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A new model for charges transport and build-up in extruded insulation (XLPE) for HVDC cables

Assane **NDOUR**, Séverine **LE ROY**, Gilbert **TEYSSEDRE**; LAPLACE - Université de Toulouse, CNRS, UPS, INPT, (France), <u>assane.ndour@laplace.univ-tlse.fr</u>, <u>severine.leroy@laplace.univ-tlse.fr</u>, <u>gilbert.teyssedre@laplace.univ-tlse.fr</u> Raphaël **GUFFOND**, Julien **FERNANDEZ**; Nexans, (France), <u>raphael.guffond@nexans.com</u>, julien.fernandez@nexans.com

ABSTRACT

This paper presents a bipolar charge transport model based on new assumptions of energy levels distribution of traps and allowing to predict the XLPE electrical behaviour under DC stress. The model assumes that shallow traps are distributed over a single energy level and can participate in transport with a hopping mobility, whereas an exponential distribution is used to model the repartition of deep traps. Trapping, detrapping and recombination of charges are taken into account. Results show that the model (simulated under COMSOL Multiphysics®) reproduces the main characteristics of space charge density obtained by PEA measurement on degassed XLPE plates samples.

KEYWORDS

Charge transport modelling, Cross-linked polyethylene (XLPE), Insulating polymers, Dielectric characterizations, Space charges, Traps distribution.

INTRODUCTION

The challenge in strengthening grid interconnections between countries and in the development of renewable energies from solar or wind sources is to transmit energy over long distances, as production areas are generally far from consumption areas. To rise to this challenge, more and more power transmission systems are based on HVDC technology, and cross-linked polyethylene (XLPE) is now the most used insulation in HVDC cables, because of its suitable electrical and thermomechanical properties for service conditions, in particular its improved thermal and mechanical resistance due to the bridges (formed during the cross-linked process) between the molecular chains of LDPE. One of the issues using a synthetic insulation under DC stress is the generation and accumulation of charges inside the insulation, which can locally increase the electric field, leading to material degradation and possible dielectric breakdown, i.e. to the failure of the transmission link. Modelling charge generation and transport phenomena is a complementary way to experimental measurements to improve the understanding of charge accumulation mechanisms and associated consequences in XLPE. In this perspective, several charge transport models have been proposed in the literature over the last decades to describe and predict the electrical behaviour of polymeric insulators (LDPE, XLPE, etc.) [1-5]. In this paper, we present a new charge transport model allowing to follow the spatio-temporal charge evolution, the local electric field distribution and the current density evolution in a degassed XLPE under thermoelectric stress. Such degassed material allows to let ionic charges aside in a first attempt. The developed model is an improvement of a BCT (bipolar charge transport) model already published in the literature

[1, 2]. The main difficulty with charge transport models is to describe as correctly as possible the trap distribution within the band gap, as this is what rules charge transport and accumulation in solid organic insulators. On the other hand, the trap description should be relatively simple, otherwise the resolution becomes too long due to model timesteps, or parameters identification is not tractable as processes are too interrelated. The original approach of our work is the type of energy levels distribution that is proposed and used to model the traps distribution in the material: for each type of electronic charges (electrons and holes), we assume a discrete level for shallow traps, mostly linked to physical defects, and an exponential distribution for deep traps due to chemical defects. Such description has been already proposed in the literature [4], although the present model accounts differently for most of the physical processes included in the model, and described in a further paragraph. The model accounts for the main physical processes for electronic charges such as charge injection and extraction at the electrodes, transport (drift and diffusion), trapping, detrapping and recombination of charges in a degassed XLPE. The fluid model is solved using a finite element method, and has been developed for planar (plates) geometry. To validate the model, experimental measurements of space charges and current are performed on degassed XLPE plane parallel samples and the obtained results are compared with those of the model

EXPERIMENTAL APPROACH

A peroxide cross-linked polyethylene (XLPE) has been chosen as model material. Plagues of cross-linkable LDPE, i.e. containing peroxide, are first obtained using a hydraulic press. Semicon electrodes (SC) based on carbon blackdoped polyethylene are added on each side of the XLPE, and the sandwich SC/XLPE/SC is crosslinked by compression molding at 190°C for 10 minutes. Adding SC electrodes allow being closer to the real configuration of an insulated XLPE cable system, and also allow having a good electrical and acoustic match during space charge measurements. The thickness of the sandwich is about 500 µm, with SC electrodes of 12 mm wide and 150 µm thick, and XLPE insulation of 70 mm wide and about 200 µm thick. After sample preparation and before experimental measurements, the samples are degassed for 3 days at 70°C to remove the XLPE cross-linking by-products, as their presence in the material and their contribution to space charge are not taken into account in the present research. Experimental space charge measurements using the Pulsed Electro-Acoustic (PEA) method and current measurements were performed on these degassed XLPE samples. The applied electric field protocol is given in Fig. 1, and consists, for a given temperature, in applying an



Fig. 1: Electric field protocol for space charge and current measurements and simulation.

increasing electric field from 20 to 40 kV.mm⁻¹. The electric field is applied for 24 hours at each level to allow the samples to reach a steady state. After the application of each electric field for 24 hours, a depolarization time of 1 hour has been performed to measure space charge and current at volt-off. Measurements have been performed for temperatures of 20, 50 and 70°C.

MODEL DESCRIPTION

The aim of our work is to develop a fluid bipolar charge transport model that contributes to the improvement of already existing ones. The model we propose in this paper combines the trap energy levels distribution from two models already developed: the two-levels of traps model [1], and the model with an exponential trap distribution [2]. Each model accounts only for electronic charges, i.e. electrons and holes.

Description of the trap distributions used as basis for our model

The first trap distribution description, which has been described in several publications, [1, 5, 6], is the two levels of trap model presented in Fig. 2.

Each charge type (electron and hole) has only two levels, one where the charge is mobile, and the other where the charge is trapped. Mobile charges in the transport level (mobile electrons in conduction band and mobile holes in valence band) have an effective mobility that accounts for the possible trapping and detrapping of charges in shallow traps, where the residence time of charges is short (10^{-12} s) [1, 7]. This mobility is hence lower than a band mobility, and is of the order of 10^{-13} - 10^{-14} m².V⁻¹.s⁻¹. A single deep trapping level for each charge species is considered.

The second description is an exponential distribution of energy states for each kind of carrier, based on ab initio calculations [8]. The exponential distribution, presented in Fig. 3, is expressed as a function of the energy level Δ by [2, 6]:

$$N_{t(e,h)}(\Delta_{e,h}) = N'_{e,h} \exp\left[-\frac{\Delta_{e,h}}{k_B T_{0(e,h)}}\right] \quad (\Delta \le \Delta_{max}) \qquad [1]$$

where $N_{t(e)}$ and $N_{t(h)}$ are the trap density distributions for electrons and holes, characterized by the shape parameter T_0 (in K) and the pre-exponential factor N' (in m⁻³.J⁻¹). k_B

the Boltzmann constant (1,38 10^{-23} J.K⁻¹). The exponential distribution is limited by a maximum trap depth Δ_{max} (in eV) corresponding to the deepest trap available in the material [6]. All charges are considered trapped at all times, and only a fraction of trapped charges, with an energy between Δ_f and $\Delta_f - k_B T$, Δ_f representing the highest occupied level, contributes to the transport. For this model, the mobility of each carrier is function of the exponential trap distribution, and is of the hopping type.

The model with two levels of traps has the advantages of being simple and is easy to parameterize to reproduce the results of experimental measurements, as all these parameters are independent. However, it is limited by its simplified description of the energy levels of the trap states. The exponential trap distribution model provides a more realistic physical description of traps distribution in the bandgap. However, because all its parameters are related, this model is much more complicated to use. In addition, the assumption that a constant fraction of trapped charges is available for transport whatever the trap filling level is also a limitation for this model.

Description of the proposed trap distribution

The present model is based on the description of trap distribution as proposed in Fig. 4. We assume that for each charge carrier:

- There is a single trapping energy level for mobile charges,



Fig. 2: Schematic representation of the two-level of traps model.



Fig. 3: Schematic representation of the exponential trap distribution for a single kind of carrier. Δ_f is the upper filled level and Δ_{max} the maximum depth of traps.

with an energy less or equal to 0.3 eV. This upper energy value has been defined according to the maximum trap depth for physical traps reported by Meunier et al. [7]. Charges on this level have a mobility of the hopping type. Contrarily to the two levels of traps model, where the mobility for charges in the 'mobile' level was of the order of 10^{-13} - 10^{-14} m².V⁻¹.s⁻¹, in the present model, the mobility (around 10^{-8} m².V⁻¹.s⁻¹ for an energy level of 0.3 eV) is closer to a band mobility.

- There is an exponential distribution for deep traps. The depth of the traps varies from a maximum energy level Δ_{max} ($\leq 1.5 \text{ eV}$) to a minimum energy level Δ_{min} , which must be greater than the hopping barrier height (w_{hop}) value for each kind of charge. The traps are first filled from the deepest energy levels towards the most shallow ones. These energy levels values have again been extracted from the literature on ab-initio simulations [7, 8, 9].

The equation governing the exponential distribution is :

$$N_{t(e,h)} = N'_{(e,h)} \exp\left(-\frac{\Delta_{e,h}}{k_B T_{0(e,h)}}\right), \left(\Delta_{min} < \Delta_{e,h} < \Delta_{max}\right)$$
[2]

where Δ_{max} and Δ_{min} (in eV) are the maximum and minimum trap depth respectively.

The integral of $N_{t(e)}$ between Δ_{max} and Δ_{min} gives the total deep trap density:

$$N'_{tot(e,h)} = \int_{\Delta \min}^{\Delta \max} N'_{(e,h)} \exp\left(-\frac{\Delta_{e,h}}{k_B T_{0(e,h)}}\right) d\Delta \qquad [3]$$
$$N'_{tot(e,h)} = N'_{(e,h)} k_B T_{0(e,h)} \left[\exp\left(-\frac{\Delta_{\min(e,h)}}{k_B T_{0(e,h)}}\right) - \exp\left(-\frac{\Delta_{\max(e,h)}}{k_B T_{0(e,h)}}\right)\right] \qquad [4]$$

The parameters N', T_0 are then chosen to have a total trap density of the order of what has been proposed in the literature for deep traps [8, 9].

The proposed model is a one-dimensional bipolar charge transport model, function of the position in the sample, and accounts for charge generation, transport, trapping, detrapping and recombination. Each physical process has a link with the trap distribution proposed above, and will be described in the following.

The equations to solve are the Poisson equation and the transport equation combined with the charge conservation equation (also called continuity equation):

$$\nabla (\varepsilon_0 \varepsilon_r E) = (+qn_{h\mu} + qn_{ht} - qn_{e\mu} - qn_{et}) = \rho \qquad [5]$$

$$\frac{\partial n_a}{\partial t} + \nabla \left(n_a \mu_a E - D_{diff_a} \nabla n_a \right) = s_a$$
[6]

q is the elementary charge (in C), n_a is the charge density (in m⁻³), *a* defines the type of charge (electron or hole), mobile (μ) or trapped (t). *t* is the time, μ_a is the mobility (in m².V⁻¹.s⁻¹) for each kind of carrier and D_{diffa} the diffusion coefficient (in m².s⁻¹). *E* is the electric field (in V.m⁻¹), ρ the net charge density (in C.m⁻³), ε_0 the vacuum permittivity, and ε_r the relative permittivity of the material (2.3 for XLPE). s_a is the source term defined below.

The mobility for each kind of charge is of the hopping type and is expressed as:



Fig. 4: Description of the proposed model. Shallow traps are modelled by a single trap level and deep traps distribution is described by an exponential function that varies from Δ_{max} to Δ_{min} (maximum and mimimum depth of traps). Δ_f is the upper filled level, i.e. the highest occupied level.

$$\mu_{(e,h)} = \frac{2\lambda_{(e,h)}\nu}{E} \exp\left(\frac{-w_{hop(e,h)}}{k_BT}\right) \sinh\left(\frac{q\lambda_{(e,h)}E}{2k_BT}\right)$$
[7]

 $\lambda_{(e,h)}$ is the hopping distance, i.e. the inter-traps distance (in m), ν the attempt to escape frequency (in s⁻¹) equal to $k_B T/h = 6.2 \ 10^{-12} \ s^{-1}$ at room temperature (300 K), $w_{hop(e,h)}$ is the hopping barrier (in eV) $\leq 0.3 \ eV$, and *T* is the temperature.

The diffusion coefficient is related to the mobility by the Einstein relation:

$$D_{diff_{(e,h)}} = \frac{k_B T}{q} \mu_{(e,h)}$$
[8]

The source terms s_a take into account all physical processes not related to transport (trapping, detrapping, recombination). An example of a source term for free electrons is given below:

$$s_{e\mu} = -B_{(e)}n_{e\mu}\left(1 - \frac{n_{et}}{N'_{tot(e)}}\right) + D_{(e)}n_{et} -S_{1_L}n_{e\mu}n_{ht} - S_{3_L}n_{e\mu}n_{h\mu}$$
[9]

The first term in the right hand side of equation [9] defines the trapping, characterized by the trapping coefficient $B_{(e,h)}$ (in s⁻¹) which depends on the total trap density and the charges mobility [10]:

$$B_{(e,h)} = qN'_{tot(e,h)} \frac{\mu_{(e,h)}}{\varepsilon_0 \varepsilon_r}$$
[10]

The second term in the right hand side of equation [9] describes the detrapping, defined by the detrapping coefficient $D_{(e,h)}$ (in s⁻¹), which is function of the upper filled limit $\Delta_{f(e,h)}$:

$$D_{(e,h)} = v \exp\left(\frac{-\Delta_{f(e,h)}}{k_B T}\right)$$
[11]

The trap filling depth, $\Delta_{f(e,h)}$, can be calculated from the equation (for electrons for example):

$$n_{et} = \int_{\Delta_f}^{\Delta_{max}} N'_{(e)} \exp\left(-\frac{\Delta_e}{k_B T_{0(e)}}\right) d\Delta \qquad [12]$$

This allows to obtain:

$$\Delta_{f(e)} = -k_B T_{0(e)} \ln \left[\exp \left(-\frac{\Delta_{\max(e)}}{k_B T_{0(e)}} \right) + \left(\frac{n_{et}}{N'_{(e)} k_B T_{0(e)}} \right) \right]$$
[13]

At t = 0, if we consider that there are no trapped charges, then $n_{et} = n_{ht} = 0$, and thus $\Delta_{f(e,h)} = \Delta_{max(e,h)}$. This means that the trap filled limit $\Delta_{f(e,h)}$ will vary upon space and time, as a function of the occupied deep trap density.

The last two terms in the right hand side of equation [9] represent the recombination phenomena. Charge recombination is considered by assuming that the recombination coefficients S_i (in m³.s⁻¹) are of Langevin form, function of the carrier mobility, thus function of the electric field and temperature:

$$S_{1_L} = \frac{q\mu_e}{\varepsilon_0\varepsilon_r}; \quad S_{3_L} = \frac{q(\mu_e + \mu_h)}{\varepsilon_0\varepsilon_r}; \quad S_{2_L} = \frac{q\mu_h}{\varepsilon_0\varepsilon_r}$$
[14]

In the model, we assumed that charge generation in the material is only due to injection at the electrodes according to a modified Schottky law. The injected current density for electrons at the cathode (x = 0) and holes at the anode (x = D) is written:

$$j_{e,h}(x_0, t) = AT^2 \cdot \exp\left(-\frac{w_{i(e, h)}}{k_B T}\right) \times \left[\exp\left(\frac{q}{k_B T}\sqrt{\frac{qE(x_0, t)}{4\pi\varepsilon_0\varepsilon_r}}\right) - 1\right]$$
[15]

with $x_0 = 0$ or $x_0 = D$. *A* is the Richardson constant ($A = 1.2 \ 10^6 \ A.m^{-2}.K^{-2}$). $w_{i(e)}$ and $w_{i(h)}$ are the injection barriers for electrons and holes (in eV). The model does not consider an extraction barrier at the electrodes, so the extraction fluxes for electrons and holes at the anode and cathode respectively follow the transport equation.

Model implementation

The model is developed with COMSOL Multiphysics® which offers several modules adapted or adaptable to the equations of our model. We have chosen the physical module "Transport of Diluted Species" (TDS) to solve the transport equation of each charge carrier (electron and hole, mobile and trapped). This module, which already includes tools to stabilize the solutions and minimize the oscillations, has the advantage of being well optimized for the modeling of transport phenomena. The mathematical module "Poisson Equation" (POEQ) is used to model the Poisson equation and to couple it to the transport equations. "Backward Differentiation Formula" (BDF) solver is used for the time integration. The sample thickness (200 μ m) is divided into 2000 finite elements of length 0.1 μ m.

RESULTS AND DISCUSSION

Simulations have been performed following the same applied electric field protocol as the experimental one. After simulation, a post-processing step is necessary in order to obtain simulated space charge results comparable to experimental ones. This step consists in adding the influence charges (i.e. capacitive charge and image charges) at each electrode [11].

Values of the model parameters used for the simulations are reported in Table 1. Space charge measurement results using the protocol of Fig. 1 at 20°C are presented in Fig. 5a as a function of time and position.

Table 1. Model parameters used for the simulations.

Parameters	Value	Units
Injection barrier heights		
$w_{i(e)}$ for electrons	1.24	eV
$w_{i(h)}$ for holes	1.16	eV
Hopping barrier heights		
$w_{hop(e)}$ for electrons	0.3	eV
$w_{hop(h)}$ for holes	0.3	eV
Inter-shallow traps distance		
$\lambda_{(e)}$ for electrons	3 × 10 ⁻⁹	m
$\lambda_{(h)}$ for holes	3 × 10 ⁻⁹	m
Minimum depth of deep traps		
$\Delta_{min(e)}$ for electrons	0.4	eV
$\Delta_{min(h)}$ for holes	0.4	eV
Maximum depth of deep traps		
$\Delta_{max(e)}$ for electrons	1.5	eV
$\Delta_{max(h)}$ for holes	1.5	eV
Pre-exponential factors		
$N'_{(e)}$ for electrons	1.8×10^{42}	m ⁻³ .J ⁻¹
$N'_{(h)}$ for holes	$3.0 imes 10^{42}$	m ⁻³ .J ⁻¹
Shape parameters		
$T_{0(e)}$ for electrons	1600	К
$T_{0(h)}$ for holes	1300	К

The charge density profile shows a charge injection at the electrodes dominated by positive charges. The mobility of these positive charges is apparently higher than that of the negative charges, as they seem to reach the cathode soon after voltage application for an applied electric field of 20 kV.mm⁻¹. This is more difficult to observe for higher applied electric fields. We observe a progressive penetration of negative charges with time and with the increase of the electric field. This dynamic allows electrons to progressively compensate the dominance of positive charges in the material. The simulation results for the same protocole are presented in Fig. 5b. The simulated space charge density globally reproduces the interesting characteristics of the measurement results: massive injection and dominant accumulation of positive charges, higher apparent mobility of positive charges, progressive penetration of negative charges in the material with time and with increasing the electric field.

Fig. 6a, Fig. 6b and Fig. 6c compare the simulated current densities with the current densities obtained by measurements at 20°C for each applied field. Experimentally, we observe a decrease of the current with time for 20 kV.mm⁻¹, which becomes relatively stable for the other electric fields. This decrease corresponds probably to the displacement current, i.e. orientation polarization phenomena, which is high at short time. For all applied electric fields, the simulated current increases at short time and then becomes stable, at a level higher than the measured current. As polar processes are not accounted for in the model, it is not possible to reproduce the experimental behaviour at short time. However, the order of magnitude of these simulated currents.





The proposed model is qualitatively and quantitatively able to reproduce the experimental space charge density values. Concerning the current, the simulation results indicate higher values than the experimentally measured currents; however, it is interesting to note that these values tend to get closer as the applied electric field increases. One of the assumption was that a model with only electronic carriers (i. e. electrons and holes) could reproduce the space charge and current behaviour of a fully degassed XLPE. This seems to be true, as most of the features of space charge dynamics have been reproduced. Moreover, although the mobility of charge carriers is relatively high compared to the one included in the other two types of charge transport models [1, 2], the present model is able to reproduce the charge accumulation experimentally observed. Simulations performed using the same protocol with the other two models (two-level of traps model with optimized parameters for LDPE [1], and model with an exponential trap distribution with parameters $T_{0(e,h)}$, $N'_{(e,h)}$, $\Delta_{max(e,h)}$ and $w_{i(e,h)}$ from Table 1) give completely different results than our model and do not reproduce the space charge and current behaviour measured in our XLPE sam ples.

In order to further validate our model, the same set of parameters (Table 1) is used to simulate the space charge behaviour at 50°C. The comparison between the





experimental data and the simulated ones are presented in Fig. 7 a and b respectively. In contrast to the results at 20°C, the measurement at 50°C shows an intensive injection of negative charges at the cathode as soon as the electric field (20 kV.mm⁻¹) is applied. At the anode, the injection of holes greatly increases with the applied electric field. This generation of holes and their increased mobility in the insulation allows these positive charges to



Fig. 7 : Spatio-temporal profiles of the net charge density from (a) experimental measurement, and (b) simulation results, for degassed XLPE sample of 200 μm thickness, at 50°C. The polarization time at each applied electric field (20, 30 and 40 kV.mm⁻¹) is 24h. A depolarization period of 1h is introduced after each 24h during polarization.

accumulate in the majority of the material bulk, thus hiding the presence and dynamic of electrons. This last behaviour is not reproduced by the model (using the same parameters as those used at 20°C). The model does however reproduce some important features of the charge behaviour, for example the positive and negative charge fronts that are observed at the beginning of the electric field application and the intensive injection of electrons at the cathode. The steady state is reached faster than in experiments.

CONCLUSION

A fluid bipolar charge transport model, based on the assumption of a single trapping energy level for mobile charges and an exponential distribution for deep traps, is described and the simulation results of this model for a degassed XLPE sample are compared to the experimental results of space charge and current. The obtained results show that overall, the proposed model (with the used parameters set) correctly reproduces the space charge

density distribution at 20°C and moderately reproduces the space charge behaviour at 50°C. The simulated current densities show significantly higher values than the measured current densities, with an increase at short time that is not observed experimentally. The set of parameters used has not yet been optimized for all experimental available data. An optimization tool will now be used in order to find the better set of parameters reproducing most of our experimental data. Moreover, the model will now be adapted to a one-dimensional cylindrical geometry, function of the cable radius, in order to be representative of degassed model cables. The last step will be to consider non-degassed XLPE, i.e. to add the ionic transport.

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