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# Introduction of charge transport simulation models that fully consider the ionization process

Yifei He, *Student Member, IEEE*, Kai Wu, *Senior Member, IEEE*, Yang Wu, Chunyang Zhang, Zepeng Lv, *Member, IEEE*, and Davide Fabiani, *Senior Member, IEEE*

**Abstract**—Bipolar carrier models for charge transport simulation in polymers have been developed for several years, but rarely consider the effect of ionization charges inside the polymer. In this report, based on the measurement results of actual ionization charges transport by blocking electrode injection, a modified bipolar carrier transport model is proposed, in which the influence of ionization charge is also considered. The model takes into account the recombination between the ionization charges and the injected carriers as well as the secondary ionization of the recombination products and develops a bipolar carrier transport model that fully considers the influence of the ionization charges. For practical engineering purposes, some simplifications are made to the precision model obtaining an approximated engineering model that can be more simply directly used. At the same time, the criterion of whether the engineering model can be used to replace the precision model is given. This work fills a crucial gap in the existing bipolar carrier transport model.

**Index Terms**—bipolar transport, mobility, conductivity of ionization charges, precision model, engineering model

## I. INTRODUCTION

High-voltage direct current (HVDC) transmission technology is widely used in modern power systems because of its advantages of low loss and low interference. High-voltage direct current cables represented by polyethylene cables are also widely used. The safe and reliable operation of the cable is related to the stability of the system, but the accumulation of space charges under DC voltage may cause serious electric field damage to the cable structure. For weak parts such as connector accessories, the distortion of the electric field may be more serious [1,2]. Therefore, at the beginning of the HVDC cable design, the field strength difference of the overall cable structure can be calculated in advance through model simulation, which can effectively find the field strength distortion point, which is of great help to the optimization of the cable structure design [3]. It is also of great benefit to the subsequent safe and reliable operation of the entire power system.

Since Alison proposed the bipolar carrier transport model for charge transport simulation in 1994, the numerical simulation technology has made great progress [4]. These models can be roughly divided into two categories [5]. One is an engineering model based on the conductivity gradient, and the other is a precision model that considers the series of transport processes such as carrier injection, transport, trapping, de-trapping, and extraction in detail. The engineering model directly fits the electrical conduction current measurement results of the material and simulates the space charge by setting the temperature gradient to generate the electrical conductivity gradient, and further calculates the electric field [6-8]. Such simulation is closer to the actual situation of engineering applications, while the calculation is convenient and easy to use. However, the existing engineering model cannot distinguish between the charge generated by the difference in conductivity and the charge injected from the electrode [9]. At the same time, because the extraction at the electrode is not considered, it is difficult to calculate the heterocharge in the simulation, being this latter is crucial for the reliability of the insulation system. The precision model fully considers the various charge transport carriers considering the entire physical process of charge transport in the insulation bulk [10-12]. Therefore, the simulation results and the experimental results are in good agreement. However, it is difficult to directly measure the correlation coefficients of physical processes such as trapping, de-trapping, and extraction through accurate experiments [13]. Therefore, a large number of empirical parameters are used in the simulation. The accuracy of these parameters directly affects the final simulation results, but cannot be verified, so it is difficult to directly use them in engineering. The most important point is that no matter whether it is an engineering model or a precision model, there is an extreme lack of discussion about the effect of ionization charges on charge transport [14]. The ionization charges are non-negligible part of the carriers, which have a direct effect on the electric field distribution, but it is difficult to accurately distinguish them from the charges injected from the electrode,

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and calculate the magnitude of the conductivity of ionization charges. There are relatively few simulation studies on ionization charges. Roy's team set the initial ion concentration and ion mobility to a fixed value for simulation and compared the charge distribution when the ionization charges are considered or not [15,16]. It was found that the bulk current increased, and the accumulation of ionization charges boosted the injection at the electrode. However, the model only allows positive or negative ions to move at the same time, which may limit the applicability of the model. Yin Yi's team first classified the impurities into A-type and B-type according to whether the impurity ionized holes or electrons, and then compared the simulation and experiment to determine the main impurity components in different materials [17,18]. However, the expression of the ionization charges current in the simulation introduces many new empirical parameters, and the recombination process between carriers is not discussed in detail at the same time. Other scholars have made significant contributions to simulating ionization charges as well. For instance, Zheng utilized modified model calculations to determine that ionization charges are the primary source of hetero-charge accumulation in polypropylene [19]. Zhan conducted a detailed analysis of the calculation method for ionization charges concentration using the Onsager mechanism and simulated charge distribution in XLPE accordingly [20].

In summary, the charge transport process is highly complex and involves ionization, injection, and their interactions, which depend on many parameters. However, it is difficult to determine the value of all these parameters. In the previous experimental work [21,22], our method can successfully separate the injected part and the ionized part of the carriers. This provides another approach to simplify the calculation model for engineering applications relying on the parameters which can be measured.

In this paper, we will describe two numerical models, one more detailed, called precision model, that fully considers the impact of ionization charges on charge transport, and another, slightly simplified, called engineering model, obtained from the precision model. We respectively fitted the experimental expressions of mobility and conductivity of ionization charges as a function of field strength, fully considered the recombination and secondary ionization processes between electrons/holes and ions, and established a new precision model. At the same time, for engineering practical purposes, we have simplified some procedures, so that the model can be used for engineering without significant loss of accuracy. At the same time, we propose new criteria to determine under which conditions the simplification of the engineering model is valid and under which conditions it may fail.

## II. MODEL DESCRIPTION

### A. Basic settings in two new models

Both new models are based on the original bipolar carrier transport model [4]. The expression used to calculate the charge transport of each carrier is as follows:

$$\begin{cases} \frac{\partial n_a(x,t)}{\partial t} + \frac{\partial f_a(x,t)}{\partial x} = S_a(x,t) \end{cases} \quad (1)$$

$$\begin{cases} \frac{\partial E(x,t)}{\partial x} = \frac{\rho_{all}(x,t)}{\epsilon_0 \epsilon_r} \end{cases} \quad (2)$$

$$f_a(x,t) = \pm(\mu_a(x,t)n_a(x,t)E(x,t) - D_f \frac{dn_a(x,t)}{dx}) \quad (3)$$

where  $a$  represents different types of carriers, including electrons, holes, and positive and negative ions.  $n$  is the charge density and  $f$  is the current density.  $\epsilon_r$  is the relative permittivity.  $\mu$  is the mobility of different carriers and  $S$  is the source term. In traditional method, only the injected charges are considered and the source term contains the progress of trapping, detrapping, and recombination. For injected electrons,  $S$  can be calculated as:

$$S_{eu} = -eS_{e\mu,ht}n_{em}n_{ht} - Be\epsilon n_{e\mu}(1 - \frac{en_{et}}{N_e}) + v \exp(\frac{-eW_{et}}{k_b T})n_{et} \quad (4)$$

where  $S_{eu,ht}$  represents the combination coefficient between the injected electrons and the trapped holes,  $Be$  represents the trapping coefficient,  $N_e$  represents the density of traps available to trap electrons,  $n_{et}$  represents the density of electrons in those traps,  $W_{et}$  represents the trap depth of electrons, and  $v$  is the escape frequency.

During the production of polymer bases such as polyethylene and ethylene propylene rubber, impurities are introduced into the polymers due to cleanliness issues during production, packaging, storage, and transportation. The impurity molecules, when subjected to electrothermal action, may undergo the following three changes: dissociation into a positive and a negative ion; ionization of an electron as well as a positive ion; and ionization of a hole as well as a negative ion. The positive ions, negative ions, electrons, and holes produced in this process are involved in the charge transport process and contribute to the bulk current inside the polymer. In fact, from the results of the blocking experiments, it can be seen that the conductivity of the charges generated during the ionization process is close to that of the injected charges[21], and it is generally believed that the ions are large and slow-moving, so it can be judged that the charge generated during the ionization process is still mainly electrons and holes. Based on this we believe that we cannot use the simple term 'ionic current' to characterize the current generated by the charges produced during ionization, since this part of the charges include both ions and electrons and holes. Here we make the statement that the term 'ionization charges' is used in the text to denote the collection of positive ions, negative ions, electrons, and holes produced during the ionization process, the term 'ionization charges current' is used to denote the current produced by the movement of these charges and the term 'conductivity of ionization charges' is used to denote the conductivity of these charges.

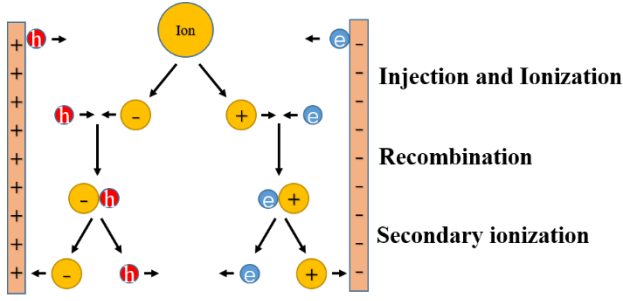


Fig. 1. Schematic diagram of the charge transport process after considering the effect of ionization charges

As shown in Figure 1, the specific behavior of ionization charges in the charge transport process is as follows: dissociable molecules are in a state of chemical equilibrium, and these ions are tightly bound together by Coulomb attraction and need to overcome the energy barrier to separate within the polymer matrix. The electric field helps to separate the ions and counterions, and this process is defined as the ionization process. The dissociated ions move towards the electrode with opposite polarity under the influence of the electric field, and during this process, they may recombine with injected electrons and holes. The neutral molecules formed after recombination can undergo secondary ionization under higher energy excitation, re-dissociating into positive ions and electrons or negative ions and holes. To establish a charge transport model that takes into account the influence of ionization charges, it is necessary to quantitatively characterize all the processes described above.

It is worth mentioning that in the previous study [23,24], we accurately measured the functional relationship between apparent mobility and field strength, which can be directly used in simulation calculations. The apparent mobility calculation captures the macroscopic process of carrier movement within insulating materials. When fitting mobility results using the hopping conductivity equation, the average distance of carrier hopping and the average energy required are determined. The equation considered for mobility is the following [25]:

$$\mu = \left( \frac{2\lambda v}{E} \right) \exp\left(-\frac{\Delta}{kT}\right) \sinh\left(\frac{eE\lambda}{2kT}\right) \quad (5)$$

where  $\lambda$  denotes the electron/hole leap distance and  $\Delta$  denotes the energy required for the leap.

As such, the source term  $S$  only takes into account the recombination process, while trapping and de-trapping processes are considered in the calculation of apparent mobility. Corresponding to Eq. 4, all terms related to  $n_{et}$  and  $W_{et}$  should no longer be considered. The calculation of the source term  $S$  at this point is simplified as:

$$S_{eq} = -eS_{e,h}n_{em}n_{ht} \quad (6)$$

The focus here is on the treatment of the ionization charges part. The first is the determination of the initial ionization charges concentration. We believe that the initial concentration of ionization charges should be a dynamically balanced value and is directly related to the electric field value in the region. The process of ionization equilibrium is illustrated with the help

of Fig. 2. In each mesh cell of the computational process, if the number of ionization charges is greater than this initial value, no processing is done; if the number of ionization charges is less than this initial value, continue ionization to this initial value. At the same time, an ionization barrier is introduced when calculating the initial value, so that the initial value of ionization is related to the field strength. The expression for calculating the initial value of the ionization charges is as follows:

$$\frac{dn_{ion+}}{dt} = \frac{dn_{ion-}}{dt} = N_0 v_0 \exp\left(-\frac{eW_{dis} - \sqrt{\frac{e^3 E}{\pi\epsilon}}}{kT}\right) \quad (7)$$

where  $N_0$  represents the total amount of material that can be ionized in the steady state.  $v_0$  is a constant, and its value is equal to  $kT/h$ .  $W_{dis}$  is the ionization barrier.  $k$  is Boltzmann's constant and  $h$  is Planck's constant.

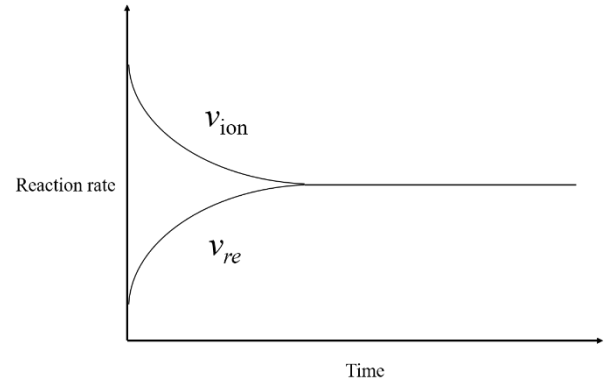


Fig. 2. Diagram of ionization equilibrium,  $v_{ion}$  represents the rate of molecular ionization into positive and negative ionization charges, while  $v_{re}$  represents the rate of recombination of positive and negative ionization charges to form neutral molecules.

Regarding the ionization charges migration process, in previous studies, we designed a blocking experiment and used a triple-layer structure to directly measure the relationship between the ionization charges current and the field strength. In the simulation calculation, we directly fit this functional relationship to calculate the conductivity of ionization charges. This not only ensures the authenticity of the ionization charges current calculation but also does not introduce new empirical parameters into the model. The expression of the fitted ionization charges current is as follows:

$$J_{ion} = \frac{dq}{dt} = A' \exp\left(-\frac{\varphi}{kT}\right) \sinh(B'|E|) \quad (8)$$

where  $J_{ion}$  is the current density of ionization charges,  $q$  is the charge density per unit area,  $\varphi$  represents the average energy required for ionization charges transition,  $A'$  and  $B'$  are both fitting coefficients, where  $B'$  is positively correlated with the average distance of ionization charges transition. The unit of  $A'$  is  $A/m^2$ , the unit of  $B'$  is  $m/V$ , and the unit of  $\varphi$  is  $eV$ . Combining the exponential term into the constant  $A'$ , the final form of the fitting expression for calculating the conductivity of ionization

charges is obtained. Here, it is not yet possible to distinguish between the density and mobility of the ionization charges, but only the product of the two can be measured:

$$\begin{aligned} n_{ion}(E, T) \times \mu_{ion}(E, T) &= \gamma_{ion} \\ &= \frac{J_{ion}}{|E|} = \frac{A \sinh(B|E|)}{|E|} \end{aligned} \quad (9)$$

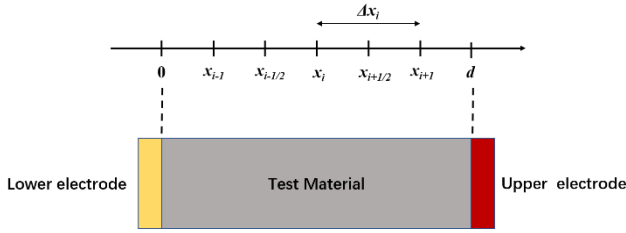


Fig. 3. Schematic representation of the space grid

The solution process for (1), (2), and (3) can be illustrated with the help of Fig. 3. While the solution method for the injected carriers remains the same as the classical method, here we focus only on the solution method for the ion part. First, the conduction equation in the set of equations is solved using the first-order windward algorithm, where the concentration of the cell in front of the direction of carrier motion is chosen to describe the conduction current  $j$ :

$$\begin{cases} j_{i+1/2}^k = n_i^k \cdot e \cdot \mu_{i+1/2}^k \\ j_{i-1/2}^k = n_{i-1}^k \cdot e \cdot \mu_{i-1/2}^k \end{cases} \quad \text{for positive ions} \quad (10)$$

$$\begin{cases} j_{i+1/2}^k = n_{i+1}^k \cdot e \cdot \mu_{i+1/2}^k \\ j_{i-1/2}^k = n_i^k \cdot e \cdot \mu_{i-1/2}^k \end{cases} \quad \text{for negative ions} \quad (11)$$

where  $k$  denotes the time step and  $i$  denotes the position where the computational unit is located.

Because the product of  $n$  and  $u$  is directly measured in experiments for each field strength and temperature, this product can be directly inserted into (8) to solve for the conduction current, as shown in (9), without separating  $n$  and  $u$ . Then, the charge concentration  $n$  can be calculated using the first-order difference method:

$$n_i^{k+1} = n_i^k - \frac{dt}{dx} \left( j_{i+1/2}^k - j_{i-1/2}^k \right) \quad (12)$$

The solution for  $j$  is obtained through the solution of the conduction equation (as shown in (10) and (11)), allowing for the calculation of ionization charges concentration in each cell and the corresponding source term  $S$ . Subsequently, the electric field distribution can be solved using Poisson's equation. This method enables the calculation of ionization charges even if separated  $n$  and  $u$  values cannot be directly obtained through experimental data fitting. The system of equations provides a solution process to calculate the ionization charges component.

In the model, the source term needs to be recalculated after

taking the effect of ionization charges into account. After introducing the effect of ionization charges, the interaction between ionized and injected charges is taken into account in the calculation of the source term, which consists of two parts: one is the recombination between the ionization charges and the injected charges, and the other is the secondary ionization process of the neutral molecules produced by the recombination. Notably, the conductivity of ionization charges is derived from macroscopic measurements, and only uncombined ionization charges can reach the interface in a triple-layer blocking experiment. Hence, the source term calculation does not need to consider the combination between positive and negative ions. In our new model, the source term's final calculation expression is as follows, using injected electrons and ionized positive ions as examples:

$$\begin{cases} S_{eu} = -eS_{hu}n_{eu} - eS_{sh}n_{eu}n_{hi}(1-DL2) \\ S_{hi} = -eS_{sh}n_{eu}n_{hi}(1-DL2) \end{cases} \quad (13)$$

where  $n_{hu}$ ,  $n_{eu}$ ,  $n_{hi}$ ,  $n_{ei}$  represent the concentrations of injected holes, injected electrons, positive charges from ionization and negative charges from ionization, respectively.  $S_{sh}$  represents the recombination coefficient between injected electrons and ionized positive ions,  $DL2$  represents the secondary ionization coefficient. The barrier for separating already dissociated ionization charges will be lower than that required to remove a charge carrier that has combined with such ionization charges thereby neutralizing them. Therefore, the secondary ionization should be more difficult than the separation of ionization charges termed primary ionization. The calculation method for  $DL2$  is the same as the method used for calculating the initial ion concentration in (7), except that the secondary ionization process requires a higher energy excitation to occur, resulting in a larger secondary ionization barrier compared to the ionization barrier.

$$DL2 = v_0 \exp\left(-\frac{eW_{ie2} - \sqrt{\frac{e^3 E}{\pi \epsilon}}}{kT}\right) \quad (15)$$

where  $W_{ie2}$  is the secondary ionization barrier.

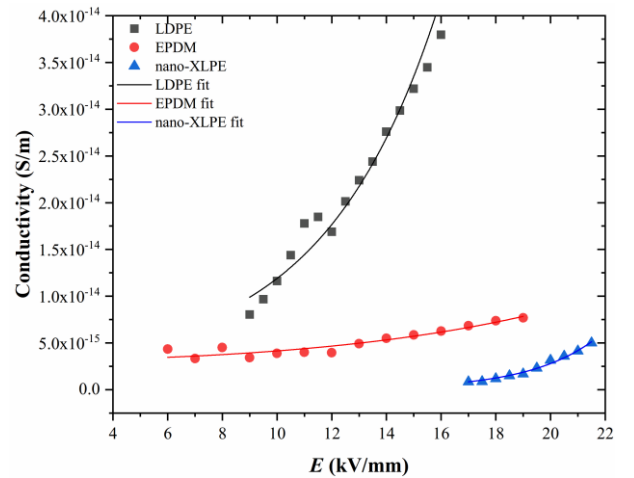


Fig. 4. Comparison of the conductivity of ionization charges of the three materials

The conductivity of ionization charges of three common insulating materials -- low-density polyethylene (LDPE), ethylene propylene diene monomer (EPDM), and cross-linked polyethylene with nanoparticles (nano-XLPE) -- measured in the experiment varies with the field strength as shown in Fig. 4. The LDPE and nano-XLPE are from Wanma Material Co., Ltd., and both have the same base resin of No. 2200 h. The nanofiller in XLPE was SiO<sub>2</sub>, the doping ratio was 1%, and the particle size was 50-100 nm. The EPDM comes from Shanghai Cable Research Institute. Use (9) to fit the experimental results, and calculate the fitting parameters A and B. The fitted curve is also plotted in Fig. 4.

The fitting coefficients of the conductivity of ionization charges in the three materials are shown in Table I. Both A and B in the table are dimensionless constants.

**TABLE I**  
COEFFICIENTS OF CONDUCTIVITY OF IONIZATION CHARGES.

	LDPE	EPDM	nano-XLPE	UNIT
A	$1.346 \times 10^{-8}$	$2.035 \times 10^{-8}$	$1.282 \times 10^{-11}$	S/m
B	$2.876 \times 10^{-7}$	$1.35 \times 10^{-7}$	$4.536 \times 10^{-7}$	m/V

### B. Difference between the precision model and the engineering model

The precision model considers the recombination between carriers, including the recombination of electrons and holes, the recombination of electrons and positive ions, the recombination of holes and negative ions, and the recombination between positive and negative ions. The recombination of electrons and positive ions and the recombination of holes and negative ions will produce neutral intermediate products. The model also carefully calculates the secondary ionization process in which the neutral products continue to ionize under the electric field. The expression of the second ionization is the same as that of the first ionization, and the parameter of the second ionization barrier is introduced here. This barrier value is greater than the barrier value during the initial ionization. For convenience of use, the engineering model does not consider the recombination and secondary ionization process.

At the same time, a flux limiter is set up in the paper to ensure that the charge that moves out of each area will not be greater than the one already existing there.

## III. SIMULATION RESULTS

In this section, the conductivity of the three materials is first calculated by our new model, and then the simulation results are compared with the experimental results from previous studies to verify the validity of the newly added part of the model, i.e., the ionization charges part. After that, a precision model and an engineering model are developed to simulate the charge density of three common insulation materials (LDPE, EPDM, LDPE) in a single-layer structure. The computational

results of the two models are compared, and criteria are set to determine when the engineering model can be used instead of the precision model.

### A. Model validation

All parameters used in the model are shown in Table II. To simplify the calculation, the same values are used for some parameters of positive carriers and negative carriers in the paper, such as their recombination coefficients with ions, but in practice, they may be slightly different. The previous analysis believes that nano-XLPE has a large number of ionization charges under high field strength. These ionization charges recombine with injected carriers, and the secondary ionization of neutral products after recombination is more difficult than the first ionization [23]. As a result, the mobility of injected carriers decreases.

**TABLE II**  
PARAMETERS USED FOR THE SIMULATIONS

Symbol	VALUE			UNIT
	LDPE	EPDM	NANO-XLPE	
<b>injection barrier heights</b>				
$\omega_{ei}$ for electrons	1.20	1.20	1.20	eV
$\omega_{hi}$ for holes	1.20	1.205	1.20	eV
<b>hopping distance</b>				
$\lambda_e$ for electrons	20.44	7.93	13.51	nm
$\lambda_h$ for holes	27.33	17.96	19.27	nm
<b>hopping energy</b>				
$\Delta_e$ for electrons	0.82	0.81	0.85	eV
$\Delta_h$ for holes	0.97	0.93	0.91	eV
<b>Extraction coefficient</b>				
$D_e$ for electrons	0.1	0.1	0.1	
$D_h$ for holes	0.1	0.1	0.1	
<b>Initial ion concentration</b>				
$N_0$	9 $\times 10^8$			
<b>Ionization barrier</b>				
$\omega_{te}$	1.15			eV
<b>Recombination coefficient</b>				
$S$ for electrons and holes	$2 \times 10^{-3}$	$2 \times 10^{-3}$	$2 \times 10^{-3}$	
$S_i$ for positive and negative ions	0	0	0	
$S_{xe}$ for electrons and positive ions	0.1	0.05	0.1	
$S_{xh}$ for holes and negative ions	0.1	0.05	0.1	
<b>Secondary ionization barrier</b>				
$\omega_{te2}$	1.17	1.17	1.25	eV

To evaluate the accuracy of the new precise model, simulations were performed to calculate the conductivity of three materials as a function of field strength at room temperature. The results were then compared with experimental conductivity values. The model used the current on the electrode divided by the average electric field to calculate the conductivity. To achieve this, the current on the electrode was divided into two parts: the extraction current on the electrode and the induced current from the change in induced charge on the electrode. The conductivity was then calculated using the following formula:

$$\begin{cases} Ih = fh + \frac{dS_{cd}}{dt} & (16) \\ \gamma = \frac{Ih}{E} & (17) \end{cases}$$

Where  $Ih$  is the current on the electrode,  $fh$  is the extraction current,  $S_{cd}$  is the induced charge, and  $E$  represents the average field strength.

In a previous study, it was observed that the conductivity of the three materials increased with increasing field strength in experimental tests, but the magnitude of the increase varied for each material. Specifically, EPDM had the smallest increase in conductivity, while LDPE and nano-XLPE had larger increases [21]. It was also observed that the conductivity curves of LDPE and EPDM intersected in the field strength range of 10-20 kV/mm. The simulation results using the newly established charge transport model successfully reproduced these experimental results. The calculated conductivity values for the three materials were in the same order of magnitude as the experimental results and closely matched them. Additionally, the pattern of conductivity variation with field strength for the three materials in the simulation results was consistent with that observed in the experiment, and the intersection point between LDPE and EPDM in the simulation results also appeared in the 10-20 kV/mm range. The high agreement between the measured conductivity of the three materials and the simulation results verifies the validity of the newly established charge transport model that fully considers the influence of ionization charges.

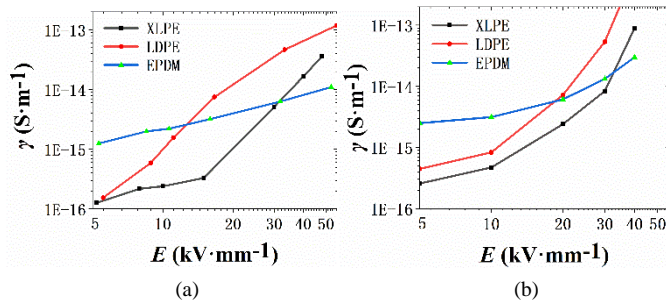


Fig. 5. Schematic diagram showing the relationship between the conductivity of the three materials as a function of field strength. (a) the experimental results, and (b) the simulation results.

The parameters of mobility of injected charges and conductivity of ionization charges obtained from experimental

fitting are directly applied to the bipolar carrier model in the simulation, and the relationship between the conductivity of the three materials with the electric field is calculated, showing a high degree of consistency with the experimental results. Therefore, we believe that the precision model can accurately reproduce the experimental results, fully consider the influence of the ionization charges in the dielectric, and can be used as a tool to accurately calculate the polymer electric field distribution.

### B. Comparison Between the Two Models

After verifying the rationality of some parameters of ionization charges, using these parameters, two charge transport models were developed, as previously mentioned. The precision model fully considers the effects of ionization charges, while the engineering model does not consider the recombination and secondary ionization processes, as summarized in Table III. It is worth mentioning that this latter even if simplified, takes into account ionization charges and can be more efficiently applied in the engineering field. The main purpose is, however, to propose the method, not to fit it to a particular experimental result.

TABLE III

COMPARISON OF PRECISION MODEL AND ENGINEERING MODEL

	PRECISION MODEL	ENGINEERING MODEL
Calculate conductivity of ionization charges	YES	YES
Consider the recombination of positive and negative ions and electrons/holes	Yes	No
Consider the secondary ionization process	Yes	No

The calculation results of the precision model and engineering model of the three materials are shown in Fig. 6. It can be seen from the diagram that under the field strength of 30kV/mm, the calculation results of the precision model of the three materials show homocharge near the electrode. On the contrary, the engineering model simulation results of the three materials showed different states. The results of the engineering model on LDPE are basically consistent with the precision model, except that the amount of charge of the same polarity is relatively reduced. The engineering model results on EPDM also show the same charge polarity, but the amount of charge is larger, and its distribution tends to move toward the inside of the sample. The calculation result of the nano-XLPE engineering model is completely different from that of the

precision model. The accumulated charge near the electrode is completely converted to heterocharge. This shows that at room temperature, LDPE and EPDM simulations can basically use the engineering model to replace the precision model, but nano-XLPE does not work, and the engineering model has a large deviation in this case.

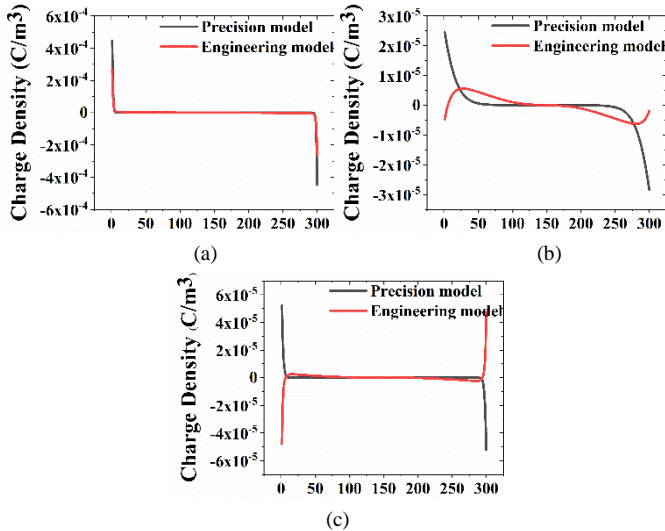


Fig. 6. Comparison of the simulation results between the three-materials precision model and the engineering model. Figures a, b, and c represent LDPE, EPDM, and nano-XLPE, respectively.

Experimental measurements show that the ionization charges in nano-XLPE have a great influence on the entire process of charge transport. However, in the engineering model, because the recombination between ions and electron holes and the effect of secondary ionization are ignored, the influence of conductivity of ionization charges has become the main factor that determines the accumulation of charge. A large number of positive and negative ionization charges move to the vicinity of the electrode with opposite polarity under the action of the electric field, forming the heterocharge accumulation. Because there are too many ionization charges, the approximation adopted by the engineering model at this time will greatly deviate the simulation results from reality. Therefore, it is necessary to propose a criterion to determine when the engineering model can be used.

Through the previous discussion, we know that in the existing model, the most important factor affecting the charge distribution and electric field distribution is the part of the ionization charges. Because ionization and injection current behavior with the electric field can be calculated with the model, we can discuss whether the engineering model can be used directly by comparing the ionization charges current and injection current. The Schottky injection is used to calculate the injection current, while the experimentally measured conductivity of ionization charges is used to calculate the ionization charges current, as in (9).

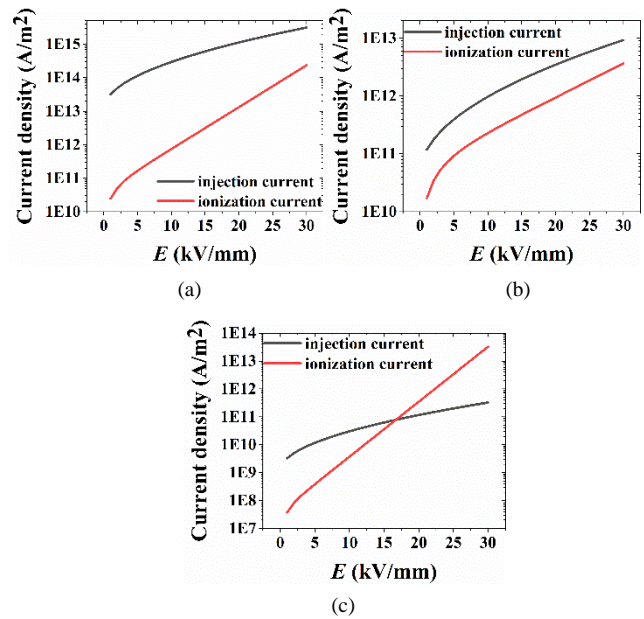


Fig. 7. Comparison of the injection current and ionization charges current in three materials. Figures a, b, and c represent LDPE, EPDM, and nano-XLPE, respectively.

It can be clearly seen from the figure that the injection current of LDPE is far greater than the ionization charges current and greater than one order of magnitude. The injection current and ionization charges current in EPDM is basically of the same order of magnitude. In nano-XLPE, however, the behavior is different, i.e., the ionization charges current is lower at low fields, and larger at high fields. This corresponds exactly to the difference between the precision model and the engineering model in the three materials. Therefore, the relationship between the injection current and the ionization charges current can be used as a criterion for whether the engineering model can be used to replace the precision model. To show the relationship between the ionization charges current and the injection current more intuitively, we separately took out the ionization charges current and the injection current of the three materials under a 28 kV/mm field strength and calculated their ratio. The calculation results are shown in Table IV.

TABLE IV

THE RATIO OF THE IONIZATION CHARGES CURRENT TO THE INJECTION CURRENT OF THE THREE MATERIALS

	LDPE	EPDM	NANO-XLPE
Injection current at 28 kV/mm	$2.601 \times 10^{15}$	$7.734 \times 10^{12}$	$2.685 \times 10^{11}$
Ionization charges current at 28 kV/mm	$1.322 \times 10^{14}$	$2.785 \times 10^{12}$	$1.314 \times 10^{13}$
Ratio	19.675	2.777	0.020

Therefore, before starting the simulation, the injection current and ionization charges current in the material should be



calculated. If the injection current is more than one order of magnitude greater than the ionization charges current, the engineering model can be used instead of the precision model. In this case, the calculation results of both models are almost identical. If the injection current is greater than the ionization charges current, but the values of the two are similar, the engineering model can also be used. The calculation result in this case slightly deviates from the precision model, but it is still within the acceptable range. If the injection current is lower than the ionization charges current, results will deviate from the model, therefore the simplified engineering model cannot be used for calculation.

#### IV. CONCLUSION

In this paper, we have presented two charge transport models that consider the impact of ionization charges in polymers. One is a precision model that considers the generation of ionization charges, the recombination of ionization charges and injected electrons and holes, and secondary ionization processes. The other, called the engineering model, neglects the recombination and secondary ionization and can be convenient for practical engineering applications. In both models, the expressions for the conductivity of ionization charges were obtained by directly fitting the experimental data in a way that guarantees the accuracy of the calculations concerning the ionization part. At the same time, the reliability of the precision model is verified by calculating the value of conductivity and comparing it with the experimental results in the previous study.

After that, the criterion of whether the engineering model can be used to replace the precision model is proposed, that is, the relationship between the ionization charges current and the injection current in the material. If the injection current is greater than the ionization charges current or the two are close at the same field strength, the engineering model can be used instead of the precision model. If the ionization charges current is greater than the injection current, the engineering model that ignores the recombination and secondary ionization cannot be used to replace the precision model.

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#### REFERENCES

- [1] C. Onneby, E. Martensson, U. Gafvert, A. Gustafsson and L. Palmqvist, "Electrical properties of field grading materials influenced by the silicon carbide grain size," *IEEE Int. Conf. Solid Dielectr. (ICSD)*, 2001, pp. 43-45.
- [2] K. Wu and C. Cheng, "Interface charges between insulating materials," *IEEE Trans. Dielectr. Electr. Insul.*, vol. 24, no. 4, pp. 2633-2642, 2017.
- [3] T. Christen, "HVDC insulation boundary conditions for modeling and simulation," *IEEE Transactions on Dielectrics and Electrical Insulation*, vol. 22, no. 1, pp. 35-44, 2015-02-01 2015, doi: 10.1109/tdei.2014.004559.
- [4] J. M. Alison and R. M. Hill, "A Model for Bipolar Charge-Transport, Trapping and Recombination in Degassed Cross-Linked Polyethene," (in English), *J Phys D Appl Phys*, vol. 27, no. 6, pp. 1291-1299, Jun 14, 1994, doi: Doi 10.1088/0022-3727/27/6/029.
- [5] Y. Zhan *et al.*, "Comparison of two models on simulating electric field in HVDC cable insulation," *IEEE Transactions on Dielectrics and Electrical Insulation*, vol. 26, no. 4, pp. 1107-1115, 2019-08-01 2019, doi: 10.1109/tdei.2019.007878.
- [6] P. H. F. Morshuis, R. Bodega, D. Fabiani, G. C. Montanari, L. A. Dissado, and J. J. Smit, "Calculation and Measurement of Space Charge in MV-size Extruded Cables Systems under Load Conditions," in *2007 IEEE International Conference on Solid Dielectrics*, 2007-07-01 2007: IEEE, doi: 10.1109/icsd.2007.4290861.
- [7] E. Ildstad, F. Mauseth, and G. Balog, "Space charge and electric field distribution in current loaded polyethylene insulated HVDC cables," *Int. Symp. HV Eng*, 2003, p. 366
- [8] D. Fabiani, G. C. Montanari, R. Bodega, P. H. F. Morshuis, C. Laurent, L. A. Dissado, "The effect of temperature gradient on space charge and electric field distribution of HVDC cable models", *Proc. IEEE Int. Conf. Prop. App. Diel. Mat.*, pp.65-68, 2006.
- [9] S. L. Roy, G. Teyssède, and C. Laurent, "Modelling space charge in a cable geometry," *IEEE Transactions on Dielectrics and Electrical Insulation*, vol. 23, no. 4, pp. 2361-2367, 2016-08-01 2016, doi: 10.1109/tdei.2016.7556514.
- [10] S. Le Roy, G. Teyssedre, and C. Laurent, "Numerical methods in the simulation of charge transport in solid dielectrics," *IEEE Transactions on Dielectrics and Electrical Insulation*, vol. 13, no. 2, pp. 239-246, 2006-04-01 2006, doi: 10.1109/tdei.2006.1624268.
- [11] N. Liu, C. Zhou, G. Chen, and L. Zhong, "Determination of threshold electric field for charge injection in polymeric materials," *Appl. Phys. Lett.*, vol. 106, no. 19, p. 192901, 2015
- [12] F. Baudoin, S. Le Roy, G. Teyssedre and C. Laurent, "Bipolar Charge Transport Model with Trapping and Recombination: An Analyze of the Current vs. Applied Electric Field Characteristic," *2007 IEEE International Conference on Solid Dielectrics*, 2007, pp. 19-22, doi: 10.1109/ICSD.2007.4290742.
- [13] S. L. Roy, T. T. N. Vu, and G. Teyssedre, "Modelling charge transport in a HVDC cable using different softwares: from fluid models to macroscopic model," in *2019 2nd International Conference on Electrical Materials and Power Equipment (ICEMPE)*, 2019-04-01 2019: IEEE, doi: 10.1109/icempe.2019.8727386.
- [14] G. Teyssedre and C. Laurent, "Charge transport modeling in insulating polymers: from molecular to macroscopic scale," *IEEE Transactions on Dielectrics and Electrical Insulation*, vol. 12, no. 5, pp. 857-875, 2005-10-01 2005, doi: 10.1109/tdei.2005.1522182.
- [15] S. Le Roy and G. Teyssedre, "Ion generation and transport in low density polyethylene under electric stress," (in English), *C Elect Insul Diel P*, pp. 63-66, 2015. [Online].
- [16] S. L. Roy, F. Baudoin, C. Laurent, and G. Teyssedre, "Introduction of Ionic Contributions to a Charge Transport Model for Dielectrics," in *2020 IEEE 3rd International Conference on Dielectrics (ICD)*, 2020-07-05 2020: IEEE, doi: 10.1109/icd46958.2020.9342023.
- [17] J. Wu, L. Lan, Z. Li, and Y. Yin, "Simulation of space charge behavior in LDPE with a modified of bipolar charge transport model," in *Proceedings of 2014 International Symposium on Electrical Insulating Materials*, 2014-06-01 2014: IEEE, doi: 10.1109/iseim.2014.6870721.
- [18] L. Lan, J. Wu, Y. Yin, and Q. Zhong, "Investigation on heterocharge accumulation in crosslinked polyethylene: Experiment and simulation," *Japanese Journal of Applied Physics*, vol. 53, no. 7, p. 071702, 2014-07-01 2014, doi: 10.7567/jjap.53.071702.
- [19] Zheng Y, Huang H, Zhong X, et al. Simulation of charge transport in polypropylene-based nano-composites[J]. *Journal of Physics D: Applied Physics*, 2021, 54(23): 235501.
- [20] Zhan Y, Chen G, Hao M, et al. Space charge measurement and modelling in cross-linked polyethylene[J]. *Energies*, 2020, 13(8): 1906.
- [21] Y. F. He *et al.*, "Comparison of Transportation Carriers in the Insulating Materials for HVDC Cable Joint," (in English), *Ieee T Dielect El In*, vol. 28, no. 2, pp. 562-568, Apr 2021, doi: 10.1109/Tdei.2020.009269.
- [22] Y. Wu *et al.*, "Distinction between the Contributions of Ionized and Injected Charges in Oil Immersed Paper," in *IEEE Transactions on Dielectrics and Electrical Insulation*, vol. 28, no. 1, pp. 318-325, February 2021, doi: 10.1109/TDEL.2020.009141.
- [23] R. Su, K. Wu, and L. A. Dissado, "Investigation of effects of charge injection and intrinsic ionic carriers in low-density polyethylene and cross-linked polyethylene," *J.Appl. Phys.*, 2020, 127(16):165103
- [24] C. Cheng *et al.*, "A new method for carrier mobility measurement in oil immersed cellulose paper insulation," *IEEE Trans. Dielectr. Electr. Insul.*, vol. 26, no. 1, pp. 308-313, Feb. 2019.

[25] L. A. Dissado and J. C. Fothergill, *Electrical Degradation and Breakdown in Polymers*, Peter Peregrinus, London, 1992.



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