Analysis of Discontinuous Galerkin Methods for Multicomponent Reactive Transport Problems

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Abstract—Primal discontinuous Galerkin (DG) methods, including the Oden-Babuška-Baumann version of DG, are formulated for solving multicomponent reactive transport problems in porous media. Using the information of chemical stoichiometry, an efficient approach is proposed for a special case of multicomponent reactive transport without immobile species. A priori error analysis is conducted to establish the convergence of DG methods for multicomponent reactive transport systems, which is optimal in h and nearly optimal in p. © 2006 Elsevier Ltd. All rights reserved.

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1. INTRODUCTION

Reactive transport phenomena arise from many natural and engineered systems. Numerical modeling of reactive transport in porous media plays important roles in hydrology, earth sciences, environmental protection, chemical engineering, petroleum industry, and tissue engineering. However, realistic simulations for simultaneous multiphase multicomponent transport and chemical reaction present significant computational challenges [1–12]. For example, transport simulations often demand a high accuracy of numerical solutions. Many realistic transport problems in porous media involve a very long period of time. Small errors in each time step may cause substantial accumulated inaccuracy, sometimes leading to physically meaningless results. This also necessitates numerical schemes being locally conservative, as transport phenomena are based on the principle of mass conservation. In addition, effective adaptivities are often required to efficiently simulate reactive transport, because the transport systems often exhibit rich time-dependent local behaviors, such as concentration plumes, sharp fronts, shocks, and layers.

The discontinuous Galerkin (DG) methods [13–19] exhibit many of the desired properties needed to solve multicomponent reactive transport problems. DG methods are high-order accurate methods, and they satisfy local mass conservation in each element. Moreover, the methods are flexible in treating general nonconforming meshes with variable degrees of approximation. Besides providing an excellent parallel efficiency, this flexibility also makes the implementation

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of $hp$-adaptivity for DG substantially easier than that for conventional approaches. With appropriate meshing, DG methods are capable of delivering exponential rates of convergence. Another advantage of DG for reactive transport problems is the small numerical diffusion in DG solutions, which is especially important for advection-dominated transport problems involving sharp concentration fronts. Furthermore, DG handles rough coefficient problems and captures discontinuities in solutions very well by the nature of discontinuous function spaces.

DG has recently been applied for flow and transport problems in porous media [20–24], and an optimal convergence in $L^2(H^1)$ was demonstrated for flow and transport problems [17,21,25,26]. The $hp$-convergence behaviors in the $L^2(L^2)$ norm have been analyzed for the symmetric DG [25,26]. In addition, explicit $a$ posteriori error estimates of DG for reactive transport have been studied [27–29]. In this paper, we extend the results on $a$ priori error estimation to multi-component reactive transport systems.

The paper is organized as follows: in the following section, we state the governing equations for multiple component reactive transport systems. The DG schemes for the transport problems are formulated in Section 3, together with a few known properties of DG. In Section 4, we derive $a$ priori error estimates. Finally, in Section 5, our results are summarized, and future work is described.

2. GOVERNING EQUATIONS

2.1. The Advection-Diffusion-Reaction Equations

We consider the multiple component reactive transport system for a single flowing phase and possibly multiple stationary phases in porous media. We remark that the results in this paper directly extend to multiple flowing phases provided that a local phase equilibrium is assumed between flowing phases, where transport may be described with a pseudosingle phase using a phase-summed reactive transport equation. Except for possible linear equilibrium type adsorptions, the reaction process is assumed to be a local nonequilibrium system [30], i.e., all reactions may fail to attain equilibrium locally during the course of transport. We assume that the given Darcy velocity field $u$ satisfies $\nabla \cdot u = q$, where $q$ is the imposed external total flow rate.

The chemical system is comprised of $N_S$ species. We allow for possible linear equilibrium type adsorptions, which are treated by using retardation factors. Except for these adsorptions, all species considered are either in a flowing phase (mobile species) or in a stationary phase (immobile species or minerals). If the same physical species occurs in both flowing and stationary phases, we treat it as two distinct species, one in each phase, in the modeling equations. In this case, the interphase mass transfer of the physical species is incorporated into the modeling system as a chemical reaction. Let $N_M$ denote the number of immobile species and $I_F$ the corresponding index set. Similarly, let $N_F$ denote the number of mobile species and $I_M$ the corresponding index set.

Let $T$ be the final simulation time. The domain $\Omega$ is assumed to be polygonal and bounded in $\mathbb{R}^d$, $d = 1, 2, 3$. Its boundary $\partial \Omega = \bar{\Gamma}_\text{in} \cup \bar{\Gamma}_\text{out}$ contains the inflow boundary $\Gamma_\text{in}$ and the outflow/noflow boundary $\Gamma_\text{out}$, defined by

$$\Gamma_\text{in} = \{x \in \partial \Omega : u \cdot n_{\partial \Omega} < 0\},$$
$$\Gamma_\text{out} = \{x \in \partial \Omega : u \cdot n_{\partial \Omega} \geq 0\},$$

where $n_{\partial \Omega}$ denotes the unit outward normal vector to $\partial \Omega$.

The classical advection-diffusion-reaction equations governing the reactive transport process for a single flowing phase in porous media are as follows:

$$\frac{\partial \phi_\alpha c_\alpha}{\partial t} + \nabla \cdot (uc_\alpha - D_\alpha(u)\nabla c_\alpha) = s_\alpha + r_\alpha, \quad (x,t) \in \Omega \times (0,T], \quad \alpha \in I_F, \quad (2.1)$$
$$\frac{\partial \phi_\alpha c_\alpha}{\partial t} = s_\alpha + r_\alpha, \quad (x,t) \in \Omega \times (0,T], \quad \alpha \in I_M, \quad (2.2)$$
where the unknown variables are \( c_\alpha \) (\( \alpha = 1, \ldots, N_S \)), the concentrations of all species (amount per volume). Here \( \phi_\alpha \) is the effective porosity (the product of porosity and the individual retardation factor) for the species \( \alpha \) and it is assumed to be time independent and uniformly bounded from above and below. \( D_\alpha(u) \) is the dispersion-diffusion tensor for the species \( \alpha \), and it is assumed to be uniformly symmetric positive definite and bounded from above. \( r_\alpha = r_\alpha(c_1, c_2, \ldots, c_{N_S}) \) is the reaction term for the species \( \alpha \), which will be described in the sequel. In (2.1), \( s_\alpha = q^* c_\alpha + s_\alpha, \) pure is the source term. The imposed external total flow rate \( q \) is a sum of sources (injection) and sinks (extraction). \( c_\alpha^* \) is the injected concentration \( c_{w,\alpha} \) if \( q > 0 \) and is the resident concentration \( c_\alpha \) if \( q \leq 0 \). In (2.2), the source term \( s_\alpha \) is simply the pure transport source \( s_\alpha, \) pure.

Equations (2.1) and (2.2) may be obtained from the mass conservation of each species. They govern the advection-diffusion-reaction process and predict the concentration profiles, provided the velocity field is given. It is parabolic but normally advection-dominated. We consider the following boundary conditions for this problem:

\[
\begin{align*}
(u c_\alpha - D_\alpha(u) \nabla c_\alpha) \cdot n_\partial \Omega &= c_{B,\alpha} u \cdot n_\partial \Omega, & \quad (x, t) &\in \Gamma_{in} \times (0, T], \quad \alpha \in I_F, \\
-D_\alpha(u) \nabla c_\alpha \cdot n_\partial \Omega &= 0, & \quad (x, t) &\in \Gamma_{out} \times (0, T], \quad \alpha \in I_F,
\end{align*}
\]

where \( c_{B,\alpha} \) is the inflow concentration for the species \( \alpha \). The initial concentrations are specified in the following way:

\[
c_{\alpha}(x, 0) = c_{0,\alpha}(x), \quad x \in \Omega, \quad \alpha \in I_M \cup I_F.
\]

### 2.2. Reaction Terms

We consider general multicomponent nonlinear reactions. The only assumption we make is that the reaction rates are locally Lipschitz continuous functions of concentrations. Most commonly used geochemical and biogeochemical reaction models satisfy this assumption. We remark that the strong assumption that reaction rates are (globally) Lipschitz continuous functions of concentrations as in [21, 31] has a limited usage in practice because, for example, any reaction of order greater than 1 is not Lipschitz continuous, but is locally Lipschitz continuous.

Let \( N_R \) be the number of total reactions. Note that we do not assume linear independence of the reaction set. Denote by \( \hat{r}_\beta \) (\( \beta = 1, 2, \ldots, N_R \)) the extent of reaction (or reaction coordinate) for the reaction \( \beta \). Let \( V \) be the associated stoichiometric matrix for the reaction system, i.e., \((V)_{ij}\) is the stoichiometric coefficient of the \( i^{th} \) species in the \( j^{th} \) reaction. Then, we have

\[
r = V \hat{r},
\]

where \( r = (r_1, r_2, \ldots, r_{N_S})^T \), \( \hat{r} = (\hat{r}_1, \hat{r}_2, \ldots, \hat{r}_{N_R})^T \). By the assumption that each term \( \hat{r}_\beta \) (\( \beta = 1, 2, \ldots, N_R \)) is a locally Lipschitz continuous function of \( (c_1, c_2, \ldots, c_{N_S}) \), it is easy to see that each \( r_\alpha \) (\( \alpha = 1, 2, \ldots, N_S \)) is also a locally Lipschitz continuous function of \( (c_1, c_2, \ldots, c_{N_S}) \).

**EXAMPLE.** To illustrate the above notations, we provide a simple example for the aqueous system consisting of \( \text{Ca}^{2+}, \text{H}^+, \text{OH}^-, \text{CO}_3^{2-}, \text{HCO}_3^-, \text{H}_2\text{CO}_3, \text{H}_2\text{O}, \text{Ca} \text{CO}_3(s) \) and with the following reactions.

\[
\begin{align*}
\text{CaCO}_3(s) &\rightleftharpoons \text{Ca}^{2+} + \text{CO}_3^{2-} & \hat{r}_1, \\
\text{HCO}_3^- &\rightleftharpoons \text{CO}_3^{2-} + \text{H}^+ & \hat{r}_2, \\
\text{H}_2\text{CO}_3 &\rightleftharpoons \text{CO}_3^{2-} + 2\text{H}^+ & \hat{r}_3, \\
\text{H}^+ + \text{OH}^- &\rightleftharpoons \text{H}_2\text{O} & \hat{r}_4.
\end{align*}
\]

Let the indices for the species of \( \text{Ca}^{2+}, \text{H}^+, \text{OH}^-, \text{CO}_3^{2-}, \text{HCO}_3^-, \text{H}_2\text{CO}_3, \text{H}_2\text{O}, \text{Ca} \text{CO}_3(s) \) be 1–8, respectively. We then have \( N_R = 4, N_S = 8, N_F = 7, N_M = 1, I_F = \{1, 2, 3, 4, 5, 6, 7\} \),
\[ I_M = \{8\}, \text{ and} \]
\[
\mathbf{r} = \begin{pmatrix}
  r_1 \\
  r_2 \\
  r_3 \\
  r_4 \\
  r_5 \\
  r_6 \\
  r_7 \\
  r_8 \\
\end{pmatrix} = \begin{pmatrix}
  1 & 0 & 0 & 0 \\
  0 & 1 & 2 & -1 \\
  0 & 0 & 0 & -1 \\
  1 & 1 & 1 & 0 \\
  0 & -1 & 0 & 0 \\
  0 & 0 & -1 & 0 \\
  0 & 0 & 0 & 1 \\
  -1 & 0 & 0 & 0 \\
\end{pmatrix} \begin{pmatrix}
  \hat{r}_1 \\
  \hat{r}_2 \\
  \hat{r}_3 \\
  \hat{r}_4 \\
\end{pmatrix} = \mathbf{V} \mathbf{r}.
\]

3. DISCONTINUOUS GALERKIN SCHEMES

3.1. Notations

Let \( \mathcal{E}_h \) be a family of nondegenerate and possibly nonconforming partitions of \( \Omega \) composed of linear segments if \( d = 1 \), triangles or quadrilaterals if \( d = 2 \), or tetrahedra, prisms, or hexahedra if \( d = 3 \). Here, \( h \) is the maximum element diameter for the mesh. The nondegeneracy requirement (also called regularity) is that the element is convex and that there exists \( \rho > 0 \) such that, if \( h_j \) is the diameter of \( E_j \in \mathcal{E}_h \), then each of the subtriangles (for \( d = 2 \)) or subtetrahedra (for \( d = 3 \)) of element \( E_j \) contains a ball of radius \( \rho h_j \) in its interior. We assume that no element crosses the boundaries \( \Gamma_{\text{in}} \) and \( \Gamma_{\text{out}} \). The set of all interior faces (faces are understood as points or edges in one or two spatial dimensions, respectively) for \( \mathcal{E}_h \) is denoted by \( \Gamma_h \). On each face \( \gamma \in \Gamma_h \), a unit normal vector \( \mathbf{n}_\gamma \) is chosen. The sets of all faces on \( \Gamma_{\text{out}} \) and on \( \Gamma_{\text{in}} \) for \( \mathcal{E}_h \) are denoted by \( \Gamma_{h,\text{out}} \) and \( \Gamma_{h,\text{in}} \), respectively, for which the normal vector \( \mathbf{n}_\gamma \) coincides with the outward unit normal vector.

For \( \omega \geq 0 \), we define

\[
H^\omega(\mathcal{E}_h) := \{ \phi \in L^2(\Omega) : \phi|_E \in H^\omega(E), E \in \mathcal{E}_h \}.
\]  

(3.1)

The discontinuous finite element space is taken to be

\[
\mathcal{D}_r(\mathcal{E}_h) := \{ \phi \in L^2(\Omega) : \phi|_E \in \mathcal{P}_r(E), E \in \mathcal{E}_h \},
\]  

(3.2)

where \( \mathcal{P}_r(E) \) denotes the space of polynomials of (total) degree less than or equal to \( r \) on \( E \). Note that, though the results in this paper are based on the complete polynomial space \( \mathcal{P}_r \), they may be easily extended to the tensor-product polynomial space \( Q_r \).

We now define the average and jump for \( \phi \in H^\omega(\mathcal{E}_h), \omega > 1/2 \). Let \( E_i, E_j \in \mathcal{E}_h \) and \( \gamma = \partial E_i \cap \partial E_j \in \Gamma_h \) with \( \mathbf{n}_\gamma \) exterior to \( E_i \). Denote

\[
\{ \phi \} := \frac{1}{2} \left( (\phi|_{E_i})|_\gamma + (\phi|_{E_j})|_\gamma \right),
\]  

(3.3)

\[
[\phi] := (\phi|_{E_i})|_\gamma - (\phi|_{E_j})|_\gamma.
\]  

(3.4)

Denote the upwind value of a concentration \( c \) as follows:

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

The usual Sobolev norm on a domain \( E \subset \Omega \) is denoted by \( \| \cdot \|_{m,E} \) [32]. The broken norms are defined, for \( m \geq 0 \), as

\[
\| \phi \|_{m,E}^2 := \sum_{E \in \mathcal{E}_h} \| \phi \|_{m,E}^2.
\]  

(3.5)
The inner product in \((L^2(E))^d\) or \(L^2(E)\) is indicated by \((\cdot, \cdot)_E\), and the inner product in the boundary function space \(L^2(\gamma)\) is denoted by \((\cdot, \cdot)_\gamma\). The inner product over the entire domain \((\cdot, \cdot)_\Omega\) is also written simply as \((\cdot, \cdot)\). We define a cut-off operator \(\mathcal{M}\) by

\[
(M(c))_\alpha(x) = \min(c_\alpha(x), M), \quad \forall \alpha,
\]

where \(M\) is a large positive constant. If concentrations are all nonnegative (as they are supposed to be physically), the definition of the cut-off operator \(\mathcal{M}\) may be also written as

\[
(M(c))_\alpha(x) = \min(c_\alpha(x), M), \quad \forall \alpha.
\]

### 3.2. Continuous-in-Time Schemes

For convenience of presentation, we write \(c = (c_1, c_2, \ldots, c_{N_s})^T\), and \(w = (w_1, w_2, \ldots, w_{N_s})^T\). We introduce the bilinear form \(B(c, w; u)\) as

\[
B(c, w; u) := \sum_{\alpha \in I_F} \left\{ \sum_{E \in \mathcal{E}_h} \int_E (D_\alpha(u) \nabla c_\alpha - c_\alpha u) \cdot \nabla w_\alpha + \int_\Omega c_\alpha q^- w_\alpha \\
- \sum_{\gamma \in \Gamma_h} \int_\gamma \{D_\alpha(u) \nabla c_\alpha \cdot n_\gamma\} [w_\alpha] - s_{\text{form}} \sum_{\gamma \in \Gamma_h} \int_\gamma \{D_\alpha(u) \nabla w_\alpha \cdot n_\gamma\} [c_\alpha] \right. \\
+ \sum_{\gamma \in \Gamma_{h, \text{int}}} \int_\gamma c^\alpha_u \cdot n_\gamma [w_\alpha] + \sum_{\gamma \in \Gamma_{h, \text{out}}} \int_\gamma c_\alpha u \cdot n_\gamma w_\alpha + J_0^\sigma(c_\alpha, w_\alpha) \left. \right\}.
\]

Here, \(s_{\text{form}} = -1, 0,\) or \(1\). In this paper, \(B(c, w; u)\) is also written as \(B_{NS}(c, w; u)\) when \(s_{\text{form}} = -1\). The injection source term \(q^+\) and the extraction part \(q^-\) are defined as usual

\[
q^+ := \max(q, 0), \quad q^- := \min(q, 0).
\]

The interior penalty term \(J_0^\sigma(c_\alpha, w_\alpha)\) is defined by

\[
J_0^\sigma(c_\alpha, w_\alpha) := \sum_{\gamma \in \Gamma_h} \frac{r^2 \sigma_{\gamma, \alpha}}{h_\gamma} \int_\gamma [c_\alpha] [w_\alpha],
\]

where \(\sigma\) is a discrete positive function that takes a constant value \(\sigma_{\gamma, \alpha}\) on the face \(\gamma\) for the species \(\alpha\). The linear functional \(L(w; u, c)\) is defined as

\[
L(w; u, c) := \sum_{\alpha \in I_F \cup I_M} \int_\Omega (s_{\text{pure, } \alpha} + r_\alpha (M(c))) w_\alpha \\
+ \sum_{\alpha \in I_F} \int_\Omega c_{w, \alpha} q^+ w_\alpha - \sum_{\alpha \in I_F} \sum_{\gamma \in \Gamma_{h, \text{in}}} \int_\gamma c_{B, \alpha} u \cdot n_\gamma w_\alpha.
\]

We give a weak formulation for the reactive transport problem.

**Lemma 3.1. Weak Formulation.** If \(c\) is a solution of (2.1)–(2.4) and \(c\) is essentially bounded, then \(c\) satisfies

\[
\sum_{\alpha \in I_F \cup I_M} \left( \frac{\partial c_\alpha}{\partial t}, w_\alpha \right) + B(c, w; u) = L(w; u, c), \\
\forall w \in (H^s(\mathcal{E}_h))^N, \quad s > \frac{3}{2}, \quad \forall t \in (0, T],
\]

provided that the constant \(M\) for the cut-off operator is sufficiently large.
Proof. Let \( w_\alpha \in H^s(\mathcal{E}_h) \), \( s > 3/2 \) for each \( \alpha \), and take \( E \in \mathcal{E}_h \). Multiplying equations (2.1) and (2.2) by \( w_\alpha |_E \), and integrating by parts, we have

\[
\left( \frac{\partial \phi_\alpha c_\alpha}{\partial t}, w_\alpha \right)_E - \int_E (u c_\alpha - D_\alpha(u) \nabla c_\alpha) \cdot \nabla w_\alpha + \int_{\partial E} (u c_\alpha - D_\alpha(u) \nabla c_\alpha) \cdot n_{\partial E} w_\alpha = \int_E s_\alpha w_\alpha + r_\alpha w_\alpha, \quad (x, t) \in \Omega \times (0, T], \quad \alpha \in I_F,
\]

\[
\left( \frac{\partial \phi_\alpha c_\alpha}{\partial t}, w_\alpha \right)_E = \int_E s_\alpha w_\alpha + r_\alpha w_\alpha, \quad (x, t) \in \Omega \times (0, T], \quad \alpha \in I_M.
\]

Summing over all elements in \( \mathcal{E}_h \) and over all species in \( I_M \cup I_F \), noting that the traces of each concentration and its normal flux are continuous across element interfaces, and applying the boundary conditions, we obtain the desired result. \( \blacksquare \)

The continuous-in-time DG approximation \( \textbf{C}^{DG}(\cdot, t) \in (\mathcal{D}_r(\mathcal{E}_h))^{N_s} \) of (2.1)–(2.5) is defined by

\[
\sum_{\alpha \in I_F \cup I_M} \left( \frac{\partial \phi_\alpha C^{DG}_\alpha}{\partial t}, w_\alpha \right) + B \left( \textbf{C}^{DG}, \textbf{w}; \textbf{u} \right) = L \left( \textbf{w}; \textbf{u}, \textbf{C}^{DG} \right),
\]

\[
\forall \textbf{w} \in (\mathcal{D}_r(\mathcal{E}_h))^{N_s}, \quad \forall t \in (0, T],
\]

(3.8)

\[
\sum_{\alpha \in I_F \cup I_M} \left( \phi_\alpha C^{DG}_\alpha, w_\alpha \right) = \sum_{\alpha \in I_F \cup I_M} \left( \phi_\alpha c_0, w_\alpha \right),
\]

\[
\forall \textbf{w} \in (\mathcal{D}_r(\mathcal{E}_h))^{N_s}, \quad t = 0.
\]

(3.9)

We note that OBB-DG (the Oden-Babuška-Baumann formulation of DG [14]) has \( s_{\text{form}} = -1 \) and \( \sigma_\gamma = 0 \) in the bilinear form; NIPG (the nonsymmetric interior penalty Galerkin method [17]) has \( s_{\text{form}} = -1 \) and \( \sigma_\gamma \geq 0 \); SIPG (the symmetric interior penalty Galerkin method [19,25,26]) has \( s_{\text{form}} = 1 \) and \( \sigma_\gamma > 0 \); and IIPG (the incomplete interior penalty Galerkin method [25,26,33]) has \( s_{\text{form}} = 0 \) and \( \sigma_\gamma > 0 \). A DG solution always exists for the multicomponent reactive transport system.

Lemma 3.2. Existence of Solution. The discontinuous Galerkin scheme (3.8),(3.9) has a unique solution for all \( t > 0 \).

Proof. Let \( \{v_i\}_{i=1}^{M_B} \) be a basis of \( (\mathcal{D}_r(\mathcal{E}_h))^{N_s} \) and write

\[
\textbf{C}^{DG} = \sum_{i=1}^{M_B} \zeta_i(t)v_i(x).
\]

Then (3.8) and (3.9) reduce to an initial value problem

\[
A \frac{d\zeta}{dt} = -B\zeta + R(\zeta),
\]

\[
A\zeta(0) = b,
\]

where the mass matrix \( A \) is block diagonal, symmetric, and positive definite. From the property of the cut-off operator \( \mathcal{M} \) (to be presented in Lemma 4.1) and the assumption of local Lipschitz continuity for the reaction functions, we know that \( R(\zeta) \) is (globally) Lipschitz continuous. It follows from the theory of ordinary differential equations that \( \zeta(t) \) exists and is unique for \( t > 0 \). \( \blacksquare \)

We emphasize the important feature of local mass conservation that holds for the four primal DG schemes.
Lemma 3.3. Local Mass Balance. The DG approximation of a concentration satisfies on each element $E$ the following local mass balance property:

$$
\int_E \frac{\partial \phi_\alpha}{\partial t} C^{DG}_\alpha - \int_{\partial E \setminus \partial I} \{ D_\alpha(u) \nabla C^{DG}_\alpha \cdot n_{\partial E} \} + \int_{\partial E \cap \Gamma_{h,\text{in}}} c_{B,\alpha} u \cdot n_{\partial E} \\
+ \int_{\partial E \cap \Gamma_{h,\text{out}}} C^{DG}_\alpha u \cdot n_{\partial E} + \int_{\partial E \cap \Gamma_{h}} C^{DG}_\alpha u \cdot n_{\partial E} \left( C^{DG}_\alpha \right)_{E} \\
+ \sum_{\gamma \in \partial E \cap \partial \Omega} \frac{\tau_{\gamma}}{h_{\gamma}} \int_{\gamma} \left( C^{DG}_\alpha \right)_{E} - \left( C^{DG}_\alpha \right)_{\Omega \setminus E} \\
= \int_E \left( C^{DG}_\alpha q^{-} + c_{w,\alpha} q^{+} \right) + \int_E \left( s_{\text{pure},\alpha} + r_{\alpha} (M(C^{DG})) \right),
$$

for each $\alpha \in I_F$; and

$$
\int_E \frac{\partial \phi_\alpha}{\partial t} C^{DG}_\alpha = \int_{\Omega} \left( s_{\text{pure},\alpha} + r_{\alpha} (M(C^{DG})) \right),
$$

for each $\alpha \in I_M$.

Proof. The desired mass balance relationships follow immediately from scheme (3.8) and (3.9) by fixing an element $E$ and a species $\alpha \in I_F \cup I_M$, and taking $w \in (D_r(E_h))^{N_S}$ with $w_{\alpha}|_E = 1$, $w_{\beta}|_{\Omega \setminus E} = 0$ and $w_{\beta} = 0$, $\forall \beta \neq \alpha$.

3.3. DG for a Special Case

If there is no immobile species, and the effective porosities and the dispersion-diffusion tensors are the same for all species, we may simplify the system of multicomponent transport equations by using the information of chemical stoichiometry. Under these assumptions, the transport equations become

$$
\frac{\partial \phi c_\alpha}{\partial t} + \nabla \cdot (u c_\alpha - D(u) \nabla c_\alpha) = s_\alpha + r_{\alpha}, \quad \alpha \in I_F.
$$

Writing $c = (c_1, c_2, \ldots, c_{N_S})^T$, $s = (s_1, s_2, \ldots, s_{N_S})^T$, and using the standard notation of $\nabla$ applied to $c$, we have

$$
\frac{\partial \phi c}{\partial t} + \nabla \cdot (u c - D(u) \nabla c) = s + r. \quad (3.10)
$$

Recall that $r = (r_1, r_2, \ldots, r_{N_S})^T$ is the source due to reactions. The extent of reaction is $\hat{r} = (\hat{r}_1, \hat{r}_2, \ldots, \hat{r}_{N_R})^T$. $V$ is the associated stoichiometric matrix for the reaction system, and $r = V\hat{r}$. It is always possible to perform a Gauss-Jordan reduction on $V$ to obtain a reduced form $V_r$, i.e.,

$$
V_r = \begin{pmatrix} I_{N_I \times N_I} & \hat{V} \\ 0 & 0 \end{pmatrix}
$$

and

$$
V = P^{-1}V_r,
$$

where $P$ is a nonsingular $N_S \times N_S$ matrix, $\hat{V}$ is an $N_I \times (N_R - N_I)$ matrix, and $N_I$ is the number of independent reactions.

Left-multiplying the matrix $P$ on both sides of (3.10), we have

$$
\frac{\partial \phi Pc}{\partial t} + \nabla \cdot (u (Pc) - D(u) \nabla (Pc)) = Ps + Pr.
$$

Noticing that

$$
Pr = PV\hat{r} = V_r\hat{r} = \begin{pmatrix} I_{N_I \times N_I} & \hat{V} \\ 0 & 0 \end{pmatrix} \hat{r},
$$
and using notations of $c^r = P_c$, $s^r = P_s$, we have the reduced form of the reactive transport equations.

$$\frac{\partial c^r}{\partial t} + \nabla \cdot (uc^r - D(u)\nabla c^r) = s^r + \left( I_{N_f \times N_f}^{N_f \times N_f} \hat{V} \right) \hat{r},$$

(3.11)

where $\hat{r}$ is a locally Lipschitz continuous function of $c^r$. Applying the DG scheme to the reduced equation (3.11), we have an improved DG algorithm for the multicomponent reactive transport system. In the new approach here, only $N_f$ equations are coupled due to reactions; the remaining ($N_S - N_f$) equations do not contain chemistry and can be solved independently. On the other hand, DG applied to the original equations needs a solution of $N_S$ coupled algebraic equations. Obviously, this reduced approach is more efficient, especially for the case where the number of species is much greater than the number of independent reactions.

4. A PRIORI ERROR ANALYSIS

4.1. Preliminaries

It is easy to show the following uniform Lipschitz continuity of the cut-off operator $M$.

**Lemma 4.1. Property of Operator $M$.** The cut-off operator $M$ defined in (3.6) is uniformly Lipschitz continuous with a Lipschitz constant of one; that is,

$$\|M(c) - M(w)\|_{L^\infty(\Omega)} \leq \|c - w\|_{L^\infty(\Omega)}.$$  

(4.1)

We shall use the following inverse inequalities, which can be derived using the method in [34]. Let $E \in \mathcal{E}_h$, $v \in P_r(E)$, and $h_E$ be the diameter of the element $E$. There exists a constant $K$, independent of $v$, $r$, and $h_E$, such that

$$\|D^q v\|_{0, \partial E} \leq K \frac{r}{h_E^{1/2}} \|D^q v\|_{0, E}, \quad q \geq 0,$$

$$\|D^{q+1} v\|_{0, E} \leq K \frac{r^q}{h_E} \|D^q v\|_{0, E}, \quad q \geq 0.$$  

(4.2)

The following $h^p$-approximation results, which can be proved using the techniques in [35,36], are useful for deriving error estimates of SIPG, IIPG, and NIPG. Let $E \in \mathcal{E}_h$ and $\psi \in H^\omega(E)$. There exists a constant $K$, independent of $\psi$, $r$, and $h_E$, and a sequence of $z^p_r \in P_r(E)$, $r = 1, 2, \ldots$, such that

$$\|\psi - z^h_r\|_{q, E} \leq K \frac{h_E^{\mu-q}}{r^{\omega-q}} \|\psi\|_{\omega, E}, \quad 0 \leq q < \mu,$$

$$\|\psi - z^h_r\|_{q, \partial E} \leq K \frac{h_E^{\mu-q-1/2}}{r^{\omega-q-1/2}} \|\psi\|_{\omega, E}, \quad 0 \leq q < \mu - \frac{1}{2},$$  

(4.3)

where $\mu = \min(r + 1, \omega)$. For error analysis of OBB-DG, we recall the approximation properties of a special interpolant in $\mathcal{D}_r(\mathcal{E}_h)$ [17] as follows.

**Lemma 4.2. Approximation Properties.** Let $\mathcal{E}_h$ consist of triangles, parallelograms ($d = 2$), or tetrahedra ($d = 3$). Let $c \in H^s(\mathcal{E}_h)$ for $s \geq 2$ and let $r \geq 2$. If, in addition, $D(u) \in (W^{1,\infty}(\mathcal{E}_h))^d \times d$, there exists an interpolant of $c$, $\hat{c} \in \mathcal{D}_r(\mathcal{E}_h)$, such that for each element $E \in \mathcal{E}_h$ and each face $\gamma$ of the element $E$

$$\int_{\gamma} D(u)\nabla (\hat{c}|_E - c) \cdot n_{\partial E} = 0,$$

where $n_{\partial E}$ is the outward vector unit normal to $\partial E$. Furthermore, $\hat{c}$ is optimally close to $c$,

$$\|\nabla^i (\hat{c}|_E - c)\|_{0, E} \leq K \frac{h_E^{\mu-i}}{r^{s-3/2-\delta}} \|c\|_{s, E}, \quad i = 0, 1, 2,$$

and

$$\|D(u)\nabla (\hat{c}|_E - c) \cdot n_{\partial E}\|_{L^2(\partial E)} \leq K \frac{h_E^{\mu-3/2}}{r^{s-3/2}} \|c\|_{s, E},$$

where $\delta = 0$ if $i = 0$ or 1, $\delta = 1/2$ if $i = 2$, $\mu = \min(r + 1, s)$, and $K$ is independent of $h_E$ and $r$. 

4.2. $L^2(H^1)$ and $L^\infty(L^2)$ Error Estimates

Throughout this section, we denote by $K$ a generic positive constant that is independent of $h$ and $r$, and by $c$ a fixed positive constant that can be chosen arbitrarily small.

**Theorem 4.3. Error Estimates for OBB-DG.** Let $\mathcal{E}_h$ consist of triangles, parallelograms ($d=2$), or tetrahedra ($d=3$). Let $\mathbf{c}$ be the solution to (2.1)–(2.5), and assume $c_\alpha \in L^2(0,T;H^s(\mathcal{E}_h))$, $\frac{\partial c_\alpha}{\partial t} \in L^2(0,T;H^s(\mathcal{E}_h))$, and $c_{0,\alpha} \in H^s(\mathcal{E}_h)$ for each $\alpha$. We further assume that $\mathbf{c}$, $\mathbf{u}$, and $q$ are essentially bounded, and that the reaction rates are locally Lipschitz continuous functions of $\mathbf{c}$. Let $\mathbf{C}^{DG}$ be the OBB-DG approximation of $\mathbf{c}$. If the constant $M$ for the cut-off operator is sufficiently large, then there exists a constant $K$, independent of $h$ and $r$, such that

$$
\sum_{\alpha \in I_F \cup I_M} \| C^{DG}_\alpha - c_\alpha \|_{L^\infty(0,T;L^2)} + \sum_{\alpha \in I_F} \left\| D_\alpha^{1/2} (\mathbf{u}) \nabla (C^{DG}_\alpha - c_\alpha) \right\|_{L^2(0,T;L^2)} \\
\leq K \frac{h^\mu}{r^{s-3/2}} \sum_{\alpha \in I_F \cup I_M} \left( \| c_\alpha \|_{L^2(0,T;H^s)} + \| \frac{\partial c_\alpha}{\partial t} \|_{L^2(0,T;H^s)} + \| c_{0,\alpha} \|_s \right) \\
+ K \frac{h^{\mu-1}}{r^{s-5/2}} \sum_{\alpha \in I_F} \| c_\alpha \|_{L^2(0,T;H^s)},
$$

where $r \geq 2$, $s \geq 3$, and $\mu = \min(r + 1, s)$.

**Proof.** Let $\hat{\mathbf{c}} = (\hat{c}_1, \hat{c}_2, \ldots, \hat{c}_N)^T$, where $\hat{c}_\alpha$ is the special interpolant of $c_\alpha$ as in Lemma 4.2 for each $\alpha$. Define

$$
\mathbf{E} = \mathbf{C}^{DG} - \mathbf{c},
$$

$$
\mathbf{E}^I = \mathbf{c} - \hat{\mathbf{c}},
$$

$$
\mathbf{E}^A = \mathbf{E}^I + \mathbf{E} = \mathbf{C}^{DG} - \hat{\mathbf{c}}.
$$

Subtracting (3.7) from (3.8), and choosing $\mathbf{w} = \mathbf{E}^A$, we have

$$
\sum_{\alpha \in I_F \cup I_M} \left( \frac{\partial \phi_\alpha E^A_\alpha}{\partial t} , E^A_\alpha \right) + B_{NS} (\mathbf{E}^A, \mathbf{E}^A; \mathbf{u}) \\
= L (\mathbf{E}^A; \mathbf{u}, \mathbf{C}^{DG}) - L (\mathbf{E}^A; \mathbf{u}, \mathbf{c}) + \sum_{\alpha \in I_F \cup I_M} \left( \frac{\partial \phi_\alpha E^I_\alpha}{\partial t} , E^A_\alpha \right) + B_{NS} (\mathbf{E}^I, \mathbf{E}^A; \mathbf{u}).
$$

(4.4)

The first term of (4.4) can be written as

$$
\sum_{\alpha \in I_F \cup I_M} \left( \frac{\partial \phi_\alpha E^A_\alpha}{\partial t} , E^A_\alpha \right) = \frac{1}{2} \sum_{\alpha \in I_F \cup I_M} \frac{d}{dt} \left\| \sqrt{\phi_\alpha} E^A_\alpha \right\|_{L^2(\Omega)}^2.
$$

The second term can be simplified by using the fact that the two diffusion terms on element interfaces cancel each other

$$
B_{NS} (\mathbf{E}^A, \mathbf{E}^A; \mathbf{u}) = \sum_{\alpha \in I_F} \left\{ \sum_{E \in \mathcal{E}_h} \int_E \left( D_\alpha (\mathbf{u}) \nabla E^A_\alpha - E^A_\alpha \mathbf{u} \right) \cdot \nabla E^A_\alpha - \int_\Omega q^- (E^A_\alpha)^2 \\
+ \sum_{\gamma \in \Gamma_h} \int_\gamma (E^A_\alpha)^* \mathbf{u} \cdot \mathbf{n}_\gamma \left[ E^A_\alpha \right] + \sum_{\gamma \in \Gamma_{h,\text{out}}} \int_\gamma \mathbf{u} \cdot \mathbf{n}_\gamma (E^A_\alpha)^2 \right\}.
$$
Integrating the advection term by parts and using the fact that $\nabla \cdot u = q$, we have

$$2 \sum_{E \in \mathcal{E}_h} \int_E E^A_\alpha u \cdot \nabla E^A_\alpha = \sum_{E \in \mathcal{E}_h} \int E \cdot \nabla (E^A_\alpha)^2$$

$$= \sum_{\gamma \in \Gamma_h} \int_{\gamma} u \cdot n_\gamma \left( (E^A_\alpha)^2 \right) + \sum_{\gamma \in \Gamma_{h, in} \cup \Gamma_{h, out}} \int_{\gamma} u \cdot n_\gamma (E^A_\alpha)^2$$

$$- \sum_{E \in \mathcal{E}_h} \int_E (E^A_\alpha)^2 q.$$ 

Noting that $[c^2] = 2\{c\} |c|$ and $(c^* - \{c\}) \text{sign}(u \cdot n_\gamma) = (1/2)\{c\}$, we obtain

$$B_{NS} (E^A, E^A; u) = \sum_{\alpha \in \mathcal{I}_F} \left\{ \sum_{E \in \mathcal{E}_h} \int_E \nabla E^A_\alpha \cdot \nabla E^A_\alpha + \frac{1}{2} \sum_{\gamma \in \Gamma_{h, in} \cup \Gamma_{h, out}} \int_{\gamma} \left| u \cdot n_\gamma \right| (E^A_\alpha)^2$$

$$+ \frac{1}{2} \sum_{\gamma \in \Gamma_h} \int_{\gamma} \left| E^A_\alpha \right|^2 + \frac{1}{2} \int_{\Omega} \left| q \right| (E^A_\alpha)^2 \right\}.$$ 

The first two terms on the right-hand side of (4.4) may be bounded using the property of the cut-off operator $\mathcal{M}$, the Cauchy-Schwarz inequality, and the approximation results.

$$L (E^A; u, C^{DG}) - L (E^A; u, c) = \sum_{\alpha \in \mathcal{I}_F \cup \mathcal{I}_M} \int_{\Omega} \left( r_{\alpha} (\mathcal{M} (C^{DG})) - r_{\alpha} (\mathcal{M} (c)) \right) E^A_\alpha$$

$$\leq K \sum_{\alpha \in \mathcal{I}_F \cup \mathcal{I}_M} \left\| \sqrt{\phi_{\alpha}} E^A_\alpha \right\|_{L^2(\Omega)}^2 + K \frac{h^{2\mu}}{r^{2s-3}} \sum_{\alpha \in \mathcal{I}_F \cup \mathcal{I}_M} \left\| c_{\alpha} \right\|^2_s.$$ 

We estimate the third term on the right-hand side of (4.4) using the Cauchy-Schwarz and approximation inequalities.

$$\sum_{\alpha \in \mathcal{I}_F \cup \mathcal{I}_M} \left( \frac{\partial \phi_{\alpha}}{\partial t} E^I_\alpha, E^A_\alpha \right) \leq \sum_{\alpha \in \mathcal{I}_F \cup \mathcal{I}_M} \left( K \left\| \sqrt{\phi_{\alpha}} E^A_\alpha \right\|_{L^2(\Omega)}^2 + K \frac{h^{2\mu}}{r^{2s-3}} \left\| \frac{\partial c_{\alpha}}{\partial t} \right\|^2_s \right).$$ 

The fourth term on the right-hand side of (4.4) contains seven pieces

$$B_{NS} (E^I, E^A; u) = \sum_{\alpha \in \mathcal{I}_F} \left\{ \sum_{E \in \mathcal{E}_h} \int_E \nabla E^I_\alpha \cdot \nabla E^A_\alpha - \sum_{E \in \mathcal{E}_h} \int_E E^I_\alpha u \cdot \nabla E^A_\alpha - \int_{\Omega} E^I_\alpha u \cdot \nabla E^A_\alpha$$

$$- \sum_{\gamma \in \Gamma_h} \int_{\gamma} \left( \nabla E^I_\alpha \cdot n_\gamma \right) \left[ E^A_\alpha \right] + \sum_{\gamma \in \Gamma_h} \int_{\gamma} \left( \nabla E^A_\alpha \cdot n_\gamma \right) \left[ E^I_\alpha \right]$$

$$+ \sum_{\gamma \in \Gamma_h} \int_{\gamma} E^I_\alpha u \cdot n_\gamma \left[ E^A_\alpha \right] + \sum_{\gamma \in \Gamma_{h, out}} \int_{\gamma} E^I_\alpha u \cdot n_\gamma E^A_\alpha \right\}$$

$$=: \sum_{\alpha \in \mathcal{I}_F} \sum_{i=1}^7 T_i.$$ 

We now proceed to estimate $T_i$, $i = 1, 2, \ldots, 7$. The terms $T_1$, $T_2$, and $T_3$ may be bounded using the Cauchy-Schwarz and approximation inequalities.

$$T_1 + T_2 \leq \epsilon \left\| D^{1/2} (u) \nabla E^A \right\|_0^2 + K \frac{h^{2\mu-2}}{r^{2s-3}} \left\| c_{\alpha} \right\|^2,$$

$$T_3 \leq \epsilon \int_{\Omega} \left| q \right|^2 (E^A_\alpha)^2 + K \frac{h^{2\mu}}{r^{2s-3}} \left\| c_{\alpha} \right\|^2.$$
The term $T_4$ may be bounded using the fact that the integrated diffusive flux for the interpolant error is zero on each face.

\[ T_4 = -\sum_{\gamma \in \Gamma_h} \int_{\gamma} \{ D_{\alpha}(u) \nabla E_{\alpha} \cdot n_{\gamma} \} \left( [E_{\alpha}] - a_\gamma \right) \]

\[ \leq \sum_{\gamma \in \Gamma_h} \| \{ D_{\alpha}(u) \nabla E_{\alpha}^I \cdot n_{\gamma} \} \|_{0,\gamma} \| [E_{\alpha}] - a_\gamma \|_{0,\gamma} \]

\[ \leq K \frac{h^{3/2}}{r^{3/2}} \| c_{\alpha} \|_s h^{1/2} \| D_{\alpha}^{1/2}(u) \nabla E_{\alpha} \|_0 \]

\[ \leq \epsilon \| D_{\alpha}^{1/2}(u) \nabla E_{\alpha} \|_0^2 + \frac{K h^{2/2}}{r^{2/2}} \| c_{\alpha} \|_s^2. \]

where $a_\gamma$ is a constant chosen by $a_\gamma = a_1 - a_2$, $a_i = \int_{E_i} E_{\alpha}^A \mid E_i \mid$, $i = 1, 2$, with $\gamma = \partial E_1 \cap \partial E_2$ and $n_{\gamma}$ exterior to $E_1$. The term $T_5$ is estimated by using the trace inverse inequality.

\[ T_5 \leq \sum_{\gamma \in \Gamma_h} \| \{ D_{\alpha}(u) \nabla E_{\alpha} \cdot n_{\gamma} \} \|_{0,\gamma} \| [E_{\alpha}] \|_{0,\gamma} \]

\[ \leq K rh^{-1/2} \| D_{\alpha}^{1/2}(u) \nabla E_{\alpha} \|_0 h^{1/2} \| c_{\alpha} \|_s \]

\[ \leq \epsilon \| D_{\alpha}^{1/2}(u) \nabla E_{\alpha} \|_0^2 + \frac{K h^{2/2}}{r^{2/2}} \| c_{\alpha} \|_s^2. \]

The terms $T_6$ and $T_7$ may be bounded simply by using the Cauchy-Schwarz and approximation inequalities.

\[ T_6 + T_7 \leq \epsilon \sum_{\gamma \in \Gamma_h} \int_{\gamma} |u \cdot n_{\gamma}| \left( [E_{\alpha}]^2 \right) + \epsilon \sum_{\gamma \in \Gamma_h} \int_{\gamma} |u \cdot n_{\gamma}| \left( [E_{\alpha}]^2 \right) + \frac{K h^{2/2}}{r^{2/2}} \| c_{\alpha} \|_s^2. \]

Substituting estimates back into (4.4), integrating the resultant inequality over the time interval $[0, T]$, choosing $\epsilon$ sufficiently small, and using the error bound at the initial time

\[ \| \sqrt{\phi_{\alpha} E_{\alpha}} \|_{L^2(\Omega)}(0) \leq K \frac{h^{2/2}}{r^{2/2}} \| c_{\alpha} \|_s^2, \]

we obtain

\[ \sum_{\alpha \in I_P \cup I_M} \left\{ \| \sqrt{\phi_{\alpha} E_{\alpha}} \|_{L^2(\Omega)}(t) + \sum_{\alpha \in I_P} \int_0^t \left\{ \sum_{E \in E_h} \int_E D(u) \nabla E_{\alpha} \cdot \nabla E_{\alpha} \right. \right. \]

\[ \left. + \sum_{\gamma \in \Gamma_h} \int_{\gamma} |u \cdot n_{\gamma}| \left( [E_{\alpha}]^2 \right) + \sum_{\gamma \in \Gamma_h} \int_{\gamma} |u \cdot n_{\gamma}| \left( [E_{\alpha}]^2 \right) + \int_\Omega |g| \left( [E_{\alpha}]^2 \right) \left. \right\} \right. \]

\[ \leq K h^{2/2} \left\{ \frac{1}{r^{2/2}} \| c_{\alpha} \|_s^2 + \frac{h^{2/2}}{r^{2/2}} \| \frac{\partial c_{\alpha}}{\partial t} \|_s^2 + \| \sqrt{\phi_{\alpha} E_{\alpha}} \|_{L^2(\Omega)}^2 \right\} \]

\[ + K \sum_{\alpha \in I_P} \int_0^t \left\{ \frac{h^{2/2}}{r^{2/2}} \| c_{\alpha} \|_s^2 + K \sum_{\alpha \in I_P \cup I_M} \frac{h^{2/2}}{r^{2/2}} \| c_{\alpha} \|_s^2. \right. \]

Applying Gronwall’s inequality, we conclude that

\[ \sum_{\alpha \in I_P \cup I_M} \left\{ \| \sqrt{\phi_{\alpha} E_{\alpha}} \|_{L^2(\Omega)}(0,T;L^2) + \sum_{\alpha \in I_P} \left\{ \| D_{\alpha}^{1/2}(u) \nabla E_{\alpha} \|_{L^2(0,T;L^2)} \right. \right. \]

\[ \leq K \frac{h^{2/2}}{r^{2/2}} \sum_{\alpha \in I_P} \left\{ \| c_{\alpha} \|_s + \| c_{\alpha} \|_{H^s(0,T;H^s)} + \left\| \frac{\partial c_{\alpha}}{\partial t} \right\|_{L^2(0,T;H^s)} \right. \right. \]

\[ + K \frac{h^{2/2}}{r^{2/2}} \sum_{\alpha \in I_P} \left\{ \| c_{\alpha} \|_{L^2(0,T;H^s)}. \right. \]
The theorem follows by the triangle inequality, the assumption that \( \phi_\alpha \) is uniformly bounded from below by a positive number, and the fact that
\[
\| \psi \|_{L^\infty(0,T;H^r)} \leq K \left( \left\| \frac{\partial \psi}{\partial t} \right\|_{L^2(0,T;H^r)} + \| \psi(\cdot,0) \|_\omega \right), \quad \forall \psi \in H^1(0,T;H^\omega(E_h)).
\]

REMARK. The above theorem gives only the \( L^\infty(L^2) \) error estimate for stationary species concentrations. Error bounds on \( L^2(H^1) \) for immobile species are unattainable because we do not have the smoothing effect of dispersion-diffusion for them. Also note that the \( L^\infty(L^2) \) error estimate for the stationary species concentrations is the best result we may obtain with respect to \( h \) in the sense that, if \( I_F = \phi \), the above theorem yields the following \( h \)-optimal result:
\[
\sum_{\alpha \in I_M} \| C_{\alpha}^{DG} - c_\alpha \|_{L^\infty(0,T;L^2)} \leq K \frac{h^\mu}{r^3-3/2} \sum_{\alpha \in I_M} \left( \| c_\alpha \|_{L^2(0,T;H^r)} + \left\| \frac{\partial c_\alpha}{\partial t} \right\|_{L^2(0,T;H^r)} + \| c_0,\alpha \|_\star \right).
\]

We comment that, using the same approach as above for treating multicomponent systems, we can also extend the \textit{a priori} error estimation results of SIPG, NIPG, and IIPG for a single-species transport \cite{26} to multicomponent systems, which are omitted in this paper for brevity. Due to the penalty terms, the special interpolant in \( D_r(E_h) \) is not necessary to establish error bounds for SIPG, NIPG, and IIPG, and it may be replaced by the standard \( hp \)-optimal interpolant (4.3), which yields sharper estimates in \( p \) and is applicable to more element types.

The reader is referred to references \cite{22,37} for computational examples of two-species systems and \cite{27,29,38} for numerical performance and implementation issues on DG’s adaptivities.

5. SUMMARY

Four primal discontinuous Galerkin schemes, i.e., OBB-DG, NIPG, SIPG, and IIPG, have been formulated for solving multicomponent reactive transport with a single flowing phase and possibly multiple stationary phases in porous media. A cut-off operator has been introduced in the discontinuous Galerkin schemes to ensure convergence for general nonlinear kinetic chemistry. Using the information of chemical stoichiometry, an efficient approach has been proposed for a special case without immobile species. Error estimates in the \( L^2(H^1) \) norm for concentrations have been derived for the OBB-DG scheme, which are optimal in \( h \) and nearly optimal in \( p \). For conciseness, we have only presented the error analysis of OBB-DG. However, the analysis with multicomponent transport systems can be extended to SIPG, IIPG, and NIPG.

As an interesting future work, we plan to study the primal DG methods for multicomponent transport with mixed kinetic and local-equilibrium reactions and for the transport coupled with multiphase flow in porous media. In addition to the theoretical analysis on DGs, we are also pursuing numerical investigation of primal DG methods for various multiphase multicomponent transport systems.

REFERENCES

