Combined RKDG and LDG Method for the Simulation of the Bipolar Charge Transport in Solid Dielectrics

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Abstract—The space charge transport described by the convection-reaction equations is simulated by using the Runge-Kutta discontinuous Galerkin (RKDG) method. Compared to the traditional finite volume method, the RKDG method has higher accuracy and better performance of capturing the steep front in the charge profile. Combined with the RKDG method, the local discontinuous Galerkin (LDG) method was adopted to solve the Poisson’s equation instead of the previous boundary element method (BEM), in order that the numerical quadrature for the solution of the convection-reaction equations is replaced by analytical formulas. The bipolar charge transport under dc voltage is simulated by the RKDG+LDG method, which is more efficient and produces identical results with those of the RKDG+BEM method.

1. INTRODUCTION

The space charge dynamics plays an important role on the degradation and the breakdown of solid dielectrics under the high voltage due to the intensification of the local electric field. The transport of the different species of space charges under the electric field can be described by a set of convection-reaction equations coupled with the Poisson’s equation. In our previous work, the RKDG method was utilized to solve the convection-reaction equations [1]. Unlike the traditional QUICKEST method with the ULTIMATE flux limiter [2, 3], the RKDG method can handle the convection and the reaction terms simultaneously without incorporating the split procedure [4], and the high-order accuracy can be obtained without incorporating a wide stencil, which is more suitable for the shock capturing than the QUICKEST method [5].

For the solution of the Poisson’s equation, the local discontinuous Galerkin (LDG) method proposed by B. Cockburn et al. [5, 6] is adopted in this paper instead of the generally used boundary element method (BEM) [7], in order to replace the numerical quadrature with analytical formulas in the RKDG weak formulation of the convection-reaction equations. This combined RKDG+LDG method is verified by the simulation of the space charge transport in a low-density polyethylene (LDPE) sample under high dc voltage. The results show that the proposed method is more efficient and produces identical space charge profiles with those of the RKDG+BEM method.

2. MATHEMATICAL MODEL DESCRIPTIONS

The fluid model for the space charge transport in this paper was initially proposed by Alison and Hill [8]. It has already been widely adopted by Le Roy and Belgaroui et al. in [2, 3, 7]. The model is given as follows:

\[
\frac{\partial n_a}{\partial t} + \frac{\partial f_a}{\partial x} = S_a \quad \text{(convection-reaction equation)},
\]

\[
\frac{\partial E}{\partial x} = \frac{\rho_{all}}{\varepsilon_0 \varepsilon_r} \quad \text{(Poisson’s equation)},
\]

\[
f_a = \pm \mu_a n_a E \quad \text{(transport equation)},
\]

where \(n_a\) is the number of carriers per unit volume and the subscript \(a\) represents different carrier types. Usually, four species of carriers are taken into account to describe the charge dynamics in solid dielectrics, i.e., free electrons and holes, which represent the carriers in the shallow traps; trapped electrons and holes, which represent the immobile carriers residing in the deep traps. The source term \(S_a\) in (1) comprises the effects of trapping and recombination. Both the source term \(S_a\) and the gradient of the carrier convection flux \(f_a\) contribute to the variation of the carrier concentration according to (1). At the electrodes, the inlet boundary condition, i.e., carrier injection, for the convection-reaction equation is usually prescribed as the Schottky injection law, while the Ohm’s law is adopted as the outlet boundary condition, i.e., carrier extraction. For the definitions and the physical meanings of the model parameters, readers may refer to [1, 3, 7, 8] for details.
3. RKDG METHOD FOR CONVECTION-REACTION EQUATION

The authors of [3, 7] used the QUICKEST method with the ULTIMATE flux limiter to solve the convection-reaction Equation (1). However, it cannot accurately simulate the space charge profile with very steep wavefront, i.e., shock wave, due to that a wide stencil is adopted to interpolate the numerical flux. Moreover, the split treatment of the originally coupled convection and reaction terms brings additional errors [1].

In our previous work [1], the RKDG method was applied to the convection-reaction equation, in which the high-order piecewise continuous Legendre polynomials were chosen as the basis functions to expand the space charge profile. A special Runge-Kutta method combined with a slope limiter was used for the time discretization, which ensures the numerical stability. The source term \( S_a \) and the convection term \( \partial f_a / \partial x \) were handled simultaneously by the RKDG method without the split procedure. High-order accuracy can be obtained without incorporating a wide stencil, which is more suitable for the shock capturing than the QUICKEST method.

The basic steps of the RKDG method are as follows:

1. Discontinuous Galerkin (DG) space discretization: The carrier concentration \( n_a \) of the \( j \)-th element \( I_j = (x_{j-\frac{1}{2}}, x_{j+\frac{1}{2}}) \) can be approximated by the Legendre polynomials \( \{P_l(x)\}_{l=0, \ldots, k} \) as:

\[
n_a = \sum_{l=0}^{k} a_l P_l \left( \frac{2(x - x_j)}{\Delta_j} \right),
\]

where \( l \) is the order of the polynomial and \( \Delta_j \) is the length of \( I_j \). By taking \( \{P_l(x)\}_{l=0, \ldots, k} \) as the weighting functions, the convection-reaction Equation (1) can be weakly enforced. After the simplification by utilizing the orthogonality of the Legendre polynomials, the semi-discrete form of the convection-reaction equation can be obtained:

\[
\frac{d}{dt} a_j(t) = \frac{2l+1}{\Delta_j} \left( \frac{2}{\Delta_j} \int_{I_j} f_a P_l' \left( \frac{2(x - x_j)}{\Delta_j} \right) dx \right. \\
- \left. \int_{I_j} S_a \left( \frac{2(x - x_j)}{\Delta_j} \right) \right) + \int_{I_j} S_a P_l \left( \frac{2(x - x_j)}{\Delta_j} \right) dx,
\]

where \( \hat{f}_a \) is the numerical flux.

2. Numerical flux: The Lax-Friedrichs numerical flux was adopted in the RKDG method according to [9]. For the right boundary of the \( j \)-th element, it is given as:

\[
\hat{f}_{a_j+1/2}(n_{a_j+1/2}^-, n_{a_j+1/2}^+) = \frac{1}{2} \left[ f_a(n_{a_j+1/2}^-) + f_a(n_{a_j+1/2}^+) - C(n_{a_j+1/2}^+ - n_{a_j+1/2}^-) \right],
\]

where

\[
C = \max_x |v_a(t = 0, x)|,
\]

\( n_{a_j+1/2}^- \) and \( n_{a_j+1/2}^+ \) are the left and right limit values of \( n_a \) at \( x_{j+\frac{1}{2}} \), \( v_a(t = 0) \) is the initial carrier speed.

3. RK time discretization: According to [9], the RK time discretization should be performed in \( k+1 \) intermediate steps to match the accuracy degree of the space domain. With the charge distribution \( n_a^m \) at the time point \( m\Delta t \), the RK time stepping is as follows:

(a) Set \( n_a^{(0)} = n_a^m \);

(b) For the \( s \) intermediate steps \( (s = 1, \ldots, k + 1) \):

\[
n_a^{(s)} = \Delta t \left( \sum_{l=0}^{s-1} \alpha_s l \omega^s \right),
\]
where

$$\omega^{sl} = n_a^{(l)} + \frac{\beta_{sl}}{\alpha_{sl}} \Delta t L_j \{n_a^{(l)}\},$$  \hspace{1cm} (9)$$

$L_j \{n_a^{(l)}\}$ represents the right-hand side of (5). All is a slope limiter proposed by Biswas et al., which ensures the numerical stability of the RKDG method [10]. The determination of the coefficients $\alpha_{sl}$ and $\beta_{sl}$ is introduced by Gottlieb et al. in [11].

(c) Set $n_a^{m+1} = n_a^{(k+1)}$.

4. LDG METHOD COMBINED WITH RKDG METHOD

The purpose of adopting the LDG method for the solution of the Poisson’s equation is to promote the efficiency of the RKDG method by analytically evaluating the integrals instead of the numerical quadrature.

In the RKDG semi-discrete formulation of the convection-reaction Equation (5), there exists the integrand which is the product of the carrier concentration $n_a$ and the electric field $E$:

$$\int_{I_j} f_s P'_l \left( \frac{2(x - x_j)}{\Delta_j} \right) \, dx = \int_{I_j} \pm \mu_a n_a E P'_l \left( \frac{2(x - x_j)}{\Delta_j} \right) \, dx. \hspace{1cm} (10)$$

If the electric field $E$ is solved by the BEM, this integral should be evaluated by numerical methods, such as the Gauss-Legendre quadrature. However, for the combined RKDG+LDG method, the Legendre polynomials are selected as the basis functions for both the carrier concentration $n_a$ and the electric field $E$. This fact enables us to analytically calculate the above integral.

4.1. LDG Method for Poisson’s Equation

For the one-dimensional Poisson’s equation defined in domain $\Omega$ with the first kind condition on the domain boundary $\Gamma_D$:

$$- \frac{dq}{dx} = f \quad \text{in} \ \Omega, \hspace{1cm} (11)$$

$$q = -E = \frac{du}{dx}, \hspace{1cm} u = g_D \quad \text{on} \ \Gamma_D,$$

its weak solution satisfies the following two equations:

$$\int_{I_j} qr \, dx = ru \mid_{x_j - \frac{1}{2}}^{x_j + \frac{1}{2}} - \int_{I_j} u \frac{dr}{dx} \, dx, \hspace{1cm} (12)$$

$$\int_{I_j} q \frac{dv}{dx} \, dx = \int_{I_j} f v \, dx + vq \mid_{x_j - \frac{1}{2}}^{x_j + \frac{1}{2}}, \hspace{1cm} (13)$$

where $r$ and $v$ belongs to the space of Legendre polynomials defined on $I_j$ with the degree at most $k$, i.e., $r, v \in P^k(I_j) = \{P^k(x) : l = 0, \ldots, k\}$.

The numerical flux $\hat{u}$ in (12) and $\hat{q}$ in (13) are defined as:

$$\begin{pmatrix} \hat{q} \\ \hat{u} \end{pmatrix} = \begin{pmatrix} q \\ u \end{pmatrix} + \begin{pmatrix} C_{11} \\ -C_{12} \end{pmatrix} \begin{pmatrix} u \\ q \end{pmatrix} \quad \text{in} \ \Omega, \hspace{1cm} (14)$$

$$\begin{pmatrix} \hat{q} \\ \hat{u} \end{pmatrix} = \begin{pmatrix} q^+ - C_{11}(u^+ - g_D)n \\ g_D \end{pmatrix} \quad \text{on} \ \Gamma_D, \quad n = \begin{pmatrix} -1 \\ 1 \end{pmatrix} \quad \text{left boundary right boundary}, \hspace{1cm} (15)$$

where $C_{11} = C_{22} = \frac{1}{2}, C_{12} = C_{21} = 0, \{q\} = \frac{1}{2}(q^+_{j+\frac{1}{2}} + q^-_{j+\frac{1}{2}}), \{q\} = q^+_{j+\frac{1}{2}} - q^-_{j+\frac{1}{2}}$. $\{u\}$ and $[u]$ adopt the similar definitions as $\{q\}$ and $[q]$.

By expanding $u$ and its gradient $q$ with Legendre polynomials, all the coefficients of the basis functions can be obtained by solving (12) and (13).
4.2. Analytical Evaluation of the Integral

In the RKDG+LDG method, both the charge density $n_a$ and the electric field $E$ are expanded by the Legendre polynomials with the form as in (4). Therefore, the integral in (10) can be directly given by analytical formulas. Take the Legendre polynomial space $P_k(I_j)$ where $k = 1$ and $k = 2$ as example, the analytical solution of the integral can be given as:

$$\int_{I_j} \pm \mu_a n_a E P_l\left(\frac{2(x - x_j)}{\Delta_j}\right) \, dx = \begin{cases} 0 & l = 0 \quad \text{(for } k = 1), \\ \pm \mu_a \left(2a_0b_0 + \frac{2}{3}a_1b_1\right) & l = 1 \quad \text{(for } k = 2), \\ \pm \mu_a \left(2a_0b_1 + 2a_1b_0 + \frac{2}{3}a_1b_2 + \frac{2}{5}a_2b_1\right) & l = 2 \end{cases}$$

where $\{b_l\}_{l \geq 0}$ represent the coefficients of the Legendre polynomials for $E$.

The above analytical formulas are flexible and can be applied to various situations, due to that they are derived from the integration with respect to the product of the Legendre polynomial series which are used to approximate the arbitrary distribution of the electric field and the carrier density.

5. RESULTS AND COMPARISONS

A 118 $\mu$m LDPE sample under external dc voltage 12 kV is used as a test model for the bipolar charge transport. The adopted parameter values are the same as those in [3]. To verify the combined RKDG+LDG method with different basis function orders $k = 1$ and $k = 2$, its simulation results at $t = 20, 30, 50, 100$ s are compared with those obtained from the RKDG+BEM method. In the implementation of the RKDG+BEM method, five-point Gauss-Legendre numerical quadrature was adopted in each spacial element in. The relative errors of the electric field and the net charge density are given in Table 1. The relative errors are defined as follows:

$$\varepsilon_E = \frac{\|E_{\text{BEM}} - E_{\text{LDG}}\|_2}{\|E_{\text{BEM}}\|_2}, \quad \varepsilon_{\rho_{\text{all}}} = \frac{\|\rho_{\text{all/BE}} - \rho_{\text{all/LD}}\|_2}{\|\rho_{\text{all/BE}}\|_2}$$

It can be seen from these data that for the case $k = 1$, the RKDG+LDG method produces almost identical results as those of the RKDG+BEM method. For $k = 2$, the relative error of the electric field is still very small. Although the relative error of the net charge density increases to about 1%, the simulated charge profiles of the two methods are still very close to each other (see Figure 1). Moreover, by using the RKDG+LDG method, all of the numerical quadratures implemented in the RKDG+BEM method are replaced by analytical solutions, which saves 40% of the computation time. From our numerical tests, the difference in the computation time between the BEM and the LDG method for solving the Poisson’s equation is negligible and the increased efficiency of the RKDG+LDG method is mainly due to replacing the numerical quadratures by analytical formulas in the solution of the convection-reaction equation. Therefore, the combined RKDG+LDG method is verified and shows to be more efficient than the RKDG+BEM method.

![Figure 1: Comparison of the simulated space charge profiles by using the 2nd order RKDG+LDG and RKDG+BEM methods.](image)
Table 1: Relative errors of the electric field and the net charge density by using the RKDG+BEM and the RKDG+LDG methods.

<table>
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<th>Times(s)</th>
<th>$\varepsilon_E (k = 1)$</th>
<th>$\varepsilon_E (k = 2)$</th>
<th>$\varepsilon_{\rho_{all}} (k = 1)$</th>
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6. CONCLUSIONS

The combined RKDG and LDG method proposed in this paper has high-order accuracy and is suitable for simulating the space charge transport with steep fronts. Both the RKDG and the LDG methods are based upon the discontinuous Galerkin space discretization with the Legendre polynomials as the basis functions, which enables us to replace the numerical quadratures in the RKDG+BEM method with analytical formulas. The RKDG+LDG method is verified by the simulation of the bipolar charge transport in an LDPE sample, which produces identical results with those of the RKDG+BEM method. Due to the employment of the analytical integral, the RKDG+LDG method can promote the efficiency of the numerical scheme by saving 40% of the computation time that needed by the RKDG+BEM method.

ACKNOWLEDGMENT

This work is supported by the National Natural Science Foundation of China (50437030).

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