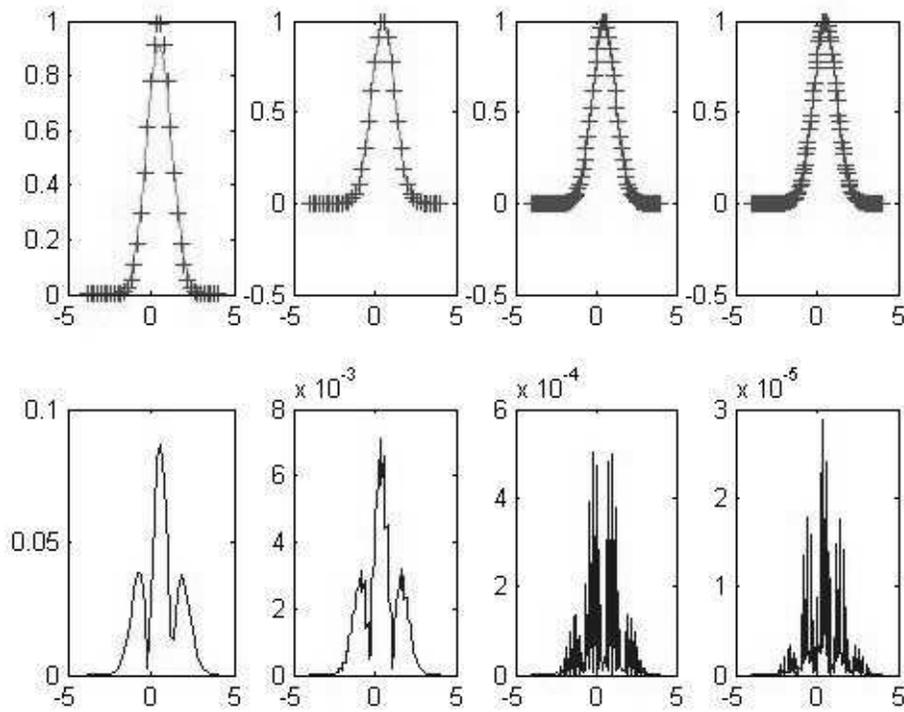


Figure 1: The DG solution (upside) and error (downside) for the concentration  $c$  at time  $t=0.5$  with spatial step  $h = 0.2$  for  $p = 0, 1, 2, 3$

$p$	$T_1$	$T_2$	$T_3$
0	$7.85e-2$	$7.68e-1$	$7.20e-3$
1	$1.67e-2$ $r = 2.3$	$5.41e-1$ $r = 0.5$	$1.84e-3$ $r = 2.0$
2	$3.22e-3$ $r = 2.4$	$3.85e-1$ $r = 0.5$	$4.53e-4$ $r = 2.19$
3	$6.20e-4$ $r = 2.5$	$2.65e-1$ $r = 0.5$	$1.12e-4$ $r = 2.0$

Table 1: The computed quantities  $T_1$ ,  $T_2$ ,  $T_3$  and convergence rates  $r$  for DG with different  $p$  when  $h = 0.2$

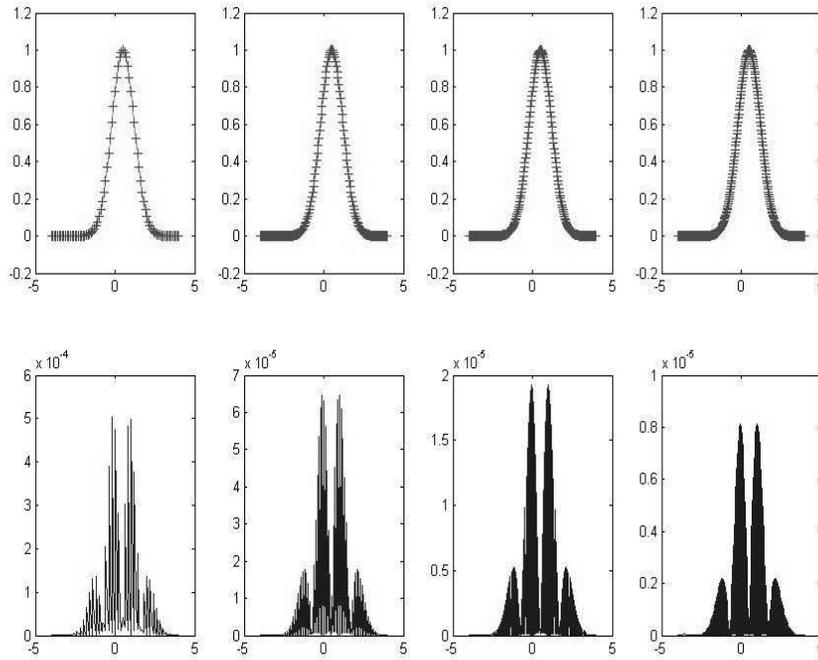


Figure 2: The DG solution (upside) and error (downside) for the concentration  $c$  at time  $t=0.5$  with spatial step  $h = 0.2, 0.1, 0.05, 0.025$  for  $p = 2$

$h$	$T_1$	$T_2$	$T_3$
0.5	$7.91e-2$	$7.65e-1$	$7.17e-3$
0.25	$1.72e-2$ $r = 2.2$	$5.39e-1$ $r = 0.5$	$1.80e-3$ $r = 2.0$
0.125	$3.27e-3$ $r = 2.4$	$3.88e-1$ $r = 0.5$	$4.49e-4$ $r = 2.0$
0.0625	$6.28e-4$ $r = 2.5$	$2.68e-1$ $r = 0.5$	$1.15e-4$ $r = 2.0$

Table 2: The computed quantities  $T_1, T_2, T_3$  and convergence rates  $r$  for DG with different  $h$  when  $p = 2$

## References

- [1] T. ARBOGAST, S. BRYANT, C. DAWSON, F. SAAF, C. WANG, AND M. WHEELER, Computational methods for multiphase flow and reactive transport problems arising in subsurface contaminant remediation, *J. Comput. Appl. Math.*, **74** (1996), 19–32.
- [2] P. C. LICHTNER, C. I. STEEFEL, AND E. H. OELKERS, Reactive transport in porous media, *Reviews in Mineralogy*, **34** (1996), 438.
- [3] J. T. ODEN, I. BABUŠKA, AND C. E. BAUMANN, A discontinuous hp finite element method for diffusion problems, *J. Comput. Phys.*, **146** (1998), 491–516.
- [4] B. RIVIÈRE, M. F. WHEELER, AND V. GIRAULT, A priori error estimates for finite element methods based on discontinuous approximation spaces for elliptic problems, *SIAM J. Numer. Anal.*, **39** (2001), 902–931.
- [5] C. JOHNSON, Discontinuous Galerkin finite element methods for second order hyperbolic problems, *Comput. Methods Appl. Mech. Engrg.*, **107** (1993), 117–129.
- [6] S. SUN, B. RIVIÈRE, AND M. F. WHEELER, A combined mixed finite element and discontinuous Galerkin method for miscible displacement problem in porous media, In Recent progress in computational and applied PDEs, conference proceedings for the international conference held in Zhangjiajie in July 2001, 321–348.
- [7] M. F. WHEELER, S. SUN, O. ESLINGER, AND B. RIVIÈRE, Discontinuous Galerkin method for modeling flow and reactive transport in porous media, In W. Wendland, editor, Analysis and Simulation of Multifield Problem, Springer Verlag, August 2003, 37–58.
- [8] B. RIVIÈRE, AND M. F. WHEELER, A posteriori error estimates and mesh adaptation strategy for discontinuous Galerkin methods applied to diffusion problems, *Comp. Math. Appl.*, **46** (2003), 141–163.
- [9] M. LARSON AND T. BARTH, A posteriori error estimation for adaptive discontinuous Galerkin approximations of hyperbolic systems. in Discontinuous Galerkin Methods, B. Cockburn, G. Karniadakis, and C. Shu, eds., Springer-Verlag in Berlin, 2000.
- [10] S. SUN AND M. F. WHEELER,  $L^2(H^1)$  norm a posteriori error estimation for discontinuous Galerkin approximations of reactive transport problems, *Journal of Scientific Computing*, **22** (2005), 511–540.
- [11] S. SUN AND M. F. WHEELER, A posteriori error analyses for symmetric discontinuous Galerkin approximations of reactive transport problems, TICAM report 03-19, Institute for Computational Engineering and Sciences, The University of Texas at Austin, Austin, Texas, 2003.
- [12] ALEXANDRE ERN AND JENNIFER PROFT, A posteriori discontinuous Galerkin error estimates for transient convection-diffusion equations, *Applied Mathematics Letters*, **18** (2005), 833–841.
- [13] S. SUN, Discontinuous Galerkin Methods for Reactive Transport in Porous Media, Ph. D. thesis, The university of Texas at Austin, 2003.
- [14] I. BABUŠKA AND M. SURI, The optimal convergence rate of the p-version of the finite element method, *SIAM J. Numer. Anal.*, **24** (1987), 750–776.